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**Contribution à la modélisation par
champ de phase du dommage
d'irradiation dans les alliages métalliques**

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Contribution to phase-field modelling of irradiation damage in metallic alloys

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Abstract

The prediction of the microstructure evolution during irradiation ageing of structural materials of nuclear reactors is a key issue for the nuclear industry. In this work, a phase field approach is used to simulate the microstructure evolution of materials under irradiation conditions at the mesoscopic scale. We are interested at first in the calculations of the sink strength which describes the ability of microstructural defects (dislocations, cavities, etc) to absorb point defects (PDs). These calculations take into account the elastic interactions between point defects and sinks and are performed in pure metals Al, Ni and Fe. Additional precision in the calculations is provided by incorporating in the model the change of the PD migration energy due to the sink strain field, also known as elastodiffusion. PDs are elastically modelled through their elastic dipole tensors and the role of the anisotropy of these dipole tensors at saddle state is investigated. The results show that the PD dipole tensor anisotropy at saddle state is a key parameter in the accurate sink strength calculations. Subsequently, our interest is focused on the development of a PF model of dislocation climb under irradiation. The model allows to simulate dislocation loop growth or shrinkage by absorption of both PDs (vacancies and self-interstitial atoms). The analysis of the validation tests shows the limit of the model, and adjustments are carried out. This new model is applied to simulate the growth of an interstitial loop in pure Fe. The temperature, dislocation density, loop orientation and elastodiffusion effects on the loop growth rate are studied. The results show, in particular, an increase of the loop growth rate with the combined effects of the increase of the temperature and the decrease of the dislocation density. The new PF model of dislocation climb under irradiation is also used to simulate the radiation induced segregation (RIS) phenomenon in Fe-Cr alloy near an interstitial dislocation loop during its growth. We show that the RIS prediction depends on the sink mobility and on the surrounding microstructure (multi-sink effects).

Keywords: modelling and simulation, metallic alloys, irradiation, point defects, sink strength, dislocation climb, radiation induced segregation, phase-field, elastodiffusion

Résumé

La prévision de l'évolution de la microstructure au cours du vieillissement par irradiation des matériaux de structure des réacteurs nucléaires est une question clé pour l'industrie du nucléaire. Dans ce travail, une approche par champ de phase est utilisée pour simuler l'évolution de la microstructure de matériaux dans des conditions d'irradiation à l'échelle mésoscopique. Nous nous intéressons tout d'abord aux calculs de la force de puits, c'est-à-dire la capacité des défauts de la microstructure (dislocations, cavités, etc) à absorber les défauts ponctuels (DPs). Ces calculs prennent en compte les interactions élastiques entre les défauts ponctuels et les puits et sont réalisés dans les métaux purs d'Al, Ni et Fe. Une précision supplémentaire dans ces calculs est fournie en incorporant dans le modèle le changement de l'énergie de migration des DPs en raison du champ de déformation dû au puits, encore appelé élastodiffusion. Les DPs sont modélisées élastiquement par leurs tenseurs dipolaires élastiques et le rôle de l'anisotropie de ces tenseurs dipolaires au point de col est étudié. Les résultats montrent que l'anisotropie du tenseur dipolaire au point col

est un paramètre clé dans les calculs précis de la force de puits. Par la suite, notre intérêt est centré sur le développement d'un modèle champ de phase de montée de dislocation sous irradiation. Le modèle permet de simuler la croissance ou le retrait d'une boucle de dislocation par absorption des deux DP's (lacunes et atomes auto-interstitiels). L'analyse des tests de validation montre la limite du modèle et des ajustements sont effectués. Ce nouveau modèle est appliqué pour simuler la croissance d'une boucle interstitielle dans le Fer pur. Les effets de la température, de la densité de dislocations, de l'orientation de la boucle et de l'élastodiffusion sur le taux de croissance de la boucle sont étudiés. Les résultats montrent notamment une augmentation du taux de croissance de la boucle avec les effets combinés de l'augmentation de la température et de la diminution de la densité de dislocations. Le nouveau modèle de montée de dislocation sous irradiation développé est également utilisé pour simuler le phénomène de ségrégation induite par irradiation (SII) près d'une boucle de dislocation interstitielle au cours de sa croissance, dans des alliages Fe-Cr. Nous montrons que la prédiction de la SII dépend de la mobilité du puits et de la microstructure environnante (effets multi-puits).

Mots clés: modélisation et simulation, alliages métalliques, irradiation, défauts ponctuels, force de puits, montée de dislocation, ségrégation induite par irradiation, champ de phase, élastodiffusion

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List of acronyms and nomenclature

AKMC	Atomistic kinetic Monte Carlo
bcc	Body centered cubic
DFT	Density functional theory
dpa	Displacements per atom
fcc	Face centered cubic
GGA	Generalized gradient approximation
LDA	Local density approximation
KMC	Kinetic Monte Carlo
MC	Monte Carlo
MFRT	Mean field rate theory
OKMC	Object kinetic Monte Carlo
PD	Point defect
PKA	Primary knock-on atom
PF	Phase field
RIP	Radiation induced precipitation
RIS	Radiation induced segregation
RT	Rate theory
RTA	Residence time algorithm
SIA	Self-interstitial atom
STGB	Symmetric tilt grain boundary
TEM	Transmission electron microscopy
T	Temperature in K
k_B	Boltzmann constant
V	Volume of the system
V_{at}	atomic volume
Ω_d	Relaxation volume of PD d
a_0	PF grid spacing
E_f^d	PD formation energy
F	Total free energy of the system
F_{chem}	Chemical energy of the system
F_{el}	Elastic energy of the system
F_{core}	Dislocation core energy
$k_{s,d}^2$	Sink strength of sink s for PD d
K_0^d	Generation rate of PD d
B_s	Bias of sink s

$\bar{X}_d$	Average atomic fraction of PD d
X_{eq}^d	Thermal equilibrium PD atomic fraction
X_d^s	Atomic fraction of PD d at the sink s
η_s	Elastic field associated to the sink s
λ_s	Shape function of the capture region of sink s
v_η	Dislocation climb velocity
μ_{chem}	Chemical potential
μ_{el}	Elastic potential
j_i^d	Flux of PD d
$j_{s,d}^{abs}$	Rate absorption of PD d by the sink s
D_{ij}^d	PD diffusion tensor
M_{ij}^d	Mobility tensor of PD d
P_{ij}^d	Elastic dipole tensor of PD d
$\mathbf{b}$	Burgers vector
$\mathbf{q}$	Wave vector
∇	Gradient operator
μ	Shear modulus
ν	Poisson coefficient
C_{ijkl}	Elastic constants tensor
S_{ijkl}	Eshelby tensor
G_{ij}	Green function
ε_{ij}^0	Eigenstrain tensor
ε_{ij}	Total strain in the system
σ_{ij}	Total stress in the system
u_i	Displacement field
δ_{ij}	Kronecker symbol
i_c	Imaginary complex number

Introduction

Structural materials of nuclear reactors are subject to rough operating conditions such as fast neutron irradiation, high temperatures and mechanical stresses. Thus, their functional properties deteriorate due to irradiation ageing which limits the operating time of components. Therefore, understanding and predicting the evolution of the properties of these structural materials are crucial issues for the safety and security of nuclear reactors.

During irradiation ageing, several phenomena are observed such as irradiation creep, swelling, [radiation induced segregation](#) (RIS), etc. These phenomena can be explained by the evolution of microstructural defects. For instance, [dislocation loop growth](#) allows to explain irradiation creep, cavity growth is responsible for swelling, and the coupling between the fluxes of point defects (PDs) and the ones of atoms allows to explain RIS. The challenge is then to predict the evolution of these microstructural defects. For this purpose, modelling techniques are developed and are good alternatives compared to experiments because of several reasons such as the cost and security. To treat the different physical phenomena occurring at different time scales and length scales such as the PD migration mechanism which occurs at the atomic scale and the dislocation loop growth which can be described at the mesoscopic scale, a multiscale approach is generally used.

The present work is dedicated to the simulation of microstructure evolution under irradiation using a phase field (PF) approach. The evolution of microstructural defects depends on their ability to absorb PDs, known as [sink strength](#). The first objective is thus to compute the sink strength by taking into account elastic interactions between PDs and sinks. The influence of the modification of the PD migration rate by an elastic strain field is investigated. Recently, PF models were developed to describe [dislocation climb](#) [1, 2, 3]. They are limited to climb via vacancy diffusion and are not adapted to irradiation conditions. The second objective is thus to develop a new PF model of dislocation climb based on the previous ones [1, 2, 3] to simulate dislocation loop evolution (growth/shrinkage) under irradiation. The final objective is to simulate the RIS phenomenon near an interstitial dislocation loop during its growth by means of the new PF model developed. This manuscript is organized as follows:

In chapter 1 microstructural defects intrinsic to the materials or formed under irradiation by PD agglomeration are described. Different simulation methods of microstructure evolution are also presented in this chapter.

The sink strength is calculated in chapter 2 for straight dislocations, low-angle symmetric tilt grain boundaries and spherical cavities in fcc (Al, Ni) and bcc (Fe) pure metals. These calculations take into account the elastic interactions between PDs and sinks like in the PF model of Rouchette et al. [4]. In addition to this model [4], elastodiffusion effects are incorporated and a particular emphasis is placed on the role of the PD anisotropy at saddle state.

In chapter 3, a new PF model of dislocation climb under irradiation is developed. This new model is based on the one developed by Geslin et al. [1] and is adapted to deal with both vacancy and self-interstitial atom (SIA) diffusion. Several tests are performed to validate this new model under irradiation conditions, and some adjustments are proposed to overcome the problems encountered. Thereafter, the model is applied to simulate the growth of an interstitial dislocation loop in pure bcc iron. The temperature, loop orientation and elastodiffusion effects on the loop growth rate are investigated.

Finally, the RIS phenomenon near an interstitial dislocation loop is simulated in chapter 4 in Fe-Cr alloys. The elastic effects are taken into account as well as the loop growth rate by means of the climb model developed in chapter 3.

Chapter 1

Microstructure evolution under irradiation and modelling techniques

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Under irradiation, microstructural defects such as dislocation loops, grain boundaries and cavities evolve through different mechanisms and this evolution leads to the change in the mechanical properties of nuclear materials. In this chapter, microstructural defects are first described. Secondly, the phenomena which are observed during the microstructure evolution are presented, as well as, the different modelling techniques which allow to predict it.

1.1 Irradiated materials

Metallic alloys are used for the reactor component structure in the nuclear industry. To ensure the safety and security of the nuclear reactors, these structural materials are chosen according to several criteria such as stability under irradiation, corrosion and swelling resistance, manufacturing cost, etc. For example, zirconium alloys and austenitic steels are used respectively for the fuel cladding structure and the internal reactor vessel structure in pressurized water reactor. Ferritic/martensitic steels and nickel based alloys are candidate materials for innovative reactor systems [5]. The prediction of the evolution of these structural materials is then a key issue for the nuclear industry. The evolution of microstructure is controlled by the evolution of its defects which can be intrinsic (lattice defects) or formed under irradiation. These different microstructural defects are described below.

1.1.1 Lattice defects

All real materials contain imperfections that can be point, line, surface or volume defects. In this thesis, the discussions will mainly focus on point defects (PDs) and dislocations (line defects).

Point defects

Two PDs are intrinsic to the material: vacancy and self-interstitial atom (SIA). Vacancy is an atom missing from a lattice site which is normally occupied in a perfect lattice. SIA is an atom that occupies a place outside the normal lattice position. In this thesis, typical fcc (Al and Ni pure metals) and bcc (Fe pure metal and Fe-Cr alloys) structure materials will be particularly studied. The possible configurations of SIA in these structures are the following: octahedral, tetragonal, dumbbell where two atoms share a single lattice site, and crowdion where $N+1$ atoms share N single lattice sites which leads to the extended distortion of the crystal lattice in the $\langle 111 \rangle$ direction (first noted by Paneth [6]). The most stable SIA configuration in fcc structure is generally the $\langle 100 \rangle$ -dumbbell [7] and in bcc structure the $\langle 111 \rangle$ -dumbbell, but in bcc iron it is the $\langle 110 \rangle$ -dumbbell which is more stable due to magnetism [8]. The PD diffusion in a crystal lattice occurs by a displacement from an equilibrium configuration to a nearest neighbor one. During this transition, the energy landscape presents a maximum and the PD configuration which corresponds to this maximum is the called [saddle state](#). The required energy for this transition is the migration energy E^m and it is the difference between the energy at the

saddle E^{sad} and stable E^e states:

$$E^m = E^{sad} - E^e \quad (1.1)$$

Vacancy migrates through the motion of an atom located initially on the final stable configuration of vacancy. The 12 (respectively 8) possible jumps in fcc (respectively bcc) structure are then accessible. The dumbbell migration mechanism is more complex than the one of vacancy. The most favorable one is a mechanism of translation-rotation from an initial orientation to a different one, for the metals specified above. Therefore, for a given initial dumbbell orientation in fcc (respectively bcc) structure, 8 (respectively 4) possible jumps are energetically accessible. The possible PD transitions in fcc (Al, Ni) and bcc (Fe) structures are depicted in Figs. 1.1 and 1.2, and all the corresponding jump directions are given in table 1.1.

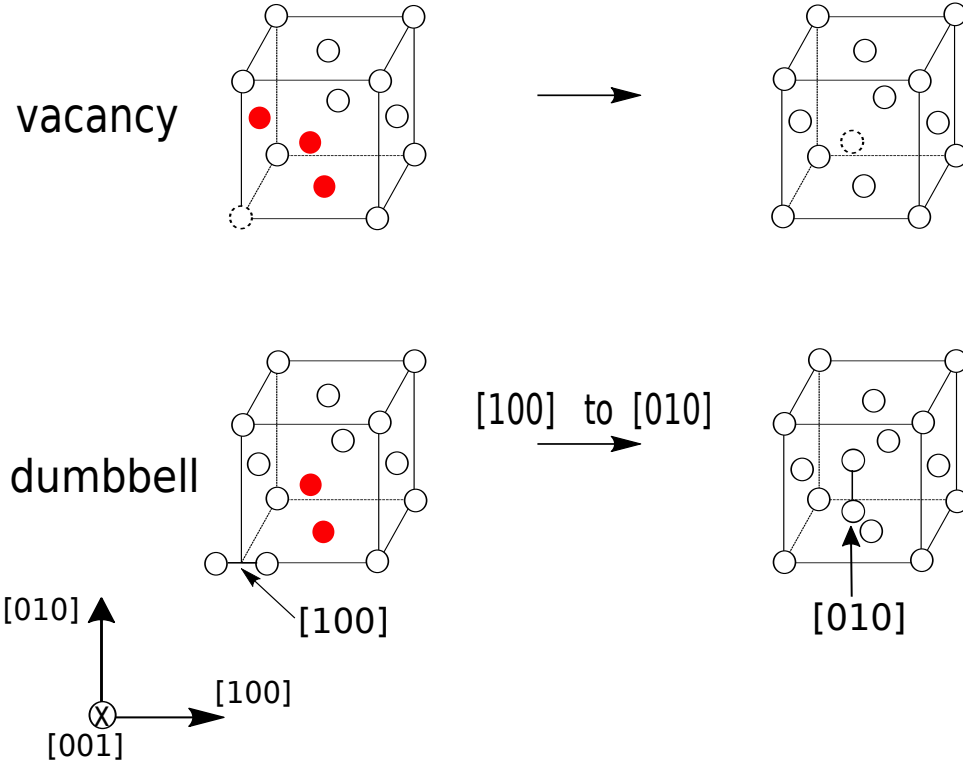


Figure 1.1: Possible PD transitions in pure fcc metals. The allowed target sites are marked in red.

Dislocations

Dislocations are linear defects which exist in materials and allow understanding plastic deformation. A dislocation is characterised by its vector line $\mathbf{l}$ and Burgers vector $\mathbf{b}$ (deformation amplitude transported by the dislocation) and there are two basic types of dislocation: edge dislocation and screw dislocation as illustrated on Fig. 1.3. In general dislocation has a mixed character. Only edge dislocations will be addressed in this

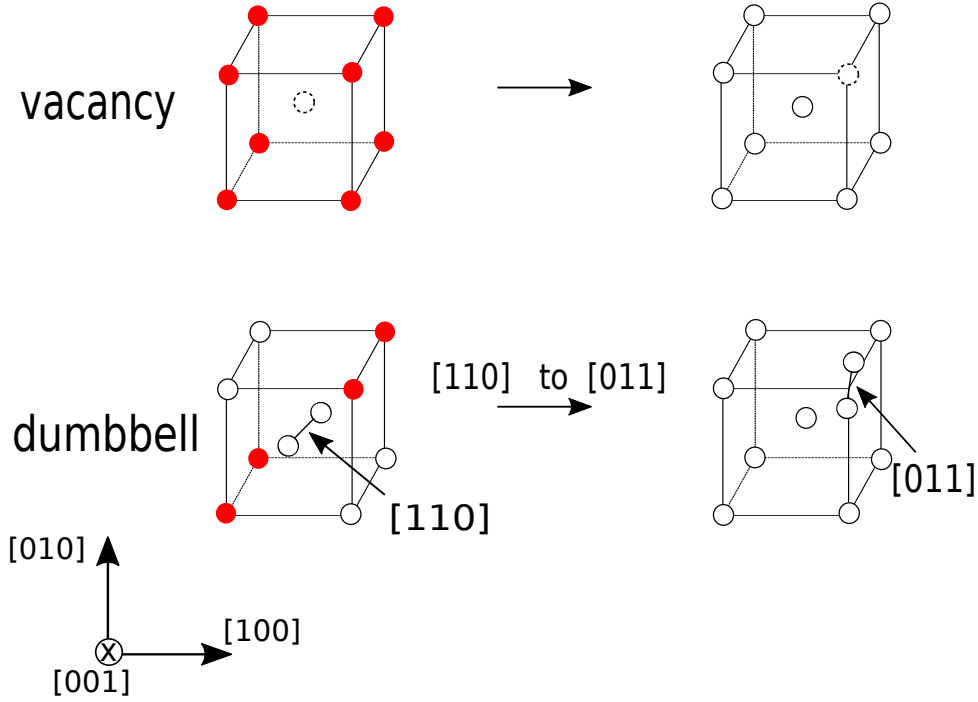


Figure 1.2: Possible PD transitions in pure bcc metal Fe. The allowed target sites are marked in red.

Table 1.1: Possible jump directions of PD in $R_0([100],[010],[001])$ space.

	Jump direction $\mathbf{h}$	
	Al and Ni (fcc)	Fe (bcc)
Vacancy	$[110]$, $[\bar{1}10]$, $[1\bar{1}0]$, $[\bar{1}\bar{1}0]$ $[011]$, $[0\bar{1}1]$, $[01\bar{1}]$, $[0\bar{1}\bar{1}]$ $[101]$, $[\bar{1}01]$, $[10\bar{1}]$, $[\bar{1}0\bar{1}]$	$[111]$, $[\bar{1}11]$, $[1\bar{1}1]$, $[11\bar{1}]$ $[\bar{1}\bar{1}1]$, $[1\bar{1}\bar{1}]$, $[\bar{1}1\bar{1}]$, $[\bar{1}\bar{1}\bar{1}]$
Dumbbell [100] in Al, Ni and [110] in Fe	$[110]$, $[\bar{1}10]$, $[1\bar{1}0]$, $[\bar{1}\bar{1}0]$ $[101]$, $[\bar{1}01]$, $[10\bar{1}]$, $[\bar{1}0\bar{1}]$	$[111]$, $[11\bar{1}]$, $[\bar{1}\bar{1}1]$, $[\bar{1}\bar{1}\bar{1}]$

manuscript. The vectors $\mathbf{b}$ and $\mathbf{l}$ define a plane which is called the glide plane of the edge dislocation. An edge dislocation can be visualized as an extra half-plane of atoms in a lattice as shown in Fig. 1.3. The ability of materials to deform depends on the mobility of dislocations. Edge dislocation can move in its glide plane which is called glide, or out of its glide plane which is called **climb**. Dislocation glide is a **conservative** motion which does not involve PD, while dislocation climb is a **non-conservative** motion which requires PD. Dislocation climb sometimes plays an important role in plastic deformation since it enables edge dislocations to circumvent otherwise insurmountable obstacles.

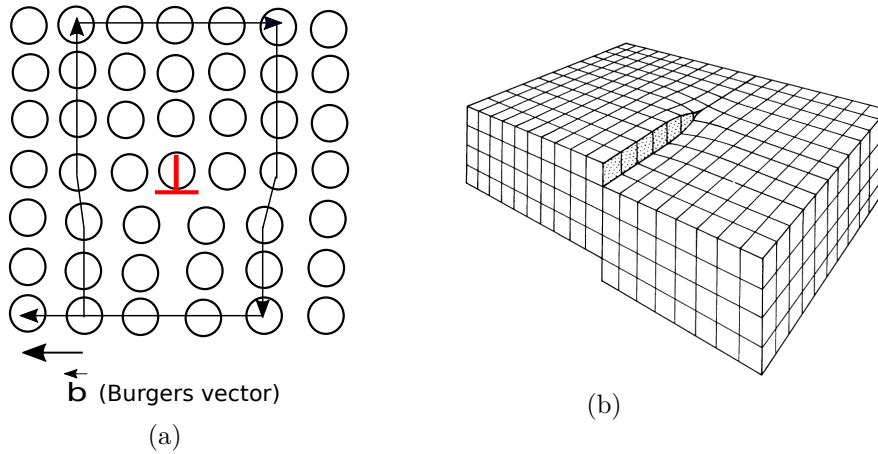


Figure 1.3: Illustration of a) an edge dislocation and b) a screw dislocation [9] in a simple cubic crystal.

Under irradiation, isolated defects will aggregate and form larger defects. A non exhaustive list of them is given below.

1.1.2 Irradiation effects

Irradiation of materials with high energy particles leads to particle-atom collisions and the atom called the primary knock-on atom (PKA) is displaced from its regular position in lattice. There is an energy transfer between the particle and the atom. If this transferred energy is smaller than the required energy to move an atom from a lattice site, then the atom keeps its position and the energy is converted in heating. On the other hand, if the transferred energy is higher than the displacement energy, the atom is ejected from its site which produces a vacancy and the atom becomes a SIA. Frenkel pairs (vacancy + SIA) are then created and this type of defect generation corresponds typically to the electron irradiation [10]. In the case where the transferred energy is high enough, the atom becomes itself a projectile. Further collisions are then possible occurring with a transfer of the excess atom displacement energy. The displacements generated by these successive atom collisions are called displacement cascades. During the cascade, isolated defects will agglomerate which leads to the formation of other defects such as dislocation loops (2D) and cavities (3D) (see Figs. 1.4 and 1.5). Dislocation loops can be of vacancy or interstitial type and their nucleation and/or growth/shrinkage can be explained by the mechanisms of PD clustering and/or PD absorption (discussed in chapter 3). Cavities are microstructural defects that consist of 3D aggregation of vacancies. During the evolution of these microstructural defects, many macroscopic phenomena are observed such as irradiation creep, swelling, radiation induced segregation (RIS), radiation induced precipitation (RIP), etc. For example, dislocation loop growth allows to explain irradiation creep and swelling is related to cavity growth. RIS (discussed in chapter 4) is a non-equilibrium phenomenon which consists in the local redistribution of alloying elements near microstructural defects such as dislocation loops, grain boundaries or cavities. The redistribution of alloying elements can lead to the observation of other physical phenomena

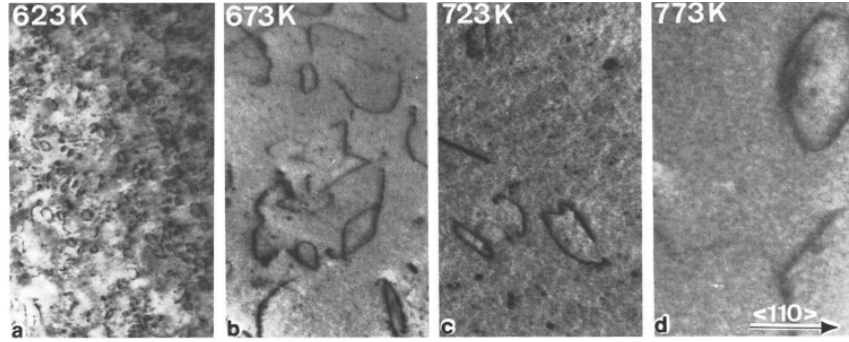


Figure 1.4: Dislocation loops observed for irradiation temperatures of 623-773 K in neutron-irradiated iron, transmission electron microscopy (TEM) observations (from [11]). The length of the arrow equals 500 nm.

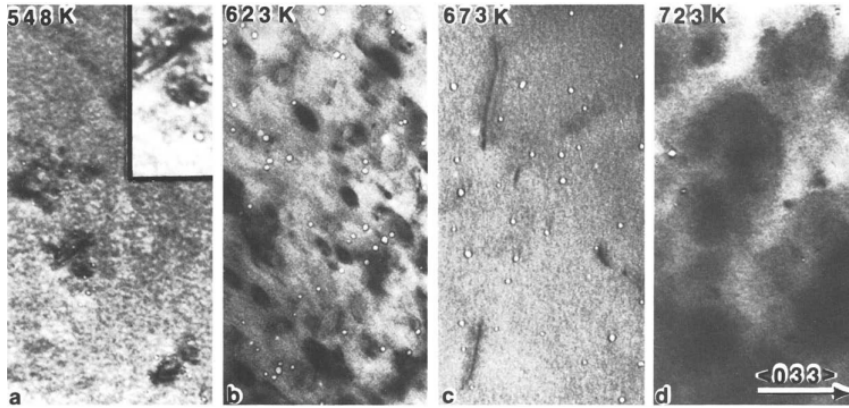


Figure 1.5: Cavity microstructures observed with TEM in neutron-irradiated iron (from [11]). The length of the arrow equals 200 nm.

such as precipitation.

In order to better understand microstructure evolution under irradiation, modelling techniques are increasingly used due to several advantages compared to experimental studies such as the cost, the security issues, the access to smaller time and space scales. Some of these modelling techniques which are mentioned in this work are presented below.

1.2 Modelling techniques of microstructure evolution

To simulate the microstructure evolution, multiscale modelling tools are developed. The physical phenomena observed under irradiation occur at different time and length scales thus, different simulation methods are developed and used. In this manuscript, the following methods are mentioned: ab initio/DFT, kinetic Monte Carlo (KMC) methods, phase field (PF) and mean field simulations. A brief description of these methods is given below.

1.2.1 Ab initio/DFT

Ab initio calculations are techniques which are based on the resolution of the Schrödinger equation (Eq. 1.2) in order to obtain atomic and molecular structures directly from the first principles of quantum mechanics:

$$H\psi = E\psi \quad (1.2)$$

where H , E and ψ are respectively the system Hamiltonian, energy and wave function. The main advantage of the methods used to solve Eq. 1.2 is the non implementation of adjustable parameters derived from experiments. However, the exact resolution of Eq. 1.2 is difficult (manybody problem) and a certain number of approximations is adopted. The first approximation conventionally used is the adiabatic approximation of Born-Oppenheimer which assumes that the motion of ions can be dissociated from that of electrons. Ions are heavier than electrons and therefore have a much slower motion than the electrons. Thus, equation 1.2 can be solved on many electrons for a given configuration of many ions. The Born-Oppenheimer approximation is not enough on its own because electrons interact strongly and their motions can not be decorrelated. Two methods are used to describe the quantum states of many electrons: the Hartree-Fock method [12] and the density functional theory (DFT) that we describe below because it is mentioned in this thesis. The density functional theory (DFT) introduced by Hohenberg and Kohn [13] states that the ground state energy of a many-electron system can be expressed as a unique function of the electron density. For this purpose, Kohn and Sham [14] proposed a reformulation of the problem by replacing the system of many electrons with a system of independent electrons evolving in an effective potential. The energy of the system is then written as a functional of the electronic state density and contains an exchange-correlation functional term. The local density approximation (LDA) or the generalized gradient approximation (GGA) are commonly used to express the functional of exchange-correlation. PF approach described in section 1.2.3 is used in this manuscript to simulate microstructure evolution and requires data from DFT calculations such as the PD formation and migration energy, or the PD elastic dipole tensor (see section 2.1.2).

1.2.2 Kinetic monte Carlo

Kinetic Monte Carlo (KMC) methods are stochastic approaches which derive from the Monte Carlo (MC) techniques and allow to simulate the microstructure time evolution. KMC methods have the advantage that spatial correlations during PD migration for instance are explicitly taking into account. These methods are applicable to multiple time and space scales. Thus, the evolution of atom or PD positions can be simulated using atomic kinetic Monte Carlo (AKMC). In the AKMC approach, the system evolution is a consequence of the PD and/or atom migrations. All the spatial correlations between successive PD jumps are accounted for, which limits the size of the studied system. To simulate larger defects such as dislocation loops and cavities formed under irradiation, object kinetic Monte Carlo (OKMC) models are used. The OKMC method proceeds like the AKMC, except that instead of making atoms and PDs evolve individually, clusters of PDs evolve on a lattice site or not as a whole as one single object. Many of the KMC techniques are based on the residence time algorithm (RTA)[15, 16, 17]. At each time

step, different events such as PD jump (AKMC) or PD cluster jump (OKMC) can occur with the event (thermally activated) frequency:

$$\Gamma_i = \nu_i \exp\left(\frac{-E_{a_i}}{k_B T}\right) \quad (1.3)$$

where ν_i is the attempt frequency, k_B is Boltzmann's constant, T the temperature and E_{a_i} the activation energy of the jump i . The probabilities of all the possible system transitions are calculated, and one of them is chosen by extracting a random number $r \in [0, 1]$, according to its probability. The associated time step δt and the average time step Δt are the following:

$$\delta t = \frac{-\ln r}{\sum_i \Gamma_i}; \quad \Delta t = \frac{1}{\sum_i \Gamma_i} \quad (1.4)$$

1.2.3 Phase field

Phase field (PF) methodologies have been proposed by Cahn and Hilliard [18] and first applied to simulate phase transformations [19, 20]. Recently, PF methods become a powerful computational approach to model and predict microstructure evolution in materials especially under irradiation [21, 22, 23], since diffusion processes are naturally incorporated. In the PF approaches, the microstructure evolution is described by a set of variable and continuous fields so called **order parameters**. For example, these order parameters can refer to the PD fractions or to the identification function of a dislocation loop (see section 2.3.1) in the system. Thus at each time step, the local state of the system (microstructure) is described by the values of the order parameters. The system evolves by the minimisation of its total free energy which is written as a function of the order parameters. The temporal and spatial evolution of the order parameters is governed by the **Cahn-Hilliard**-type equation [24] for **conserved** order parameters and by the **Allen-Cahn**-type equation [25] for **non-conserved** order parameters. An order parameter is conserved when its average value in the simulation domain is conserved during system evolution, and non-conserved in the opposite case. For example, the dislocation loop growth/shrinkage due to the PD absorption is a non-conservative process (change in the loop size/shape). Therefore, the order parameter associated to the loop is non-conserved while, the total PD fraction in the bulk and absorbed/emitted by the loop is a conserved order parameter (see section 3.2.3). Geslin et al. [1] have recently developed a PF model describing dislocation climb via the vacancy diffusion. In section 3.2.3, the model of Geslin is generalized to both vacancies and SIAs and applied to simulate the growth/shrinkage of prismatic dislocation loops. The main advantage of the PF methods is that the different elastic interactions that may exist can easily be incorporated through the **microelasticity theory** [26]. To sum up, three steps are usually followed in a PF approach: the definition of the order parameters which allow to describe the microstructure, the total free energy of the system and the evolution equations. In this manuscript, a PF approach is used to simulate microstructure evolution.

1.2.4 Mean field rate theory (MFRT)

Mean field simulations are deterministic approaches like PF methods, based on the resolution of the defect (PD, PD clusters, ...) evolution equations given in the rate theory (RT)

models of irradiated materials [27, 10]. These kinetic equations are related not to the local PD fractions but to their average value (see section 2.1.1). The mean field rate theory (MFRT) has been used successfully to predict microstructure evolution under irradiation [28, 29, 30, 31]. The MFRT methods have the advantage that large defects can be modelled which provides the opportunity to compare the numerical results with experimental observations. However, the spatial correlations in defect production are not accounted for and the model requires input parameters computed at lower scales such as the sink strengths (see Eqs. 2.1 and 2.2).

1.3 Summary

In this chapter, we have described the microstructural defects which can be intrinsic or formed under irradiation. We have seen that the formation of defects such as dislocation loops and cavities is due to PD clustering and during the evolution of these defects, several phenomena are observed such as irradiation creep, swelling and RIS. These phenomena are responsible for the change of the mechanical properties and predicting them is an important issue. The modelling techniques allowing to simulate the evolution of these defects during radiation aging have also been presented. These modelling techniques make it possible to describe phenomena occurring from the atomic scale to the macroscopic scale and multiscale approach is generally used to model the microstructure evolution.

Chapter 2

Elastodiffusion

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The ability of microstructural defects to absorb PDs (sink strength) is a key parameter to better understand and predict the evolution of these microstructural defects under irradiation. This ability strongly depends on the elastic interactions between sinks and PDs. The sink strength is computed in this chapter for different microstructural defects (edge dislocations, array of edge dislocations and cavities) by using a PF approach. The computations include the elastic interactions and the modification of the PD migration rate by a strain field.

2.1 Bibliography

2.1.1 Sink strength: definition and calculations

Under irradiation point defects (PD), vacancies and self-interstitial atoms (SIAs), are created and diffuse towards microstructural defects such as dislocations, grain boundaries, cavities, etc. These microstructural defects will evolve according to their ability to absorb PD, also known as [sink strength](#). The sink strength can be calculated using different methods: by the analytical solution of the PD diffusion equation around the considered sink [27, 32], by performing object kinetic Monte Carlo (OKMC) simulations [33, 34, 35], or by using a phase field (PF) approach [4, 36, 37, 38]. In the methods presented below, the PD diffusion is considered isotropic in an unstrained system.

In the rate theory models of irradiated materials [27, 10], the kinetic equations are related to the average atomic fraction $\bar{X}_d$ of PD d:

$$\frac{d\bar{X}_v}{dt} = K_0^v - R_{vi}\bar{X}_v\bar{X}_i - \sum_s k_{s,v}^2 D_v (\bar{X}_v - X_v^s) \quad (2.1)$$

$$\frac{d\bar{X}_i}{dt} = K_0^i - R_{vi}\bar{X}_v\bar{X}_i - \sum_s k_{s,i}^2 D_i (\bar{X}_i - X_i^s) \quad (2.2)$$

where v and i refer respectively to vacancies and SIAs. K_0^d is the generation rate of PD d ($d = v, i$), R_{vi} is the rate of mutual recombination between PD and is related to the PD diffusion coefficient D_d through the relation:

$$R_{vi} = \frac{4\pi r_c (D_v + D_i)}{V_{at}} \quad (2.3)$$

with r_c the distance of recombination and V_{at} the atomic volume. X_d^s is the atomic fraction of PD d at sink s. $k_{s,d}^2$ is the sink strength of sink s for PD d.

At steady state ($t \rightarrow \infty$), $\frac{d\bar{X}_d}{dt} = 0$. Equations 2.1 and 2.2 become, by assuming the recombination term negligible and considering one type of sink:

$$K_0^d - k_{s,d}^2 D_d (\bar{X}_d(t \rightarrow \infty) - X_d^s) = 0 \quad (2.4)$$

which leads to the following expression of the sink strength:

$$k_{s,d}^2 = \frac{K_0^d}{D_d (\bar{X}_d(t \rightarrow \infty) - X_d^s)} \quad (2.5)$$

The average atomic fraction at steady state $\bar{X}_d(t \rightarrow \infty)$ depends on the shape and volume of the sink, on the sink free region shape and volume, on the diffusion rate properties of PD, and on the possible elastic interactions between PD and sink. Several analytical expressions of the sink strength for various sinks have been obtained by solving equations 2.1 and 2.2 using different boundary conditions [27]. In table 2.1 the analytical solutions of the sink strength of a straight dislocation and a spherical cavity are given. The sink of radius r_0 is contained in a region or reservoir of radius R free of any other sink as illustrated in Fig. 2.1. The reservoir has the same symmetry as the sink. In the models of Laplace,

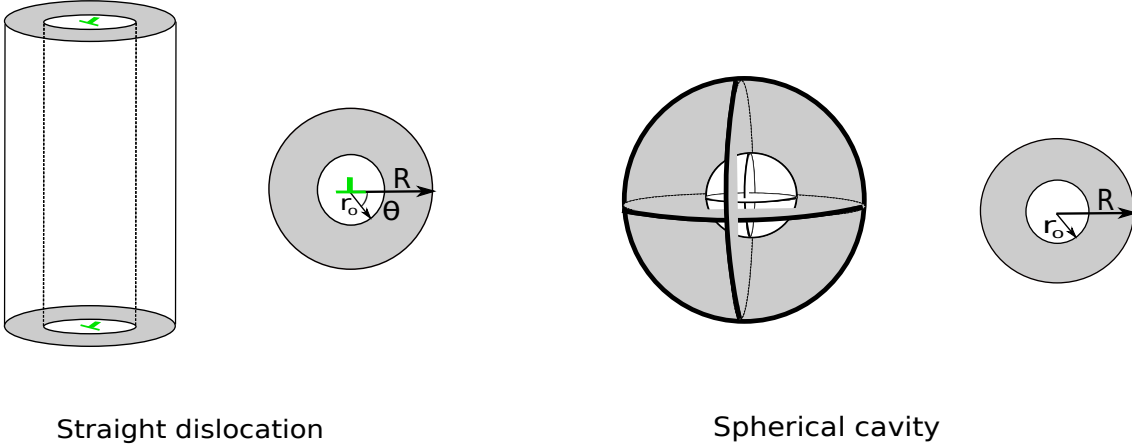


Figure 2.1: Sink geometry for analytical solutions of the sink strength (cylindrical and spherical symmetry for straight dislocation and cavity respectively).

Poisson and Wiedersich, the sink strength is obtained when the elastic interactions between PD and sink are neglected. Wiedersich's model is known to be more realistic than the models of Laplace and Poisson [27, 4]. The difficulty in the analytical models is to incorporate the elastic interactions. When the elastic interactions are taken into account, the system energy is modified as well as the PD migration energy (elastodiffusion) as described in sections 2.1.2 and 2.2.2. The model proposed by Rauh and Simon [32] for the sink strength calculation of edge dislocations takes into account the elastic interactions through an elastic drift term in the diffusion equation (see table 2.1). In this formulation, only the system energy is affected by the elastic interactions. The PD migration rate remains unchanged. The model of Rauh is limited to isotropic systems and PDs. In the case of a spherical cavity in an isotropic medium, Borodin et al. [39] have proposed a solution which incorporates the elastic interactions. The strain field generated by a spherical cavity in an isotropic medium verifies $\text{Tr}(\varepsilon_{ij}) = 0$ [40, 39]. As $\text{Tr}(\varepsilon_{ij}) = 0$, the elastic energy in the stable state given by $E = -P_{ij}^e \varepsilon_{ij}$ in the case of isotropic PD ($P_{ij}^e = P_0^e \delta_{ij}$) is then zero. P_{ij}^e is the PD **elastic dipole tensor** at the stable configuration described in section 2.1.2. The elastic drift term is consequently zero but still, some elastic interactions remain and are taken into account through the PD migration rate (see table 2.1). The PD diffusion tensor has been rewritten in order to introduce the elastic interactions between PDs and the cavity. The model is based on the one of Dederichs and Schroeder [41] (see section 2.1.2) who first proposed a model of PD diffusion in stressed systems. It must be pointed out that the solution of Borodin is very simple, it depends on the elastic dipole tensor

Table 2.1: Analytical solutions of the sink strength for a straight dislocation and a spherical cavity. r_0 is the sink radius and R the reservoir radius. ρ is the sink density equal to $(\pi R^2)^{-1}$ for a straight dislocation and $(\frac{4}{3}\pi R^3)^{-1}$ for a spherical cavity.

No elastic interactions	
Equation	k^2/ρ
Laplace	Straight dislocation, spherical cavity ($f_d = (r_0/R)^2$) $D\nabla^2 X = 0 \quad (X(r=R) \text{ fixed})$ $\frac{2\pi}{\ln(f_d^{-1/2})}, \quad \frac{4\pi r_0 R}{R-r_0}$
Poisson	$D\nabla^2 X + K_0 = 0 \quad (X(r=R) \text{ fixed})$ $\frac{2\pi}{\ln(f_d^{-1/2}) + \frac{1}{2}(f_d-1)}, \quad \frac{4\pi r_0 R}{R-r_0}$
Wiedersich	$D\nabla^2 X + K_0 = 0$ $\frac{2\pi(1-f_d)}{\ln(f_d^{-1/2}) - \frac{3}{4} + \frac{1}{4}f_d(4-f_d)}, \quad \frac{4\pi r_0(1-f_d^{3/2})}{1-1.8f_d^{1/2}+f_d^{3/2}-0.2f_d^3}$
Elastic interactions	
Straight dislocation (elastic drift term and no elastodiffusion ¹)	
Equation	k^2/ρ
Rauh and Simon [32]	$D\nabla^2 X + \nabla[X\nabla\mu_{el}] = 0,$ $z_0(R) + 2\sum_{n=1}^{\infty} (-1)^n z_n(R), \quad \frac{2\pi}{\ln(f_d^{-1/2}) - \frac{3}{4} + \frac{1}{4}f_d(4-f_d)}$
	$\mu_{el}(r, \theta) = L \frac{\sin\theta}{r}, \quad L = \frac{\mu b(1+\nu)\Omega_d}{3\pi(1-\nu)k_B T}$ $z_n(R) = \frac{2\pi I_n(L/2r_0)I_n(L/2R)}{I_n(L/2r_0)K_n(L/2R) - I_n(L/2R)K_n(L/2r_0)}$
Spherical cavity (no elastic drift term and elastodiffusion ¹)	
Equation	k^2/ρ
Borodin et al. [39]	$\frac{\partial}{\partial x_i} D_{ij} \frac{\partial X}{\partial x_j} + K_0 = 0,$ $4\pi R[1 + q(p - \frac{2\gamma}{r_0})],$ $D_{ij} = \frac{\nu_0}{2Z} \sum_{\mathbf{h}} h_i h_j \sum_{\alpha\beta} [1 + \sum_{kl} \frac{P_{kl}^{sad}(\mathbf{h})}{k_B T} \varepsilon_{kl}(\mathbf{r}^{sad})] \exp[-\frac{1}{k_B T} E_m^0(\mathbf{h}_{\alpha\beta})]$ $q = -\frac{5(2d_{2323})+2(d_{1111}-d_{1122}-2d_{2323})}{40\mu},$ $d_{ijkl} = \frac{3}{k_B T N Z} \sum_{\mathbf{h}} \sum_{\alpha\beta} e_i e_j e_k e_l P_{kl}^{sad}(\mathbf{h}_{\alpha\beta})$

¹ μ is the shear modulus, ν the Poisson ratio, T the temperature, k_B the Boltzmann constant, b the length of the Burgers vector, Ω_d the relaxation volume of the PD d , I_n and K_n are the modified Bessel functions of the n^{th} order of the first and second kind respectively (Rauh and Simon [32]), p the internal gas pressure, r_0 the cavity radius, γ the surface tension of the cavity, $P_{ij}^{sad}(\mathbf{h})$ the elastic dipole tensor at saddle state, $\varepsilon_{ij}(\mathbf{r})$ the strain field due to the cavity, $\mathbf{h}$ the possible jump direction, $\mathbf{e}$ the unit vector in the jump direction, α and β the possible PD orientations in the initial and final stable configuration respectively, N the number of nearest neighbour sites, Z the number of pairs (α, β) , ν_0 the jump frequency and $E_m^0(\mathbf{h}_{\alpha\beta})$ the PD migration energy in unstrained system. (Borodin et al. [39])

¹Elastodiffusion¹: PD migration energy modified by a strain field.

of PD at saddle point and varies as $1/r_0$ (see table 2.1). Like in the model of Rauh, the model of Borodin et al. is limited to isotropic systems.

In the OKMC simulations, different methods [34, 35, 42, 33] exist to calculate the sink strength. One of them [34, 35] consists in the following. A sink is located in a 3-dimensional box with periodic boundary conditions. PDs are generated uniformly at a constant rate K_0 and migrate in the box by successive atomic jumps until they are absorbed by the sink. The sink is assumed immobile and does not evolve by absorption of PDs. The recombination of PDs and their emission by the sink are neglected. The possible events are the creation of PD or an atomic jump from a stable position to a neighboring one. The next event is chosen according to the residence time algorithm [15, 16]. The sink strength is calculated when the steady state is reached and is given by:

$$k_{s,d}^2 = \frac{K_0}{D_d \bar{N}_d} \quad (2.6)$$

where $\bar{N}_d$ is the average number of PD d still present in the box. In the other method [42, 33], one migrating PD is present in the simulation box containing a sink at a given time. The PD trajectory is followed before it's absorbed by the sink. A new PD of the same type is introduced after the previous one has been absorbed. The sink strength is obtained as:

$$k_{s,d}^2 = \frac{2N_{dim}}{d^2 \langle n \rangle} \quad (2.7)$$

where N_{dim} is the PD migration dimensionality, d the jump length and $\langle n \rangle$ the average number of jumps before the absorption.

The PF approach to compute the sink strength is detailed in section 2.2 and the obtained expression is similar to equations 2.4 and 2.5.

Another interesting quantity is the sink bias B_s defined as [43]:

$$B_s = 1 - \frac{k_{s,v}^2}{k_{s,i}^2} \quad (2.8)$$

The sink bias allows explaining irradiation dislocation loop growth/shrinkage, irradiation void swelling, or irradiation creep [44, 28, 45]. For example, straight dislocations are known to be biased: SIAs are more absorbed than vacancies. Voids are known to produce shorter range stress fields and are usually considered as neutral sinks i.e. they absorb the same amount of vacancies and SIAs if they are produced or available at the same rate [10]. The preferential absorption of SIAs by the dislocations leads to a net flux of vacancies to voids and thus to void growth mechanism known as irradiation swelling.

The main advantage of the OKMC and PF simulations compared to the analytical solutions is the possibility to take into account the elastic interactions and anisotropic diffusion in complex microstructures.

In this section, the sink strength has been defined and the methods which allow to calculate it have also been presented. It has been shown that elastic interactions that may exist between sinks and PDs modify the sink strength. Thus to correctly calculate the sink strength, these elastic interactions must be properly described. In section 2.1.2, we present how a strain field which can be due to a sink modifies the

PD diffusion.

2.1.2 PD diffusion modified by the sink strain field

During the diffusion of PDs towards the sink, there are elastic interactions between PD and the stress field produced by the sink. As a consequence, the system energy is modified and includes an elastic energy which acts as a driving force for PD diffusion. Moreover, the migration energy of PD is also modified by the stress field, this dependence being called [elastodiffusion](#). Elastodiffusion has first been investigated by Dederichs and Schroeder [41]. Considering a crystal and PD with cubic symmetry, the PD diffusion tensor in the unstrained system is given by:

$$D_{ij}^0 = \frac{N}{6} h^2 \nu \exp(-\beta E_0^m) \delta_{ij} \quad (2.9)$$

with δ_{ij} the Kronecker symbol and $\beta = 1/k_B T$. N is the number of nearest neighbour sites, ν the attempt frequency, h the jump length. E_0^m is the PD migration energy which is the difference between the energy at the saddle and stable configurations:

$$E_0^m = E_0^{sad} - E_0^e \quad (2.10)$$

In the presence of an elastic field $\varepsilon_{kl}(\mathbf{r})$ due to the sink, the saddle and stable point energies are modified as follows at the first order (differences in the elastic properties between those of the PD and those of the matrix are neglected):

$$E^e = E_0^e - \sum_{kl} \bar{P}_{kl}^e \varepsilon_{kl}(\mathbf{r}^e) \quad (2.11)$$

$$E^{sad} = E_0^{sad} - \sum_{kl} P_{kl}^{sad}(\mathbf{h}) \varepsilon_{kl}(\mathbf{r}^{sad}) \quad (2.12)$$

$$E^m = E^{sad} - E^e = E_0^m - \left[\sum_{kl} P_{kl}^{sad}(\mathbf{h}) \varepsilon_{kl}(\mathbf{r}^{sad}) - \sum_{kl} \bar{P}_{kl}^e \varepsilon_{kl}(\mathbf{r}^e) \right] \quad (2.13)$$

where P_{kl}^e and $P_{kl}^{sad}(\mathbf{h})$ are respectively the elastic dipole tensors of PD at stable and saddle point for the jump direction $\mathbf{h}$. The PD anisotropy at stable point is ignored in this model, which justifies the choice of $\bar{P}_{kl}^e$ instead of P_{kl}^e where $\bar{P}_{kl}^e$ is given by:

$$\bar{P}_{kl}^e = \text{Tr}(P_{kl}^e) \delta_{kl} / 3, \text{Tr}(P_{ij}) = \sum_{i,j(i=j)} P_{ij} \quad (2.14)$$

It can then be demonstrated that the PD diffusion tensor is as follows:

$$D_{ij}(\mathbf{r}) = \frac{h^2 \nu}{2} \sum_{\mathbf{h}} u_i^{\mathbf{h}} u_j^{\mathbf{h}} \exp(-\beta E^m) \quad (2.15)$$

with $u_i^{\mathbf{h}}$ the i^{th} component of unit vector in the direction of the jump $\mathbf{h}$. Using the expression given by Eq. 2.13, the diffusion tensor becomes:

$$D_{ij}(\mathbf{r}) = \frac{h^2 \nu}{2} \sum_{\mathbf{h}} u_i^{\mathbf{h}} u_j^{\mathbf{h}} \exp(-\beta E_0^m) \exp\left[\beta \sum_{kl} (P_{kl}^{sad}(\mathbf{h}) - \bar{P}_{kl}^e) \varepsilon_{kl}(\mathbf{r}^e)\right] \quad (2.16)$$

assuming that $\varepsilon_{kl}(\mathbf{r}^{sad}) \simeq \varepsilon_{kl}(\mathbf{r}^e)$. This new diffusion tensor can be expressed as a function of the unstrained diffusion coefficient D^0 :

$$D_{ij}(\mathbf{r}) = \frac{3D^0}{N} \sum_{\mathbf{h}} u_i^{\mathbf{h}} u_j^{\mathbf{h}} \exp[\beta \sum_{kl} (P_{kl}^{sad}(\mathbf{h}) - \bar{P}_{kl}^e) \varepsilon_{kl}(\mathbf{r}^e)] \quad (2.17)$$

with $D^0 = \frac{N}{6} h^2 \nu \exp(-\beta E_0^m)$. In the case of isotropic PD at saddle point, $P_{kl}^{sad}(\mathbf{h}) = P_{kl}^{sad}$, relation 2.17 leads then to a diagonal diffusion tensor:

$$D_{ij}(\mathbf{r}) = \frac{3D^0}{N} \exp[\beta \sum_{kl} (P_{kl}^{sad} - \bar{P}_{kl}^e) \varepsilon_{kl}(\mathbf{r}^e)] \sum_{\mathbf{h}} u_i^{\mathbf{h}} u_j^{\mathbf{h}} \quad (2.18)$$

since

$$\sum_{\mathbf{h}} u_i^{\mathbf{h}} u_j^{\mathbf{h}} = 0, \quad \text{if } i \neq j. \quad (2.19)$$

On the contrary, for anisotropic PD at saddle point, D_{ij} can have off-diagonal terms whereas D_{ij}^0 does not. In the case where P_{kl}^{sad} depends on the initial and final PD orientations, a similar expression of Eq. 2.17 is obtained:

$$D_{ij}(\mathbf{r}) = \frac{3D^0}{NZ} \sum_{\mathbf{h}} \sum_{\xi\psi} u_i^{\mathbf{h}} u_j^{\mathbf{h}} \exp[\beta \sum_{kl} (P_{kl}^{sad}(\xi\psi) - \bar{P}_{kl}^e) \varepsilon_{kl}(\mathbf{r}^e)] \quad (2.20)$$

where ξ and ψ refer respectively to the PD orientation in the initial and final stable configurations and Z is the number of pairs (ξ, ψ) .

The P_{ij} -tensors can be determined from atomistic calculations. For this purpose, a perfect simulation cell of volume V with periodic boundary conditions is considered. One PD is introduced in the box and the supercell vectors are kept fixed. After atomic relaxation, the P_{ij} -tensors are deduced from the residual stress σ_{ij} induced by the PD on the box through the relation [46, 34, 35]:

$$P_{ij} = V(\sigma_{ij} - \sigma_{ij}^0) \quad (2.21)$$

where σ_{ij}^0 is the residual stress on the perfect supercell after relaxation. Generally, σ_{ij}^0 is not zero due to the finite convergence criteria used for the simulations. An alternative though more time consuming way is to determine P_{ij} from the strain field of the supercell if it is allowed to relax in volume and shape (see Eq. 2.25 for instance). The elastic dipole tensors can be also determined from experiments, but requires a combination of several experimental techniques [35].

The elastodiffusion effects on sink strength of various sink types have been investigated analytically [47] and using OKMC simulations [46, 34]. The results obtained mainly show that taking into account elastodiffusion can have significant effects on the sink strength. Skinner and Woo [47] have studied the elastodiffusion effects on sink strength of edge dislocations in fcc copper and bcc iron. They performed analytical calculations in the case of isotropic and anisotropic PD at saddle point. Their results showed the increase of sink strength with the PD anisotropy for both materials and the effects are more important for high dislocation densities. The PD anisotropy effects are more pronounced for vacancies than SIAs in copper while the effects are comparable for both PDs in iron. The results

obtained by Carpentier et al. [34] using OKMC simulations in Al are qualitatively the same of that obtained in copper by Skinner for edge dislocations. Carpentier et al. have also performed the OKMC simulations in the case of a spherical cavity. The results revealed the increase of the sink strength with the PD anisotropy at saddle point which leads to a cavity bias around 30 %, whereas cavity is commonly considered as an unbiased sink. Elastodiffusion effects on sink strength of grain boundaries have also been investigated by Vattré et al. [46]. In this case, the effects are visible for high grain boundary densities. The studies of Vattré [46] and Carpentier [34] also showed that the PD trajectory towards the sink is modified when elastodiffusion is taken into account. All these results show that the elastodiffusion effects on sink strength and PD trajectories depend on several parameters such as: the P_{ij} -tensors anisotropy at saddle point, the crystal anisotropy, the sink strain field properties, etc.

The elastodiffusion has been described in this section. Thus, in addition to the elastic drift term, the elastodiffusion allows to take into account the elastic effects in the PD diffusion tensor. A comparison of the sink strength calculations without and with elastodiffusion will allow to quantify the elastodiffusion effects on the sink strength. For that, we use a PF approach whose description is given in the following section (section 2.2).

2.2 PF methodology

A single crystal is considered in which one type of sink is introduced. The production of PDs is simulated through a generation rate term. PD will diffuse inside the matrix and will be absorbed by the sink. To describe the system evolution, the order parameters, the total free energy of the system and the evolution equations are defined successively, as usually done in a PF approach.

2.2.1 Order parameters

The necessary order parameters to describe the system evolution are the following:

- The site fractions of PDs X_d , $d = i$ for SIAs or v for vacancies. PDs are created at a uniform and constant generation rate K_0 (s^{-1}).
- The elastic shape function η_s associated to the sink s and which allows to generate the corresponding stress field.
- The shape function λ_s of the capture zone of sink s (equal to 0 inside the matrix and 1 in the capture zone). This parameter allows a precise control of the sink geometry, which is essential to correctly calculate the sink strength.

2.2.2 Energy of the system

The system evolves by [minimisation](#) of the total free energy F . Strictly speaking, this is only true close enough to equilibrium, an hypothesis that we assume in the following. F

includes the chemical free energy F_{chem} associated to PD and the elastic energy F_{el} :

$$F(X_d, \eta_s) = F_{chem}(X_d) + F_{el}(X_d, \eta_s) \quad (2.22)$$

In our system description, the sink evolution due to the PD absorption is not taken into account, and the sink is assumed **unchanged** and **immobile**. This assumption justifies the fact that the self-energy associated to the sink is ignored in Eq. 2.22.

Chemical free energy

In the limit of **dilute systems**, the chemical free energy of the system is written as [10]:

$$F_{chem}(X_d) = \frac{1}{V_{at}} \sum_d \int_V E_f^d X_d + k_B T [X_d \ln X_d + (1 - X_d) \ln(1 - X_d)] dV \quad (2.23)$$

where E_f^d is the PD formation energy and V is the volume of the system.

Elastic energy

The elastic energy is calculated via the **microelasticity theory** [26]. It is a function of the elastic strain which is the difference between the total strain $\varepsilon_{ij}(\mathbf{r})$ and the total eigenstrain $\varepsilon_{ij}^{0,tot}(\mathbf{r})$. The total eigenstrain is given by:

$$\varepsilon_{ij}^{0,tot}(\mathbf{r}) = \sum_d \varepsilon_{ij}^{0,X_d} X_d(\mathbf{r}) + \varepsilon_{ij}^{0,\eta_s} \eta_s(\mathbf{r}) \quad (2.24)$$

where ε_{ij}^{0,X_d} and $\varepsilon_{ij}^{0,\eta_s}$ are respectively the **eigenstrain** associated to the PD d and the sink s . The PD eigenstrain and its dipole tensor at the equilibrium state are connected by the relation:

$$P_{ij}^{e,d} = V_{at} C_{ijkl} \varepsilon_{kl}^{0,X_d} \quad (2.25)$$

where C_{ijkl} are the elastic constants of the system. In this manuscript, the system is considered **homogeneous** which means that the elastic constants are independent of space. The PD relaxation volume Ω_d is given by:

$$\Omega_d = V_{at} \text{Tr}(\varepsilon_{kl}^{0,X_d}) \quad (2.26)$$

ε_{kl}^{0,X_d} can be determined from atomic-scale calculations of the P_{ij} tensors (see Eq. 2.25). Elastic equivalences between a given sink and an inclusion are used to determine the corresponding eigenstrain $\varepsilon_{ij}^{0,\eta_s}$ [48, 40]. Examples will be given in section 2.3.1.

The expression of the elastic energy is as follows:

$$F_{el} = \frac{1}{2} \int_V C_{ijkl} [\varepsilon_{ij}(\mathbf{r}) - \varepsilon_{ij}^{0,tot}(\mathbf{r})] [\varepsilon_{kl}(\mathbf{r}) - \varepsilon_{kl}^{0,tot}(\mathbf{r})] dV \quad (2.27)$$

The total strain $\varepsilon_{ij}(\mathbf{r})$ can be decomposed into two parts, the heterogeneous part of the strain $\delta\varepsilon_{ij}(\mathbf{r})$ and the average strain $\bar{\varepsilon}_{ij}$:

$$\varepsilon_{ij}(\mathbf{r}) = \bar{\varepsilon}_{ij} + \delta\varepsilon_{ij}(\mathbf{r}) \quad (2.28)$$

it can be demonstrated that in an elastically homogeneous system,

$$\bar{\varepsilon}_{ij} = \sum_d \varepsilon_{ij}^{0,X_d} \overline{X_d(\mathbf{r})} + \varepsilon_{ij}^{0,\eta_s} \overline{\eta_s(\mathbf{r})} \quad (2.29)$$

The heterogeneous strain $\delta\varepsilon_{ij}(\mathbf{r})$ derives from the displacement field $u_i(\mathbf{r})$, and for small strains is given by:

$$\delta\varepsilon_{ij}(\mathbf{r}) = \frac{1}{2} \left[\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i} \right](\mathbf{r}) \quad (2.30)$$

The displacement field is obtained by solving the mechanical equilibrium equation:

$$\text{div } \sigma_{ij}(\mathbf{r}) = 0 \quad (2.31)$$

where $\sigma_{ij}(\mathbf{r})$ is the elastic stress:

$$\sigma_{ij}(\mathbf{r}) = C_{ijkl}(\varepsilon_{kl}(\mathbf{r}) - \varepsilon_{kl}^{0,tot}(\mathbf{r})) \quad (2.32)$$

Eq. 2.31 becomes using Eq.2.32 and Eq.2.30:

$$C_{ijkl} \frac{\partial^2 u_k(\mathbf{r})}{\partial r_j \partial r_l} = C_{ijkl} \left[\sum_d \varepsilon_{kl}^{0,X_d} \frac{\partial X_d(\mathbf{r})}{\partial r_j} + \varepsilon_{kl}^{0,\eta_s} \frac{\partial \eta_s(\mathbf{r})}{\partial r_j} \right] \quad (2.33)$$

The Fourier space is used to solve Eq.2.33 due to its simple form in this space:

$$[G_{ik}(\mathbf{q})]^{-1} \tilde{u}_k(\mathbf{q}) = -i_c C_{ijkl} \left[\sum_d \varepsilon_{kl}^{0,X_d} q_j \tilde{X}_d(\mathbf{q}) + \varepsilon_{kl}^{0,\eta_s} q_j \tilde{\eta}_s(\mathbf{q}) \right] \quad (2.34)$$

with $[G_{ik}(\mathbf{q})]^{-1} = C_{ijkl} q_j q_l$ and i_c is the imaginary complex number defined as $(i_c)^2 = -1$. $\tilde{\phi}$ is the Fourier transform of the field ϕ and $\mathbf{q}$ is the wave vector. $G_{ik}(\mathbf{q})$ is the Fourier transform of the Green function used in anisotropic elasticity. $\tilde{\phi}$ is given by:

$$\tilde{\phi}(\mathbf{q}) = \int_V \phi(\mathbf{r}) \exp(-i_c \mathbf{q} \cdot \mathbf{r}) dV \quad (2.35)$$

The elastic energy is also computed in the Fourier space and it can be demonstrated that:

$$\begin{aligned} F_{el} = & \frac{1}{2} V \sum_m C_{ijkl} \varepsilon_{ij}^{0,\theta_m} \varepsilon_{kl}^{0,\theta_m} \bar{\theta}_m - \frac{1}{2} V \sum_m \sum_n C_{ijkl} \varepsilon_{ij}^{0,\theta_m} \varepsilon_{kl}^{0,\theta_n} \bar{\theta}_m \bar{\theta}_n \\ & - \frac{1}{2} \sum_m \sum_n \int \frac{d^3 q}{(2\pi)^3} q_j \sigma_{ij}^{0,\theta_m} G_{ik}(\mathbf{q}) \sigma_{kl}^{0,\theta_n} q_l \tilde{\theta}_m(\mathbf{q}) \tilde{\theta}_n(\mathbf{q}) \end{aligned} \quad (2.36)$$

where $\sigma_{ij}^{0,\theta_m} = C_{ijkl} \varepsilon_{kl}^{0,\theta_m}$. θ_m refers to the order parameter (X_I , X_V , η_s) associated to the defect m (i, v, s). The use of the Fourier space implies periodic conditions at the boundaries of the simulation domain.

2.2.3 Kinetic equations

The PD fraction X_d is assumed to be [conserved](#) in the matrix and its evolution equation is of a [Cahn-Hilliard](#) type. The generation rate term K_0 and the absorption term $J_{s,d}^{abs}(\mathbf{r}, t)$ are added in this equation to simulate the PD creation by irradiation and absorption by the sink. The resulting equation is given by:

$$\frac{\partial X_d}{\partial t}(\mathbf{r}, t) = \sum_i \nabla_i \cdot \left[\sum_j M_{ij}^d(\mathbf{r}, t) \nabla_j \frac{\delta F(X_d, \eta_s)}{\delta X_d}(\mathbf{r}, t) \right] + K_0 - J_{s,d}^{abs}(\mathbf{r}, t) \quad (2.37)$$

with $M_{ij}^d(\mathbf{r}, t)$ the PD mobility tensor of type d which in the case of the simple free energy expressed by Eq. [2.23](#) can be written as:

$$M_{ij}^d(\mathbf{r}, t) = \frac{X_d(\mathbf{r}, t)}{k_B T} D_{ij}^d(\mathbf{r}) \quad (2.38)$$

where D_{ij}^d is the PD diffusion tensor given by equation [2.20](#). The [recombination](#) between PDs is [neglected](#) and the PD diffusion equations are solved independently. $J_{s,d}^{abs}$ is defined by using the shape function λ_s as:

$$J_{s,d}^{abs}(\mathbf{r}, t) = \lambda_s(\mathbf{r}) \lambda_{eff}(X_d(\mathbf{r}, t) - X_d^s) \quad (2.39)$$

λ_{eff} is an efficiency factor equal to $1/\delta t$ in the case of a perfect sink, δt being the time step used to solve the kinetic equation of PDs. X_d^s is the atomic fraction of PD inside the sink which is fixed at a constant value usually taken as the thermal equilibrium fraction of the PD since the sink is assumed unchanged. Substituting the total energy into Eq. [2.37](#) and taking the first variational derivatives with respect to the PD fraction X_d , we obtain:

$$\frac{\partial X_d}{\partial t}(\mathbf{r}, t) = \sum_i \nabla_i \cdot \left[\sum_j \frac{D_{ij}^d(\mathbf{r})}{V_{at} k_B T} X_d(\mathbf{r}, t) \nabla_j (\mu_{chem}^d(\mathbf{r}, t) + \mu_{el}^d(\mathbf{r}, t)) \right] + K_0 - J_{s,d}^{abs}(\mathbf{r}, t) \quad (2.40)$$

where

$$\mu_{chem}^d = V_{at} \frac{\delta F_{chem}}{\delta X_d} \quad (2.41)$$

In the low PD fraction approximation:

$$\mu_{chem}^d = E_f + k_B T \ln X_d \quad (2.42)$$

$$\mu_{el}^d = V_{at} \frac{\delta F_{el}}{\delta X_d} \quad (2.43)$$

μ_{el}^d is calculated in the Fourier space and has the following simple form:

$$\tilde{\mu}_{el}^I(\mathbf{q}) = B_{II}(\mathbf{q}) \tilde{X}_I(\mathbf{q}) + B_{IV}(\mathbf{q}) \tilde{X}_V(\mathbf{q}) + B_{I\eta_s}(\mathbf{q}) \tilde{\eta}(\mathbf{q}) \quad (2.44)$$

$$\tilde{\mu}_{el}^V(\mathbf{q}) = B_{VV}(\mathbf{q}) \tilde{X}_V(\mathbf{q}) + B_{VI}(\mathbf{q}) \tilde{X}_I(\mathbf{q}) + B_{V\eta_s}(\mathbf{q}) \tilde{\eta}(\mathbf{q}) \quad (2.45)$$

where

$$\left\{ \begin{array}{l} B_{II}(\mathbf{q}) = \sigma_{ij}^{0,X_I} \varepsilon_{ij}^{0,X_I} - q_j \sigma_{ij}^{0,X_I} G_{ik}(\mathbf{q}) \sigma_{kl}^{0,X_I} q_l \\ B_{VV}(\mathbf{q}) = \sigma_{ij}^{0,X_V} \varepsilon_{ij}^{0,X_V} - q_j \sigma_{ij}^{0,X_V} G_{ik}(\mathbf{q}) \sigma_{kl}^{0,X_V} q_l \\ B_{IV}(\mathbf{q}) = \sigma_{ij}^{0,X_I} \varepsilon_{ij}^{0,X_V} - q_j \sigma_{ij}^{0,X_I} G_{ik}(\mathbf{q}) \sigma_{kl}^{0,X_V} q_l \\ B_{VI}(\mathbf{q}) = \sigma_{ij}^{0,X_V} \varepsilon_{ij}^{0,X_I} - q_j \sigma_{ij}^{0,X_V} G_{ik}(\mathbf{q}) \sigma_{kl}^{0,X_I} q_l \\ B_{I\eta_s}(\mathbf{q}) = \sigma_{ij}^{0,X_I} \varepsilon_{ij}^{0,\eta} - q_j \sigma_{ij}^{0,X_I} G_{ik}(\mathbf{q}) \sigma_{kl}^{0,\eta_s} q_l \\ B_{V\eta_s}(\mathbf{q}) = \sigma_{ij}^{0,X_V} \varepsilon_{ij}^{0,\eta} - q_j \sigma_{ij}^{0,X_V} G_{ik}(\mathbf{q}) \sigma_{kl}^{0,\eta_s} q_l \end{array} \right. \quad (2.46)$$

The local PD flux $\mathbf{J}^d$, which is a function of driving forces is given by:

$$J_i^d(\mathbf{r}, t) = - \sum_j \frac{D_{ij}^d(\mathbf{r}) X_d(\mathbf{r}, t)}{V_{at} k_B T} \nabla_j (\mu_{chem}^d(\mathbf{r}, t) + \mu_{el}^d(\mathbf{r}, t)) \quad (2.47)$$

The evolution equations of the order parameters η_s and λ_s are not required due to the fact that they do not evolve. The sink strength $k_{s,d}^2$ can be deduced from Eq. 2.40 when steady state is reached. It is a function of the absorption rate $J_{s,d}$ and the average site fraction $\bar{X}_d$ [10]:

$$k_{s,d}^2 = \frac{J_{s,d}}{D^{0,d}(\bar{X}_d - X_d^s)} \quad (2.48)$$

with

$$J_{s,d} = \frac{1}{V} \int_V J_{s,d}^{abs}(\mathbf{r}, t) dV \quad (2.49)$$

To solve equation 2.40, the following dimensionless parameters are introduced:

$$\left\{ \begin{array}{l} \mathbf{r}^* = \mathbf{r}/a_0, \quad \nabla_i^* = a_0 \nabla_i \\ D_{ij}^{d,*} = D_{ij}^d / D^{0,d} \\ t^* = t/t_0, \quad t_0 = a_0^2 / D^{0,d} \\ K_0^* = t_0 K_0 \\ J_{s,d}^{abs,*} = t_0 J_{s,d}^{abs} \\ C_{ijkl}^* = C_{ijkl} / \left(\frac{k_B T}{V_{at}} \right), \quad \mu^* = \frac{\mu}{k_B T} \end{array} \right. \quad (2.50)$$

where a_0 is the length of a unit PF cell. The dimensionless form of Eq. 2.40 is given by:

$$\frac{\partial X_d}{\partial t^*}(\mathbf{r}^*, t^*) = \sum_i \nabla_i^* \left[\sum_j D_{ij}^{d,*}(\mathbf{r}^*) X_d \nabla_j^* (\mu_{chem}^{d,*}(\mathbf{r}^*, t^*) + \mu_{el}^{d,*}(\mathbf{r}^*, t^*)) \right] + K_0^* - J_{s,d}^{abs,*}(\mathbf{r}^*, t^*) \quad (2.51)$$

Specific numerical schemes and algorithms are required to treat Eq. 2.51. More details on this issue are given in Appendix A.

The PF methodology being described, applications are made to the sink strength calculations for various sinks in different materials in section 2.3.

2.3 Applications to pure Al, Ni (fcc) and Fe (bcc)

In this section, the PF model described in section 2.2 has been applied to investigate the elastodiffusion effects on sink strength in different pure cubic metals and for different sink types: straight dislocations, low angle tilt grain boundaries and spherical cavities. Firstly, the sinks are described and the corresponding PF stress fields are compared with the existing analytical solutions for validation. The sink strength is computed in the case of a straight dislocation and a spherical cavity to validate our model. Secondly, pure aluminium, nickel (fcc) and iron (bcc) are considered. The PD flux and atomic fraction maps are plotted to study the elastodiffusion effects on the PD trajectories and depletion region. Finally, the sink strength is computed and the results are compared with those available in the literature.

2.3.1 Sinks description, stress field and sink strength validation

The sinks are defined by the order parameters η_s and λ_s . [Isotropic material](#) is considered for stress field validation due to the fact that analytical solutions are easier to obtain in this case. The parameters used are given in table 2.2.

Table 2.2: Physical parameters for stress field validation.

T	600 K
b	0.3 nm
Shear modulus μ	33 GPa
Poisson ratio ν	0.33
Atomic volume V_{at}	$2.3 \times 10^{-29} \text{ m}^3$
Vacancy relaxation volume, Ω_v	$-0.6V_{at}$
SIA relaxation volume, Ω_I	$1.2V_{at}$

Straight dislocations

PF simulations of dislocations became possible thanks to the equivalence established by Nabarro [48] and have been performed first in [49, 50]. Nabarro has shown that a dislocation loop is elastically equivalent to a platelet inclusion with thickness d and whose border corresponds to the dislocation line (see Fig. 2.2). The eigenstrain $\varepsilon_{ij}^{0,\eta_s}$ associated to the platelet is defined as:

$$\varepsilon_{ij}^{0,\eta_s} = \frac{b_i n_j + b_j n_i}{2d} \quad (2.52)$$

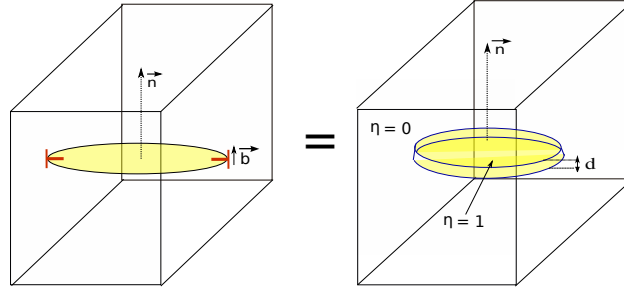
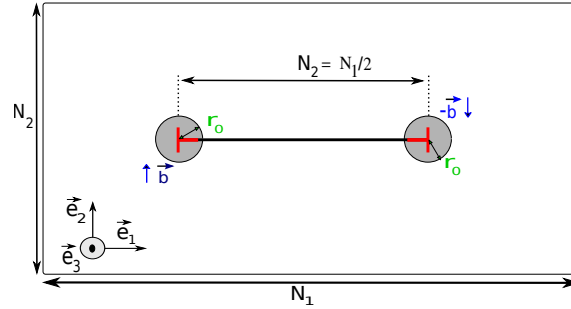


Figure 2.2: Elastic equivalence between a dislocation loop and a platelet.

where b_i and n_j are respectively the i^{th} component of the Burgers vector and the j^{th} component of the unit vector normal to the habit plane of the loop. The field η_s allows to describe the platelet: it is equal to 0 inside the matrix, and 1 inside the platelet and varies from 0 to 1 at the platelet border as illustrated in Fig. 2.2. The platelet border which corresponds to the dislocation loop core is therefore modelled as a [diffuse interface](#) of width w . The dislocation loop can be mimicked in 2 dimensions by a dipole of edge dislocations as illustrated in Fig. 2.3. η_s is given by:

Figure 2.3: 2D simulation domain of size $N_1 \times N_2$ containing a dipole of edge dislocations. r_0 is the radius of the capture region.

$$\eta_s(x_1, x_2) = \frac{1}{2} \delta(x_2 - x_2^c) \left[\tanh\left(\frac{2(x_1 - x_1^{c1})}{w}\right) - \tanh\left(\frac{2(x_1 - x_1^{c2})}{w}\right) \right] \quad (2.53)$$

where (x_1^{c1}, x_2^c) and (x_1^{c2}, x_2^c) are the coordinates of the two lines of dislocations and δ the Dirac function ($\delta(x = 0) = 1$, $\delta(x \neq 0) = 0$). An example of the profile of η_s is given in Fig. 2.4. The dislocation core width is set to $w = 4b$. The platelet thickness d and the size of a unit PF cell a_0 have been taken equal to the length of the Burgers vector b . The dislocation density ρ depends on the simulation box dimensions as ($N_1 = 2N_2$):

$$\rho = \frac{1}{N_2^2 a_0^2} \quad (2.54)$$

The capture region of the PD by the dislocation cores corresponds to 2 cylinders of radius r_0 . $\lambda(\mathbf{r})$ is equal to 0 outside the cylinder and 1 inside. The stress field has been computed

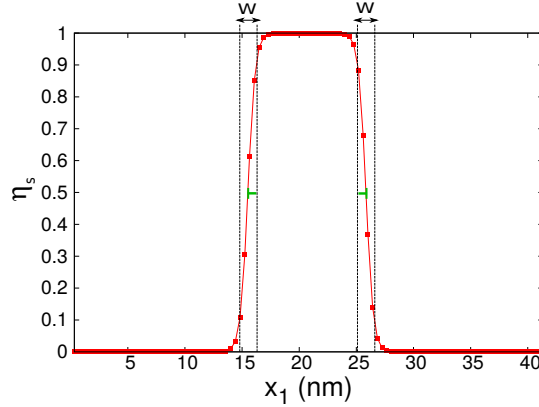


Figure 2.4: Example of η_s profile, passing through the dislocation cores along $\mathbf{e}_1$ in the case of straight dislocations.

for a simulation domain size of $330.75 \times 165.37 \text{ nm}^2$. The dislocation cores are located at $(82.68, 82.68) \text{ nm}$ and $(248.06, 82.68) \text{ nm}$. For an edge dislocation in an isotropic medium, the analytical solution of the stress field is given by:

$$\left\{ \begin{array}{l} \sigma_{11}(x_1, x_2) = -\frac{\mu b}{2\pi(1-\nu)} \frac{x_2(3x_1^2 + x_2^2)}{(x_1^2 + x_2^2)^2} \\ \sigma_{22}(x_1, x_2) = \frac{\mu b}{2\pi(1-\nu)} \frac{x_2(x_1^2 - x_2^2)}{(x_1^2 + x_2^2)^2} \\ \sigma_{12}(x_1, x_2) = -\frac{\mu b}{2\pi(1-\nu)} \frac{x_1(x_1^2 - x_2^2)}{(x_1^2 + x_2^2)^2} \\ \sigma_{33}(x_1, x_2) = \nu(\sigma_{11} + \sigma_{22})(x_1, x_2) \\ \sigma_{13} = \sigma_{23} = 0 \end{array} \right. \quad (2.55)$$

where the origin of the coordinates coincide with the position of the dislocation. The stress field obtained by PF and the analytical solution are plotted in Fig. 2.5. The profiles of Fig. 2.5 show a good agreement between the PF and the analytical solution. The radius r_0 is chosen such that the extremum values of the stress field are contained in this region as suggested in [4]. Typically, r_0 corresponds to the dislocation core width w ($r_0 = 4b$). The sink strength of cylindrical sinks (edge dislocations without elastic interactions) is plotted in Fig. 2.6. The PF results are compared to the solutions of Laplace, Poisson and Wiedersich. A good agreement is obtained with the Wiedersich solution as expected [27, 4] and allows to validate our PF approach of sink strength calculations.

Grain boundaries

A grain boundary (GB) is an interface between two crystals which differ by their orientations. A certain number of parameters are needed to crystallographically characterize a grain boundary:

- The rotation angle between the two single crystals.

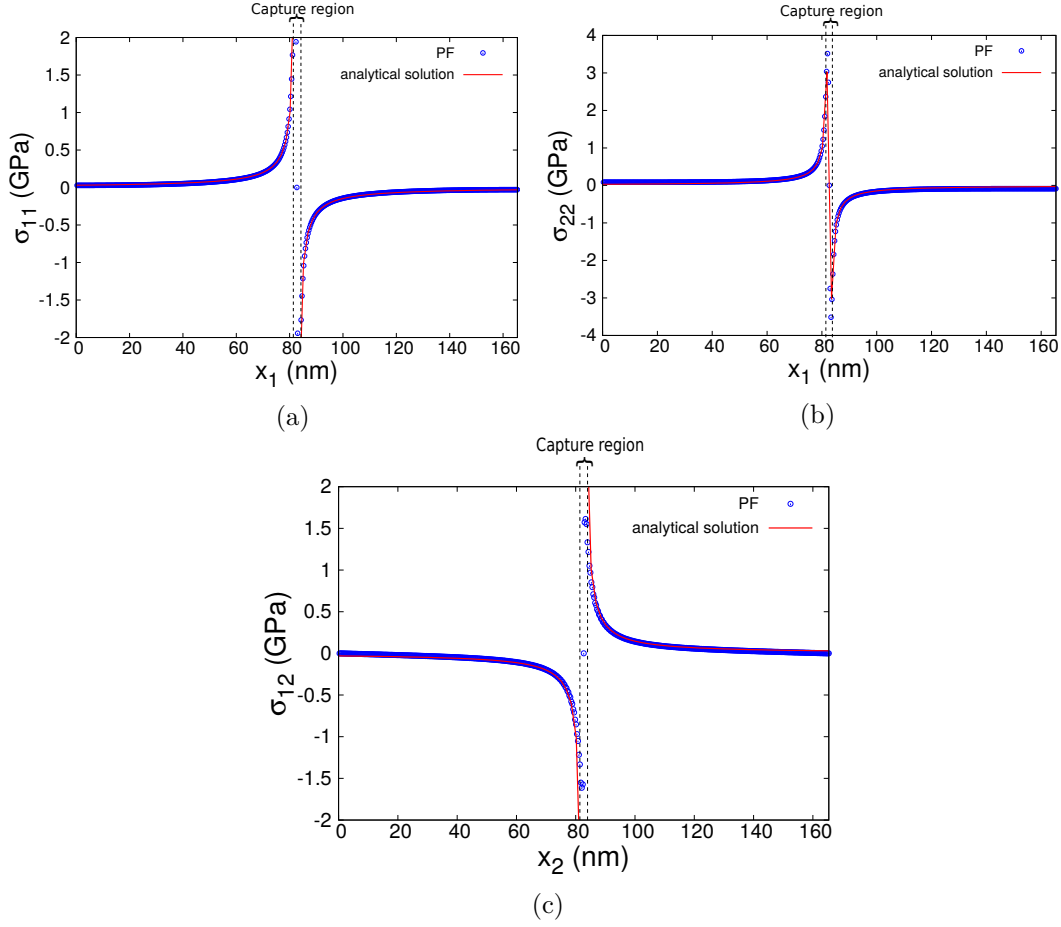


Figure 2.5: Profiles of the stress field components of edge dislocation a) σ_{11} along $\mathbf{e}_1$ ($x_2^c = 82.68$ nm), b) σ_{22} along $\mathbf{e}_1$ ($x_2^c = 82.68$ nm), and c) σ_{12} along $\mathbf{e}_2$ ($x_1^c = 82.68$ nm).

- The rotation axis, identified by its Miller indices $[uvw]$.
- The orientation of the GB plane defined by its normal (hkl) .

Thus, GB can be denoted $(hkl)[uvw]$ where (hkl) refers to the normal of the GB plane and $[uvw]$ to the rotation axis. Among the different types of GBs, the most simple ones to describe are symmetric tilt grain boundaries (STGBs), where (grains are rotated by opposite angles) the rotation axis is contained in the grain boundary plane. In the Read–Shockley model [51], STGBs with low tilt angles can be described as an [array of edge dislocations](#) separated by a distance h . The tilt angle θ is connected to h through the relation:

$$h = \frac{b}{2 \sin(\theta/2)} \simeq \frac{b}{\theta} \quad (2.56)$$

As it is possible to model dislocations using PF, we thus focused on STGBs with small tilt angles. GB is modelled in 2D, the rotation axis and the normal to the GB plane correspond respectively to the dislocation line and the Burgers vector. A PF simulation

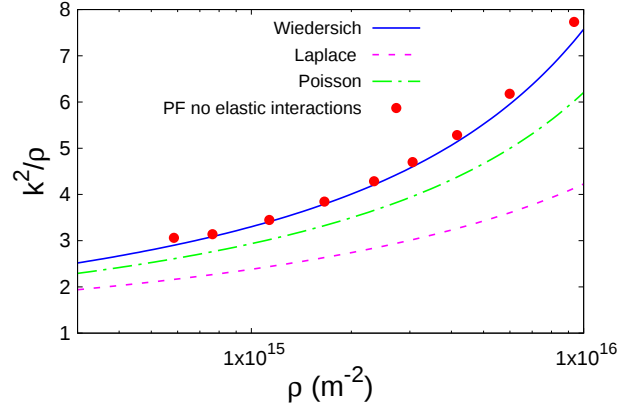


Figure 2.6: Sink strength as a function of the dislocation density without elastic interactions.

box containing a STGB with a low misorientation is illustrated in Fig. 2.7. Each dipole is defined using the parameters η and λ introduced in the case of a straight dislocation. The inter-spacing between dislocations was set to $h = 6b$ in the simulations in order to compute and validate the stress field. The simulation box size is $46.51 \times 23.25 \text{ nm}^2$. Along direction $\mathbf{e}_1$ the GBs are located at 11.62 nm and 34.88 nm. The parameters of table 2.2 have been used. The analytical solution of the stress field generated by an array of edge

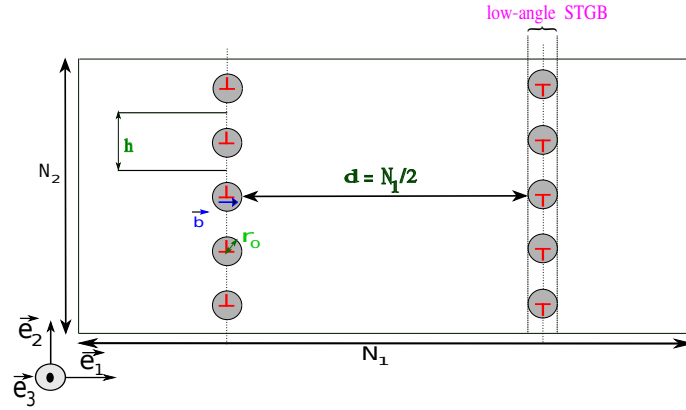


Figure 2.7: 2D simulation box of size $N_1 \times N_2$ containing an array of edge dislocation dipoles (low-angle STGBs).

dislocations is expressed as follows [52]:

$$\begin{cases} \sigma_{11}(x_1, x_2) = -\tau \sin(2\pi X_2)(\cosh(2\pi X_1) - \cos(2\pi X_2) + 2\pi X_1 \sinh(2\pi X_1)) \\ \sigma_{22}(x_1, x_2) = -\tau \sin(2\pi X_2)(\cosh(2\pi X_1) - \cos(2\pi X_2) - 2\pi X_1 \sinh(2\pi X_1)) \\ \sigma_{12}(x_1, x_2) = 2\pi\tau X_1(\cosh(2\pi X_1) \cos(2\pi X_2) - 1) \end{cases} \quad (2.57)$$

where $X_1 = x_1/h$, $X_2 = x_2/h$ and $\tau = \frac{\mu b}{2h(1-\nu)(\cosh(2\pi X_1) - \cos(2\pi X_2))^2}$.

The profiles of the stress field obtained by PF and the analytical solution are represented in Fig. 2.8. Globally, a good agreement is observed between the profiles.

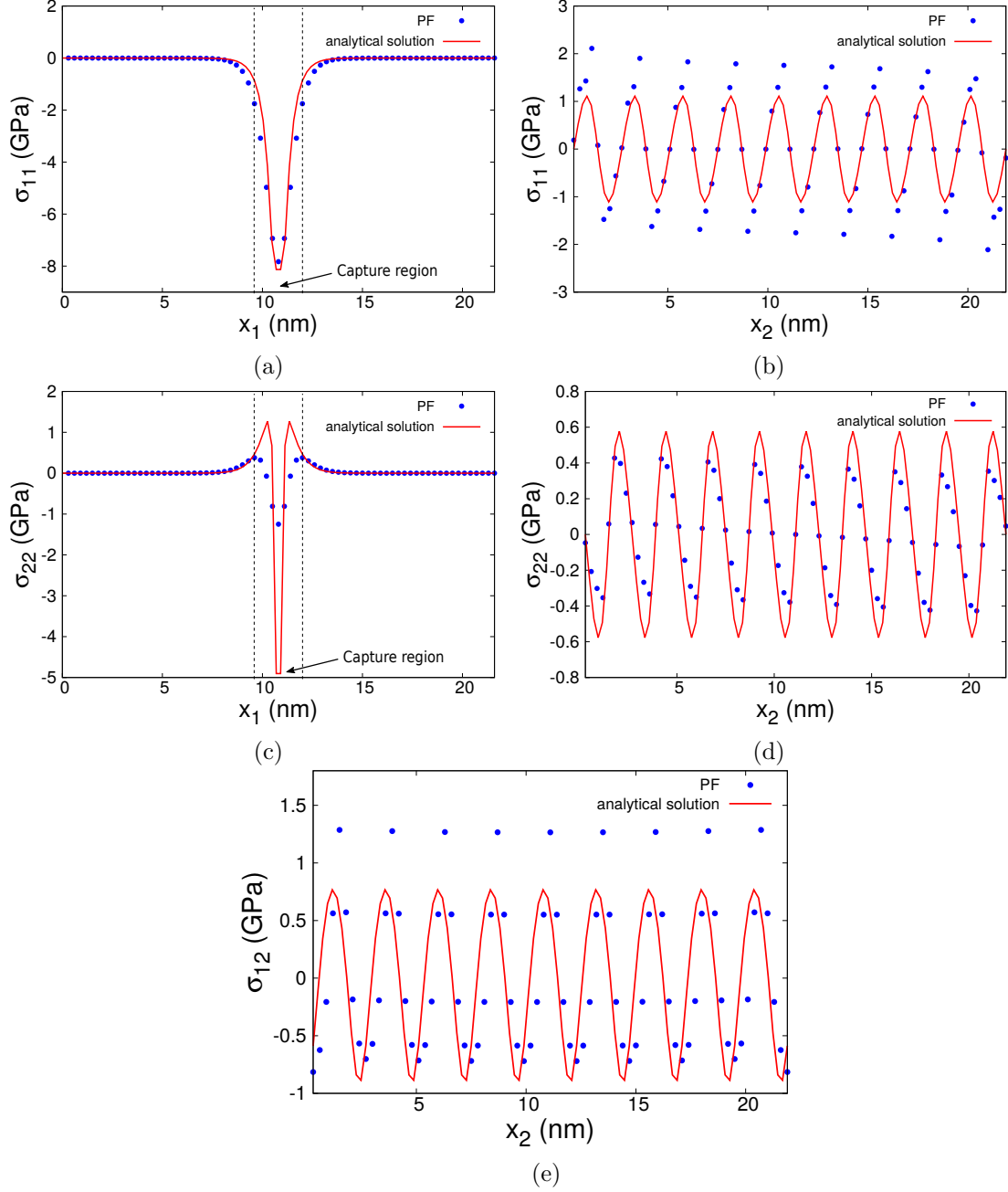


Figure 2.8: Profiles of the stress field components of low angle STGB a) σ_{11} along $\mathbf{e}_1$ at $x_2 = 10.8$ nm, b) σ_{11} along $\mathbf{e}_2$ at $x_1 = 12$ nm, c) σ_{22} along $\mathbf{e}_1$ at $x_2 = 10.8$ nm, d) σ_{22} along $\mathbf{e}_2$ at $x_1 = 12$ nm, e) σ_{12} along $\mathbf{e}_2$ at $x_1 = 12$ nm.

Spherical cavities

The elastic PF description of a cavity, like in the case of a dislocation loop, requires the knowledge of the corresponding eigenstrain. The determination of the eigenstrain of a spherical cavity in cubic medium has been done by Chiang [53] using the inclusion model of Eshelby [54]. In this model, an ellipsoidal domain Γ with the elastic constants C'_{ijkl} in an infinite material with the elastic constants C_{ijkl} is considered. The elastic constants of the domain Γ differ from those of the matrix and the domain is called an ellipsoidal inhomogeneity. The presence of this inhomogeneity induces a stress σ_{ij} with the corresponding strain ε_{ij} . The existence of an external stress σ_{ij}^A with the corresponding strain ε_{ij}^A leads to the total stress $\sigma_{ij} + \sigma_{ij}^A$ defined as:

$$\sigma_{ij} + \sigma_{ij}^A = C'_{ijkl}(\varepsilon_{kl} + \varepsilon_{kl}^A) \quad \text{in } \Gamma \quad (2.58)$$

The inclusion equivalence consists in the fact that the stress σ_{ij} due to an inhomogeneity in an external stress σ_{ij}^A can be simulated by an eigenstrain associated to inclusion with the same elastic constants as the ones of the matrix. Then, an infinite material, homogeneous with the elastic constants C_{ijkl} and containing a domain Γ with an eigenstrain $\varepsilon_{ij}^{0,\eta}$ is considered. The eigenstrain $\varepsilon_{ij}^{0,\eta}$ is introduced in order to simulate elastically the inhomogeneity. In this new system, in the presence of an external stress σ_{ij}^A , the total stress $\sigma_{ij} + \sigma_{ij}^A$ is given by:

$$\sigma_{ij} + \sigma_{ij}^A = C_{ijkl}(\varepsilon_{kl} + \varepsilon_{kl}^A - \varepsilon_{kl}^{0,\eta}) \quad \text{in } \Gamma \quad (2.59)$$

Thus, the inhomogeneity problem is elastically equivalent to the homogeneous inclusion problem if:

$$C'_{ijkl}(\varepsilon_{kl} + \varepsilon_{kl}^A) = C_{ijkl}(\varepsilon_{kl} + \varepsilon_{kl}^A - \varepsilon_{kl}^{0,\eta}) \quad \text{in } \Gamma \quad (2.60)$$

Eshelby has shown that the strain ε_{ij} and the eigenstrain $\varepsilon_{ij}^{0,\eta}$ are linked in the following way:

$$\varepsilon_{ij} = S_{ijkl}\varepsilon_{kl}^{0,\eta} \quad (2.61)$$

where S_{ijkl} is called the [Eshelby tensor](#) and is given by [53, 54]:

$$S_{ijmn} = \frac{C_{klmn}}{8\pi} \int_0^\pi \sin \tilde{\theta} d\tilde{\theta} \int_0^{2\pi} [G_{ik}^{-1}(\mathbf{q})q_j q_l + G_{jk}^{-1}(\mathbf{q})q_i q_l] d\tilde{\phi} \quad (2.62)$$

where $\tilde{\theta}$ and $\tilde{\phi}$ are the spherical coordinates in the Fourier space. In the case where a spherical cavity of radius R_{cav} is the inhomogeneity, with a surface tension γ and in which $C'_{ijkl} = 0$, equation 2.60 becomes:

$$C_{ijkl}(S_{klmn}\varepsilon_{mn}^{0,\eta} + \varepsilon_{kl}^A - \varepsilon_{kl}^{0,\eta}) = 0 \quad (2.63)$$

$$\implies C_{ijkl}(S_{klmn} - I_{klmn})\varepsilon_{mn}^{0,\eta} = -\sigma_{ij}^A \quad (2.64)$$

with I_{klmn} the unit tensor. For a cubic system and a hydrostatic pressure ($\sigma_{ij}^A = -p^A \delta_{ij}$), Eq. 2.64 becomes:

$$\varepsilon_{ij}^{0,\eta} = \frac{p^A}{(C_{11} + 2C_{12})(S_{11} + 2S_{12} - 1)} \delta_{ij} \quad (2.65)$$

In the absence of an external pressure, p^A is simply equal to:

$$p^A = \frac{2\gamma}{R_{cav}} \quad (2.66)$$

The eigenstrain $\varepsilon_{ij}^{0,\eta}$ of the cavity is thus given by:

$$\varepsilon_{ij}^{0,\eta} = \frac{2\gamma}{R_{cav}(C_{11} + 2C_{12})(S_{11} + 2S_{12} - 1)} \delta_{ij} \quad (2.67)$$

In the case of an isotropic matrix:

$$C_{11} = \lambda + 2\mu; \quad C_{12} = \lambda; \quad S_{11} = \frac{7 - 5\nu}{15(1 - \nu)}; \quad S_{12} = \frac{5\nu - 1}{15(1 - \nu)} \quad [53] \quad (2.68)$$

where λ and μ are the Lamé constants. $\varepsilon_{ij}^{0,\eta}$ is thus reduced to:

$$\varepsilon_{ij}^{0,\eta} = -\frac{2\gamma}{R_{cav}} \frac{3(1 - \nu)}{4\mu(1 + \nu)} \delta_{ij} \quad (2.69)$$

The 3D simulation box used for the stress field validation is represented in Fig. 2.9. The

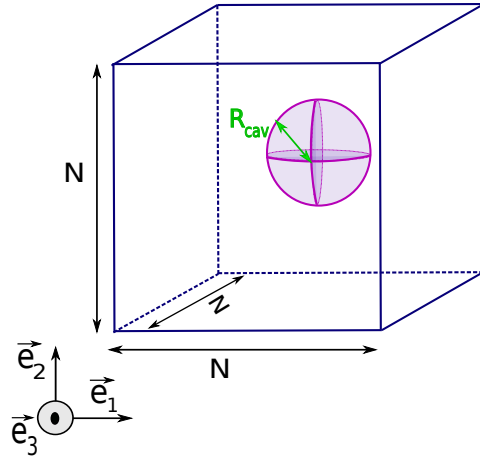


Figure 2.9: 3D simulation domain of size N^3 containing a spherical cavity.

simulation box size is N^3 cells and the cavity density corresponds to $\rho = 1/N^3$. The cavity surface is modelled as a diffuse interface and the order parameter η_s is written in the same way as in the case of dislocations:

$$\eta_s(x_1, x_2, x_3) = \frac{1}{2} \left(1 - \tanh \left[\frac{2(r - R_{cav})}{w} \right] \right) \quad (2.70)$$

with $r^2 = x_1^2 + x_2^2 + x_3^2$ and $w = 4a_0$. An example of η_s profile is shown in Fig. 2.10. The capture region corresponds to a sphere of radius r_c and is also chosen such as the extrema

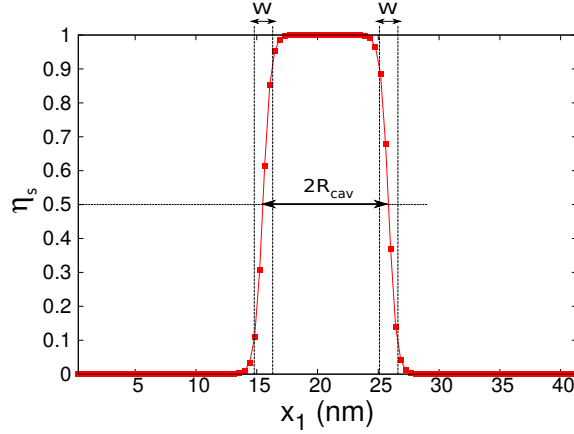


Figure 2.10: Example of η_s profile, passing through the center of the cavity along $\mathbf{e}_1$ in the case of a spherical cavity of radius R_{cav} .

values of the stress field are within this zone, $r_0 = R_{cav} + w$. The stress field is calculated in a box of size 41.344^3 nm^3 . The parameters of table 2.2 are used. The cavity radius is set at $R_{cav} = 1.2 \text{ nm}$ ($4a_0$) and γ to the typical value of 1 J.m^{-2} [39, 34]. The cavity is located in the center of the box. The analytical solution of the stress field is obtained by solving the mechanical equilibrium equation for a spherical shell with interior radius R_{cav} and exterior radius R_∞ subjected to an interior pressure $p^i = \frac{2\gamma}{R_{cav}}$ and an exterior pressure $p^e = 0$, and is given by:

$$\sigma_{ij}(x_1, x_2, x_3) = -\frac{2\gamma}{R_{cav}} \frac{R_{cav}^3}{R_\infty^3 - R_{cav}^3} \left[\left(\frac{R_\infty^3}{2r^3} + 1 \right) \delta_{ij} - \frac{3R_\infty^3 x_i x_j}{2r^5} \right] \quad (2.71)$$

with R_∞ the radius of the sphere which is equivalent to the simulation domain ($4\pi R_\infty^3/3 = (Na_0)^3$). The stress field profiles are plotted in Fig. 2.11 for the PF and analytical solutions. The fit is good for each stress component represented out of the capture region. In Fig. 2.12 the sink strength is plotted using the parameters of table 2.2. The sink strengths obtained for both PDs with elastic interactions are practically the same and correspond to the sink strengths without elastic interactions as expected. The Wiedersich and Laplace solutions (see Tab. 2.1) are also plotted, and it is seen that our results (PF) are in good agreement with the Wiedersich solution.

2.3.2 Physical parameters for applications

After the sink description and the corresponding stress field validation, the input parameters for applications to real materials are defined as follows. All the simulations were performed at temperature $T = 300 \text{ K}$ and with the dimensionless PD generation rate $K_0^* = 3 \times 10^{-8}$. The PD atomic fraction inside the sink X_d^s was taken close to zero. The elastic and Eshelby constants, the PD relaxation volume and the PD elastic dipole tensor are given in table 2.3. The elastic dipole tensors of PD in Ni and Fe were computed by DFT simulations [55] using the VASP code [56, 57]. The calculations were performed in a periodic simulation box with 256 ± 1 and 250 ± 1 atoms for Ni and Fe respectively. The projector augmented wave method (PAW) was used and the exchange-correlation functional

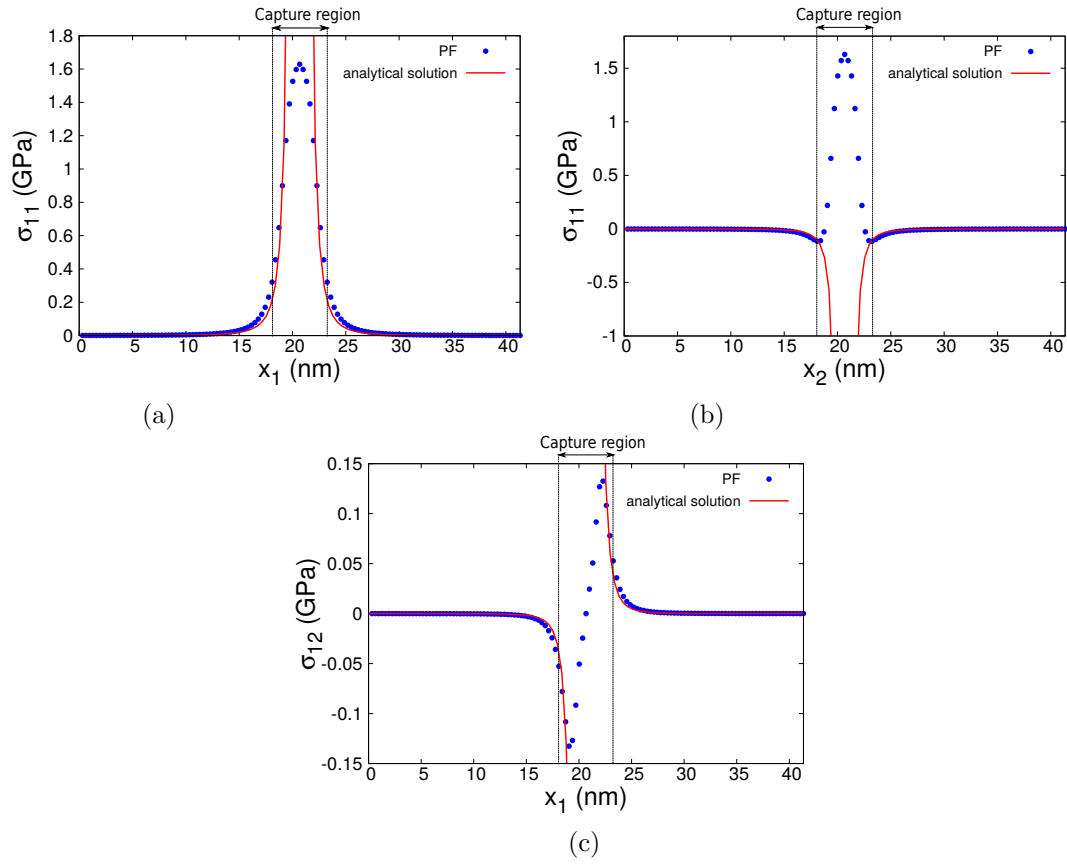


Figure 2.11: Profiles of the stress field components for a spherical cavity a) σ_{11} along $\mathbf{e}_1$ at $x_2 = 20.67$ nm, b) σ_{11} along $\mathbf{e}_2$ at $x_1 = 20.67$ nm, and c) σ_{12} along $\mathbf{e}_1$ at $x_2 = 20.67$ nm.

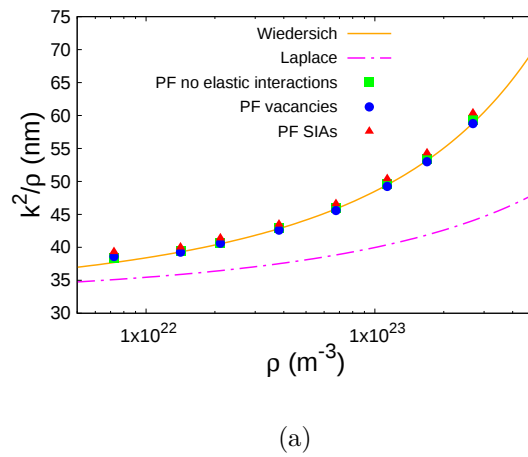


Figure 2.12: Sink strength as a function of the cavity density.

was evaluated with the Perdew-Burke-Ernzerhof (PBE). The plane wave energy cutoff was set to 350 eV for Ni and 300 eV for Fe, and the k-point grid mesh to $3 \times 3 \times 3$ grid. The migration of [100] and [110]-dumbbell respectively in (Al, Ni) and Fe is a mechanism of translation-rotation from [100] to [010] and from [110] to [011] respectively in (Al, Ni) and in Fe as described in Figs. 1.1 and 1.2. The elastic dipole tensors of each migration direction are deduced from each other by space rotations. The PF basis $R_{PF}(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ generally does not correspond to the crystallographic basis $R_0([100], [010], [001])$. Thus, all the tensors can be rewritten in the PF basis using the following relations:

$$\begin{aligned} e_i(R_{PF}) &= M_{ij}e_j(R_0) \\ P_{ij}(R_{PF}) &= M_{ik}M_{jl}P_{kl}(R_0) \\ C_{ijkl}(R_{PF}) &= M_{ig}M_{jh}C_{ghmn}(R_0)M_{km}M_{ln} \end{aligned} \tag{2.72}$$

where M_{ij} is the transformation matrix from R_0 to R_{PF} . Different cases of simulations are chosen to investigate the elastodiffusion effects:

- Case 1: no elastodiffusion ($P_{ij}^{sad} = P_{ij}^e$).
- Case 2: isotropic PD at saddle point ($P_{ij}^{sad} \equiv \frac{1}{3}Tr(P_{ij}^{sad})\delta_{ij}$).
- Case 3: full elastodiffusion (real P_{ij}^{sad} -tensors).

The comparison of the results obtained in cases 2 and 3 allows assessing the importance of the PD anisotropy at saddle point.

2.3.3 Results

The PD diffusion equation 2.51 is solved to calculate the sink strength. The sink strength is first calculated in the case of a straight dislocation and a spherical cavity for validation with the parameters of table 2.2. Secondly, the sink strength is calculated in the materials Al, Ni and Fe. Discussing the sink strength calculations in these materials, the PD flux and atomic fraction maps are represented to better understand the elastodiffusion effects.

2.3.3.1 Straight dislocation

A dipole of edge dislocations is considered as illustrated in Fig. 2.13. The glide system $\{111\}\langle\bar{1}10\rangle$ and $\{110\}\langle\bar{1}11\rangle$ in fcc (Al, Ni) and bcc (Fe) respectively are considered. Each dislocation is characterised by:

- its line vector: $\mathbf{l} = \frac{1}{\sqrt{6}}[\bar{1}\bar{1}\bar{2}]$ (fcc), $\frac{1}{\sqrt{6}}[\bar{1}\bar{1}\bar{2}]$ (bcc)
- its normal vector to the glide plane: $\mathbf{n} = \frac{1}{\sqrt{3}}[11\bar{1}]$ (fcc), $\frac{1}{\sqrt{2}}[110]$ (bcc)
- its Burgers vector: $\mathbf{b} = \pm\frac{a}{2}[\bar{1}10]$ (fcc), $\pm\frac{a}{2}[\bar{1}11]$ (bcc), a is the lattice parameter.

Table 2.3: Physical parameters for the simulations. The elastic dipole tensors are given in the basis $\mathbf{R}_0([100],[010],[001])$. $\mathbf{h}$ is the migration direction of PD.

	Al	Ni	Fe
Elastic constants C_{11} , C_{12} , C_{44} (GPa)	106.51, 60.38, 27.8 [34]	250.8, 150, 123.5 [58]	243, 145, 116 [59, 60]
Eshelby constants S_{11} , S_{12} , S_{44}	0.5212, 0.0833, 0.2393	0.4481, 0.0852, 0.2759	0.4515, 0.0852, 0.2742
Anisotropy ratio $A = 2C_{44}/(C_{11}-C_{12})$	1.21	2.45	2.37
Elastic dipole tensor Stable point $\mathbf{P}_{ij}^e$ (eV)	$\begin{bmatrix} -3.238 & 0 & 0 \\ 0 & -3.238 & 0 \\ 0 & 0 & -3.238 \end{bmatrix}$	$\begin{bmatrix} -5.448 & 0 & 0 \\ 0 & -5.448 & 0 \\ 0 & 0 & -5.448 \end{bmatrix}$	$\begin{bmatrix} -3.6368 & 0 & 0 \\ 0 & -3.6368 & 0 \\ 0 & 0 & -3.6368 \end{bmatrix}$
Vacancy	$\begin{bmatrix} -3.238 & 0 & 0 \\ 0 & -3.238 & 0 \\ 0 & 0 & -3.238 \end{bmatrix}$	$\begin{bmatrix} -5.448 & 0 & 0 \\ 0 & -5.448 & 0 \\ 0 & 0 & -5.448 \end{bmatrix}$	$\begin{bmatrix} -3.6368 & 0 & 0 \\ 0 & -3.6368 & 0 \\ 0 & 0 & -3.6368 \end{bmatrix}$
Dumbbell [100] for Al and Ni, [110] for Fe	$\begin{bmatrix} 19.652 & 0 & 0 \\ 0 & 18.518 & 0 \\ 0 & 0 & 18.518 \end{bmatrix}$	$\begin{bmatrix} 25 & 0 & 0 \\ 0 & 24.792 & 0 \\ 0 & 0 & 24.792 \end{bmatrix}$	$\begin{bmatrix} 20.6162 & -5.6702 & 0 \\ -5.6702 & 20.6162 & 0 \\ 0 & 0 & 24.8208 \end{bmatrix}$
Saddle point $\mathbf{P}_{ij}^{sad}$ (eV)			
Vacancy $\mathbf{h}[110]$ for Al, Ni and [111] for Fe	$\begin{bmatrix} -2.866 & -0.080 & 0 \\ -0.080 & -2.866 & 0 \\ 0 & 0 & 1.000 \end{bmatrix}$	$\begin{bmatrix} -5.255 & -0.213 & 0 \\ -0.213 & -5.255 & 0 \\ 0 & 0 & 2.554 \end{bmatrix}$	$\begin{bmatrix} -3.2379 & -1.6342 & -1.6342 \\ -1.6342 & -3.2379 & -1.6342 \\ -1.6342 & -1.6342 & -3.2379 \end{bmatrix}$
Dumbbell [100] to [010], $\mathbf{h}[110]$ for Al and Ni;	$\begin{bmatrix} 19.498 & 1.133 & 0 \\ 1.133 & 19.498 & 0 \\ 0 & 0 & 19.034 \end{bmatrix}$	$\begin{bmatrix} 25.438 & 1.492 & 0 \\ 1.492 & 25.678 & 0 \\ 0 & 0 & 25.411 \end{bmatrix}$	$\begin{bmatrix} 22.5000 & 2.8725 & -0.6864 \\ 2.8725 & 21.0942 & 2.8725 \\ -0.6864 & 2.8725 & 22.5000 \end{bmatrix}$
[110] to [011], $\mathbf{h}[111]$ for Fe			
Relative variation of the relaxation volume ($\Omega^{sad} - \Omega^e$)/ Ω^e for SIA; vacancy	0.0236; -0.5128	0.026; -0.5132	0.0006; -0.1096

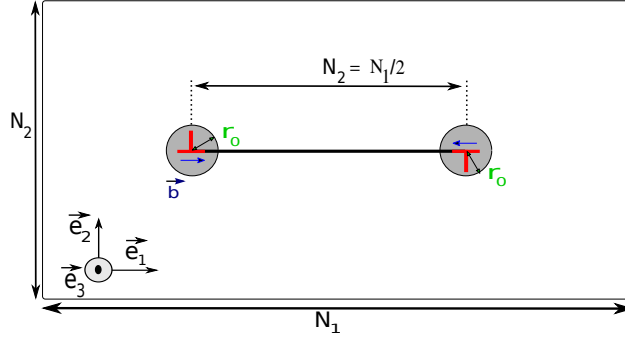


Figure 2.13: 2D simulation box containing a dipole of edge dislocations.

The PF basis R_{PF} corresponds to:

$$\left\{ \begin{array}{l} \mathbf{e}_1 = \frac{1}{\sqrt{2}}[\bar{1}10] \\ \mathbf{e}_2 = \frac{1}{\sqrt{3}}[11\bar{1}] \\ \mathbf{e}_3 = \frac{1}{\sqrt{6}}[\bar{1}\bar{1}\bar{2}] \end{array} \right. \quad (\text{fcc}), \quad \left\{ \begin{array}{l} \mathbf{e}_1 = \frac{1}{\sqrt{3}}[\bar{1}11] \\ \mathbf{e}_2 = \frac{1}{\sqrt{2}}[110] \\ \mathbf{e}_3 = \frac{1}{\sqrt{6}}[\bar{1}1\bar{2}] \end{array} \right. \quad (\text{bcc}) \quad (2.73)$$

The radius of the capture region is set to $r_0 = 4a_0$ (see section 2.3.1).

The PD fluxes are plotted in Fig. 2.14 for each material Al, Ni and Fe without (case 1) and with full elastodiffusion (case 3). Globally, for both cases, SIAs migrate preferentially towards the tension region of dislocations. On the contrary, vacancies are more attracted to the compression region as expected. When the elastodiffusion is taken into account, the flow of SIAs changes hardly for all the materials. The trajectory of vacancies in Al, Ni and Fe is more affected by the elastodiffusion especially in the compression region. The flow intensity of vacancies decreases and its orientation changes near the compression region as shown in Fig. 2.14-b), Fig. 2.14-d) and Fig. 2.14-f).

The atomic fraction maps of PDs are represented in figures 2.15 for Al, 2.16 for Ni and 2.17 for Fe. As shown by the PD flux maps, SIAs are more depleted in the compression zone of dislocations while vacancies are more depleted in the tension zone. The size of the PD depletion region increases and its shape changes with full elastodiffusion. This leads to a decrease of the average atomic fraction. The elastodiffusion effects are more pronounced for vacancies than SIAs in the case of Al and Ni (see Fig. 2.15 and Fig. 2.16). In the case of Fe, the atomic fraction maps of SIAs and vacancies are strongly affected by the elastodiffusion as shown in Fig. 2.17. The sink strength representation allows to quantify the elastodiffusion effects.

In figures 2.18, 2.19 and 2.20 the sink strengths and the corresponding biases are plotted in the studied materials. The sink strength is higher with full elastodiffusion (case 3) compared to the case without elastodiffusion (case 1) in each material and for each PD. This difference is amplified with the density of dislocations. The elastodiffusion effects are more significant for vacancies in all the materials. The intermediate case 2 which corresponds to isotropic PD at saddle point is examined to study the effects of PD anisotropy at saddle point. In case 2, the effects of elastodiffusion is due only to the change in the PD relaxation volume between stable and saddle points. The sink strengths obtained in cases 1 and 2 are very close for SIAs in all the materials. In the case of

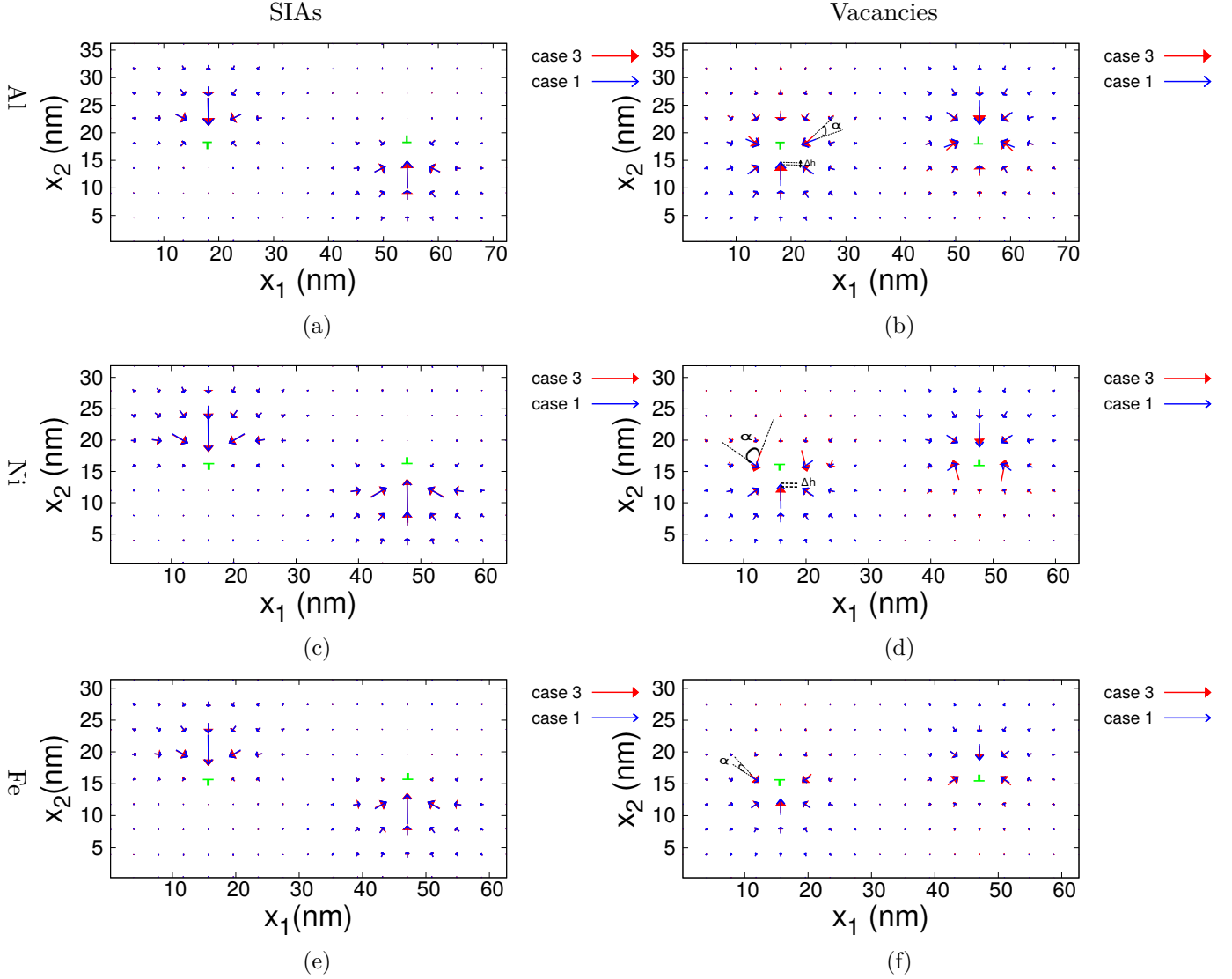


Figure 2.14: Fluxes of a) SIAs and b) vacancies in Al, c) SIAs and d) vacancies in Ni, e) SIAs and f) vacancies in Fe, without elastodiffusion (case 1) and with full elastodiffusion (case 3) for a dipole of edge dislocations. The length of the vector is proportional to the norm of the flux $\|\mathbf{J}\| = \sqrt{J_1^2 + J_2^2}$.

vacancies, it is observed a decrease of the sink strength between cases 1 and 2 as shown in Figs. 2.18-b), 2.19-b) and 2.20-b) in all the materials and this decrease is more marked in Ni. The relative difference of the relaxation volume $(\Omega^s - \Omega^e)/\Omega^e$ for SIAs in all the materials and for vacancies in Fe is less or equal to 10% (see table 2.3). Thus the elastic interactions between PDs and dislocation at stable and saddle state configurations are practically the same in case 2 which explains the small change of the sink strength between cases 1 and 2. However, the relaxation volume of vacancies in Al and Ni at saddle state is significantly lower than at stable point. This leads to a strong decrease of the elastic

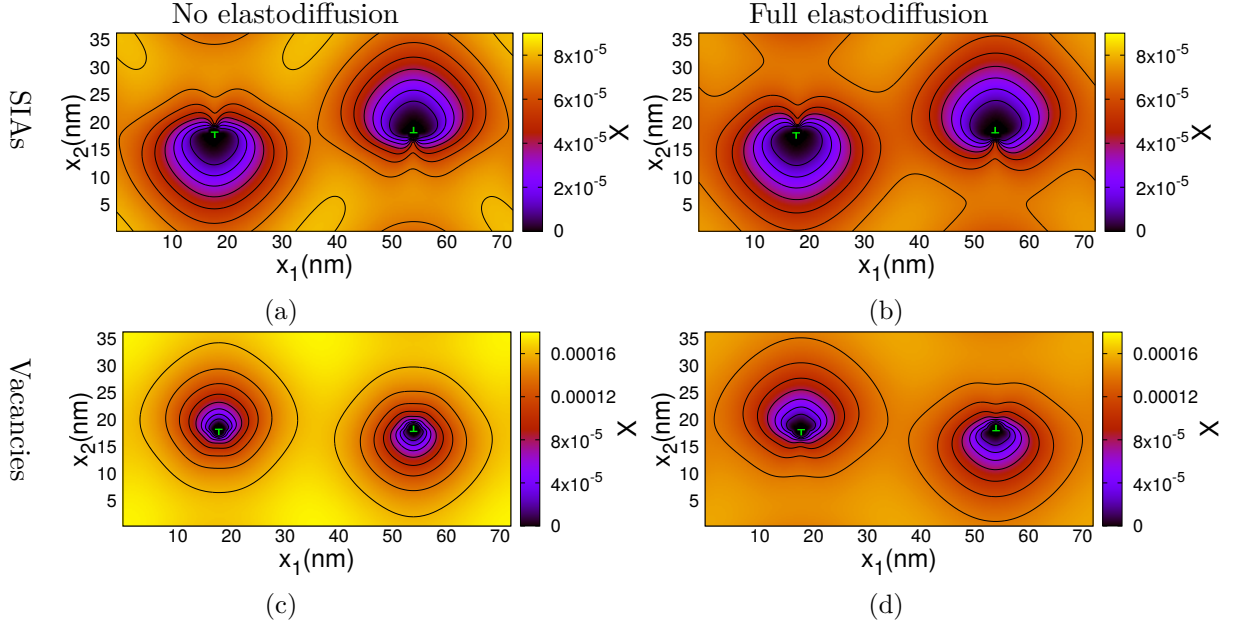


Figure 2.15: Atomic fraction maps of SIAs and vacancies respectively without elastodiffusion (case 1) a) and c), and with full elastodiffusion (case 3) b) and d) in Al for a dipole of edge dislocations.

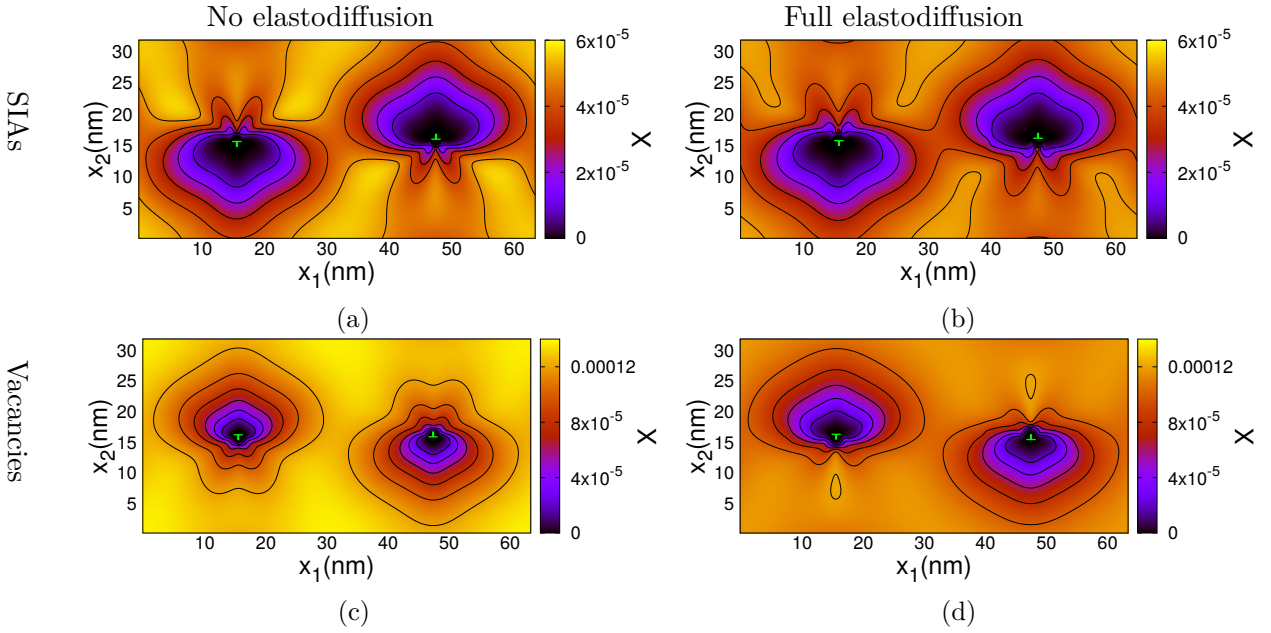


Figure 2.16: Atomic fraction maps of SIAs and vacancies respectively without elastodiffusion (case 1) a) and c), and with full elastodiffusion (case 3) b) and d) in Ni for a dipole of edge dislocations.

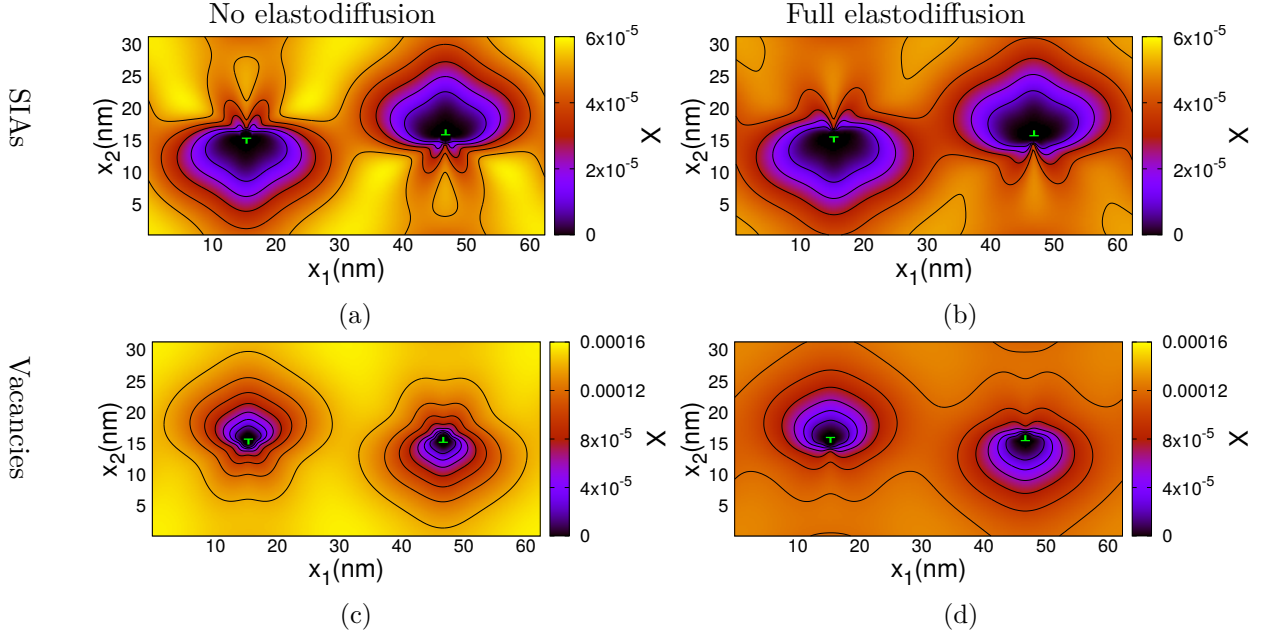


Figure 2.17: Atomic fraction maps of SIA and vacancies respectively without elastodiffusion (case 1) a) and c), and with full elastodiffusion (case 3) b) and d) in Fe for a dipole of edge dislocations.

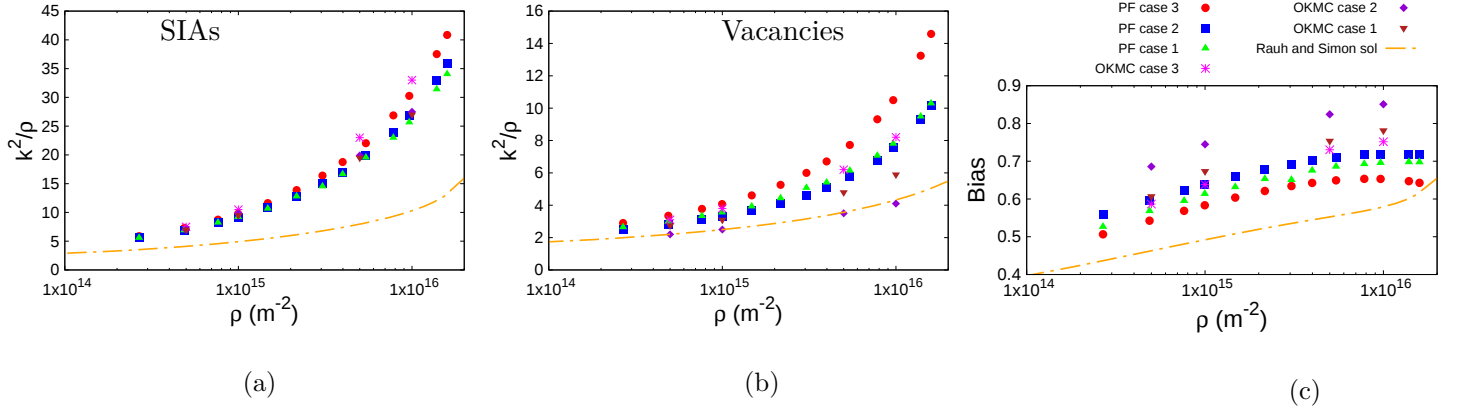


Figure 2.18: Sink strength as a function of the dislocation density for a) SIA and b) vacancies, and c) bias in Al. Case 1: no elastodiffusion, case 2: elastodiffusion with isotropic PD at saddle point, case 3: full elastodiffusion.

interactions and thus to a decrease of the sink strength in case 2 in comparison to case 1. The comparison between cases 1, 2 and 3 shows an increase of the sink strength with the PD anisotropy at saddle point. This increase is strongly significant with the dislocation density for vacancies in Al and Ni, and for both PDs in Fe. Therefore the bias decreases with the PD anisotropy at saddle point in Al and Ni as illustrated in Figs. 2.18-c) and 2.19-c). Fig.2.20-c) shows a decrease of the sink bias in Fe with full elastodiffusion due to a stronger effects for vacancies than for SIA. The solution of the sink strength proposed

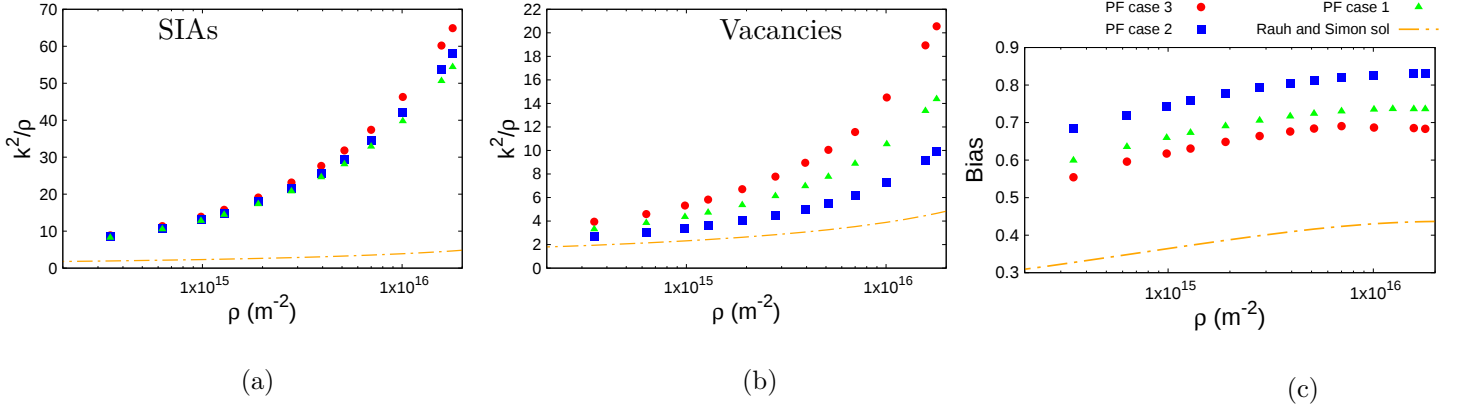


Figure 2.19: Sink strength as a function of the dislocation density for a) SIAs and b) vacancies, and c) bias in Ni. Case 1: no elastodiffusion, case 2: elastodiffusion with isotropic PD at saddle point, case 3: full elastodiffusion.

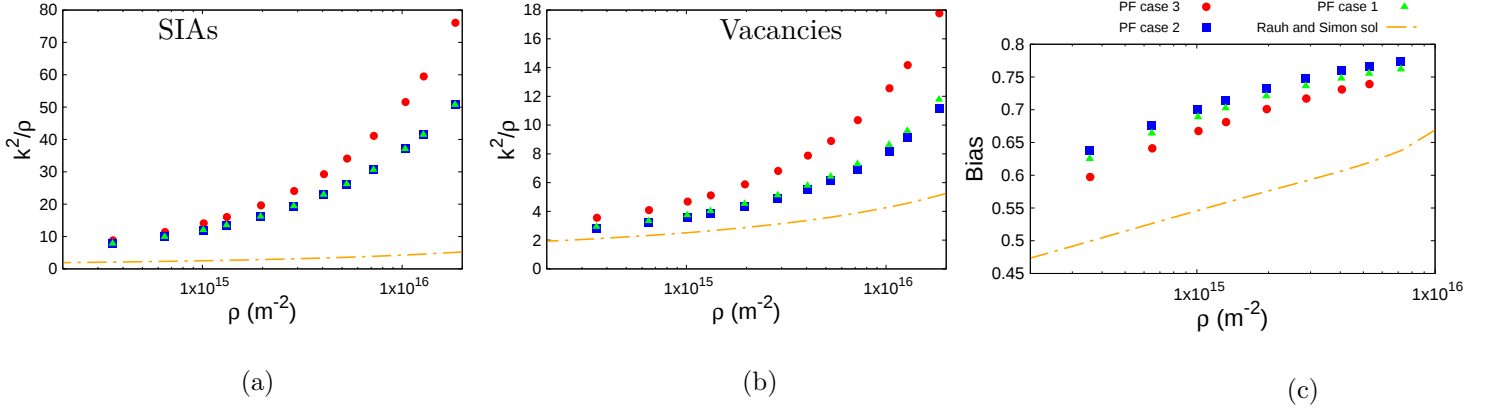


Figure 2.20: Sink strength as a function of the dislocation density for a) SIAs and b) vacancies, and c) bias in Fe. Case 1: no elastodiffusion, case 2: elastodiffusion with isotropic PD at saddle point, case 3: full elastodiffusion.

by Rauh and Simon [32] is represented in figures 2.18, 2.19 and 2.20 for each material. The results are comparable at low dislocation densities, but considerable differences are observed for high densities. These differences are due to several reasons mentioned by Rouchette [4]:

- The Rauh solution is only valid for isotropic systems and PDs.
- To obtain the Rauh solution, the choice of the boundary conditions are similar to the Laplace's model. The PD atomic fraction $\bar{X}_d(t \rightarrow \infty)$ used to compute the sink strength Eq. 2.4 corresponds to the atomic fraction at the boundaries of the reservoir $X(R)$ instead of $\bar{X}$ as in the PF model.
- The Rauh model ignores the elastic interactions between the dislocations, which limits its validation to low dislocations densities.

Thus, the Rauh and Simon solution allows to have a qualitative description of the sink

strength and bias evolution with dislocation density. The results obtained by Carpentier [34] for sink strength and bias in Al using OKMC simulations are represented in figure 2.18. The results are in good agreement for low dislocation densities but differences between OKMC and PF are observed at high densities. This discrepancy can be explained by the fact that the radius r_0 of the PD capture region used in the OKMC simulations is equal to $2b$ while in the present study it is $4b$. In our PF model, $r_0 = w$ where w is the width of dislocation core which is modelled as a diffuse interface, and it is difficult to simulate an interface with less than 3 or 4 cells.

Discussion

The results obtained above show that elastodiffusion has effects on the PD flow toward the sink, on the size and shape of the PD depletion region, and on the sink absorption and bias. The magnitude of these effects depends strongly on the PD anisotropy at saddle point. Especially the sink strength increases by taking into account the PD anisotropy at saddle point (case 3) compared to the other cases of simulations (cases 1 and 2). In all the materials, vacancies are more affected by the full elastodiffusion and a decrease of the sink bias is obtained but this decrease remains small. The saddle point anisotropy effects on the sink strength have been investigated by Skinner and Woo [47] in fcc Cu and bcc Fe at 500 K. They concluded that, the sink strength increases by a small amount for each PD and in each material. It should be noted that in the study of Skinner, a $\langle 100 \rangle$ -dumbbell is considered as SIAs in Cu and Fe while a $\langle 110 \rangle$ -dumbbell is considered in Fe for this study. The results obtained for Cu are very similar to those obtained in this study for Al and Ni. A generalization of the results could be made for materials with PDs having the same anisotropy properties at stable and saddle points. Chen [61] has shown that the PD anisotropy at saddle point effects on sink strength can be treated by defining an "effective relaxation volume". This effective relaxation volume allows to describe the PD dipole tensor anisotropy at saddle state and its choice is therefore crucial. As shown by the results obtained when the PD at saddle point is isotropic, the sink strength decreases (see Figs. 2.18 and 2.19). On the other hand the sink strength increases when the PD anisotropy at saddle state is considered.

The normalized diffusion coefficients D_{ij}/D^0 are plotted in figures 2.21, 2.22 and 2.23 to better investigate the full elastodiffusion effects on PD diffusion. As shown by equation 2.16, the diffusion coefficients result from a coupling between the P_{ij} -tensor and the strain field due to the sink. The profiles of Figs. 2.21 and 2.22 show stronger variations of the ratios D_{ij}/D^0 for vacancies than SIAs in Al and Ni, especially in Ni. These higher variations of the ratios D_{ij}/D^0 for vacancies than SIAs allow to explain the decrease of the sink bias in Al and Ni with full elastodiffusion compared to the case without. In Fe, the magnitudes of the ratios D_{11}/D^0 and D_{12}/D^0 for both PDs are very close. Significant differences are observed for the ratio D_{22}/D^0 , higher for SIAs than vacancies in some points (see Fig. 2.23-b)). But finally, a small decrease of the sink bias is observed with full elastodiffusion in Fe. The contribution of each jump direction to the diffusion coefficients (see Eq. 2.16) has been investigated. In table 2.4 the weight of each PD possible jump direction relative to the diffusion coefficients is reported. It can be seen that in Al, all the possible jump directions have almost the same contribution for both PDs (exponential expression in table 2.4). This may be due to the low anisotropy factor of Al. Contrariwise,

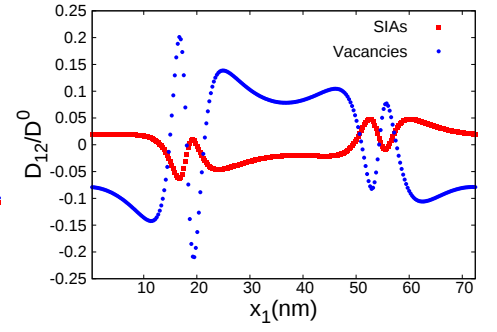
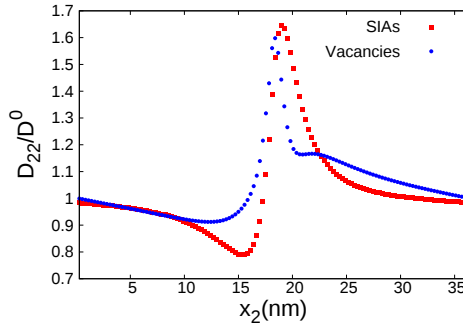
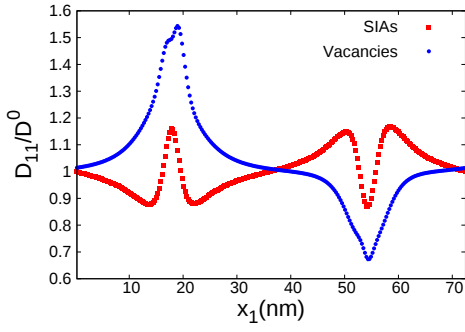
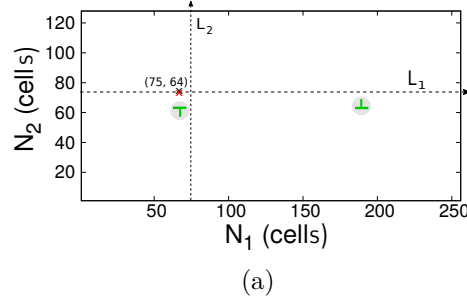


Figure 2.21: Profiles of the normalized diffusion coefficients b) D_{11}/D^0 along $\mathbf{L}_1$ ($x_2 = 21.22$ nm), c) D_{22}/D^0 along $\mathbf{L}_2$ ($x_1 = 21.22$ nm) and d) D_{12}/D^0 along $\mathbf{L}_1$ ($x_2 = 21.22$ nm) with full elastodiffusion (case 3) in Al for a dipole of edge dislocations.

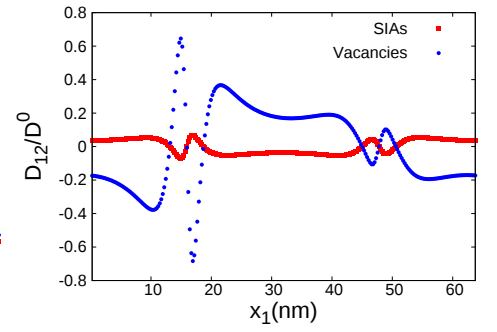
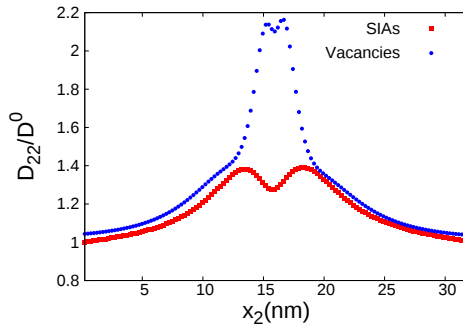
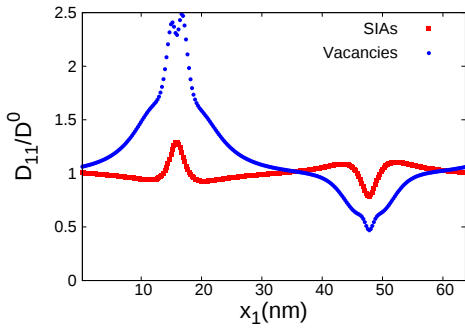


Figure 2.22: Profiles of the normalized diffusion coefficients a) D_{11}/D^0 along $\mathbf{L}_1$ ($x_2 = 18.67$ nm), b) D_{22}/D^0 along $\mathbf{L}_2$ ($x_1 = 18.67$ nm) and c) D_{12}/D^0 along $\mathbf{L}_1$ ($x_2 = 18.67$ nm) with full elastodiffusion (case 3) in Ni for a dipole of edge dislocations (see Fig. 2.21-a) for $\mathbf{L}_1$ and $\mathbf{L}_2$ axis).

in Ni and Fe where the anisotropy ratio is higher, some directions contribute much more than others, especially in Fe. Thus PD migrates preferentially in the directions where the contribution is more significant. We also calculated the sink strength for another possible glide system $\{001\}\langle 100 \rangle$ in all the metals [?]. In Fig. 2.24 the sink bias with

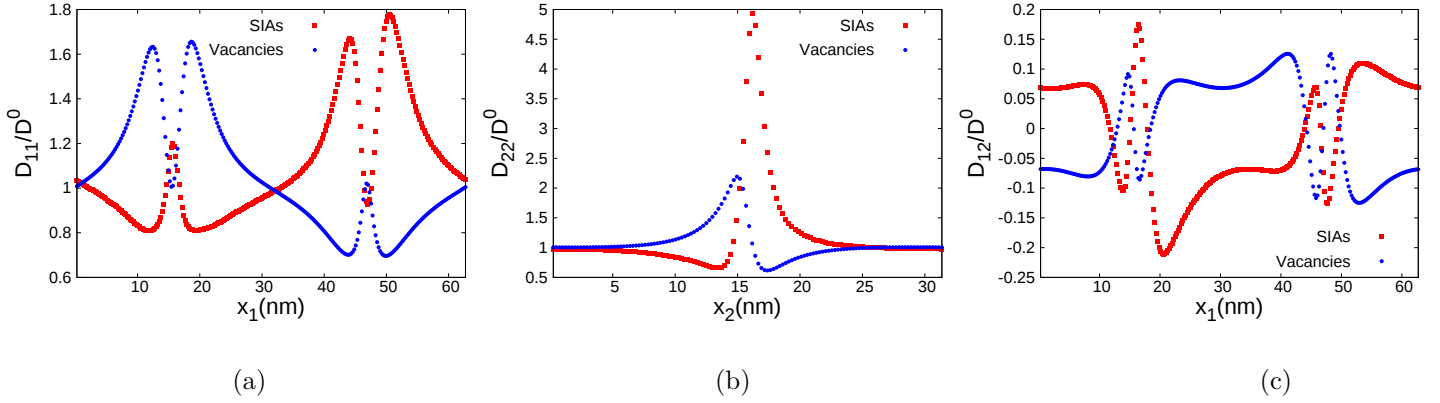


Figure 2.23: Profiles of the normalized diffusion coefficients D_{11}/D^0 along $\mathbf{e}_1$ ($x_2 = 18.67$ nm), D_{22}/D^0 along $\mathbf{e}_2$ ($x_1 = 18.67$ nm) and D_{12}/D^0 along $\mathbf{e}_1$ ($x_2 = 18.67$ nm) with full elastodiffusion (case 3) in Fe for a dipole of edge dislocations (see Fig. 2.21-a)) for $\mathbf{L}_1$ and $\mathbf{L}_2$ axis).

full elastodiffusion for the different glide systems in all the materials is plotted. The bias changes hardly in Al and Fe with the glide system while the variation is stronger in Ni. To better understand these results, the profile of the normalized diffusion coefficient

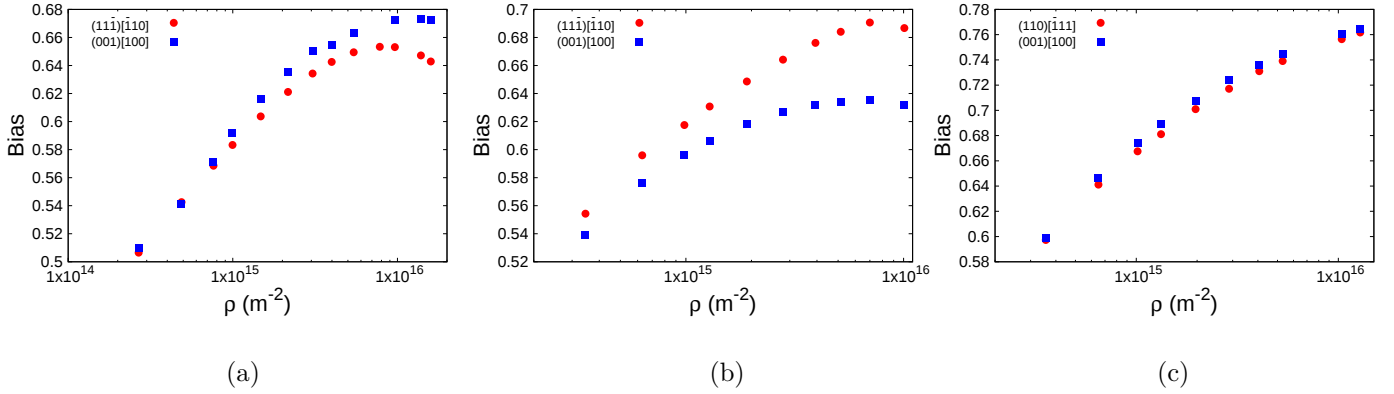


Figure 2.24: Sink bias as a function of the dislocation density for different orientations of the Burgers vector with full elastodiffusion in a) Al, b) Ni and c) Fe.

D_{11}/D^0 is plotted for each glide system in Fig. 2.25. In Al and Fe, the ratio D_{11}/D^0 varies slightly with the glide system for each PD which can explain the low bias variation in these materials. In Ni, the ratio D_{11}/D^0 is almost the same for each glide system in case of SIAs. But for vacancies the ratio D_{11}/D^0 increases highly for the glide system $\{001\}\langle 100 \rangle$ compared to the other one. This leads to the bias decrease in the glide system $\{001\}\langle 100 \rangle$ compared to the other one as shown in Fig. 2.24.

Table 2.4: Contribution of the possible jump directions $\mathbf{h}$ to the diffusion coefficients (Eq. 2.16) for a dipole of edge dislocations. $(x_{p1}, x_{p2}) = (75, 64)a_0$ (see Fig. 2.21-a)) with a_0 the size of the corresponding unit PF cell.

$\mathbf{h}$	$\beta \sum_{kl} (P_{kl}^{sad} - \bar{P}_{kl}^e) \varepsilon_{kl}(x_{p1}, x_{p2})$	$\exp(\beta \sum_{kl} (P_{kl}^{sad} - \bar{P}_{kl}^e) \varepsilon_{kl}(x_{p1}, x_{p2}))$
Al; Ni		
Vacancies		
[110] $[\bar{1}\bar{1}0]$	$-1.0269 \times 10^{-3}; 2.664 \times 10^{-2}$	0.9989; 1.0270
[1 $\bar{1}0$] $[\bar{1}10]$	$-6.6339 \times 10^{-4}; -1.3127 \times 10^{-3}$	0.9993; 0.9986
[011] $[0\bar{1}\bar{1}]$ $[01\bar{1}]$ $[0\bar{1}\bar{1}]$		
[101] $[\bar{1}01]$ $[10\bar{1}]$ $[\bar{1}0\bar{1}]$	$-5.2367 \times 10^{-3}; 0.26894$	0.9947; 1.30857
Dumbbell [100]		
[110] $[\bar{1}\bar{1}0]$	$1.2062 \times 10^{-3}; -5.2201 \times 10^{-2}$	1.00120; 0.9491
[1 $\bar{1}0$] $[\bar{1}10]$	$-3.9413 \times 10^{-3}; 0.1436$	0.9960; 1.1544
[101] $[\bar{1}0\bar{1}]$	$-8.4050 \times 10^{-4}; 3.6963 \times 10^{-2}$	0.9991; 1.0376
[$\bar{1}01$] $[10\bar{1}]$	$-8.4050 \times 10^{-4}; 4.4840 \times 10^{-2}$	0.9991; 1.0458
Fe		
Vacancies		
[111] $[\bar{1}\bar{1}\bar{1}]$ $[\bar{1}\bar{1}1]$ $[\bar{1}\bar{1}\bar{1}]$	-0.1904	0.8266
[$\bar{1}\bar{1}\bar{1}$] $[\bar{1}\bar{1}1]$ $[1\bar{1}\bar{1}]$ $[\bar{1}\bar{1}\bar{1}]$	0.3134	1.3681
Dumbbell [110]		
[111] $[\bar{1}\bar{1}\bar{1}]$ $[\bar{1}\bar{1}1]$ $[\bar{1}\bar{1}\bar{1}]$	0.4088	1.5050
[$\bar{1}\bar{1}\bar{1}$] $[\bar{1}\bar{1}1]$ $[1\bar{1}\bar{1}]$ $[\bar{1}\bar{1}\bar{1}]$	-0.4768	0.6207

In summary of this section, the sink strength of straight dislocations increases when full elastodiffusion is taken into account compared to the case where it is not in all the studied materials. The PD trajectory and depletion region are also modified. In all the materials, full elastodiffusion effects on sink strength are more significant for vacancies which leads to the decrease of the sink bias compared to the case without elastodiffusion. The plots of the diffusion coefficients with and without elastodiffusion allowed to explain these results. It has also been shown that the elastodiffusion effects depend on the glide system. In particular, the bias changes slightly with full elastodiffusion when the glide system changes from $\{111\}\langle\bar{1}10\rangle$ to $\{001\}\langle100\rangle$ in Al and from $\{110\}\langle\bar{1}11\rangle$ to $\{001\}\langle100\rangle$ in Fe. In Ni, the bias changes with the glide system is more significant. The profiles of the diffusion coefficients have also allowed to explain these bias modifications with the glide system. The case of an array of straight dislocations is studied in the following section (section 2.3.3.2).

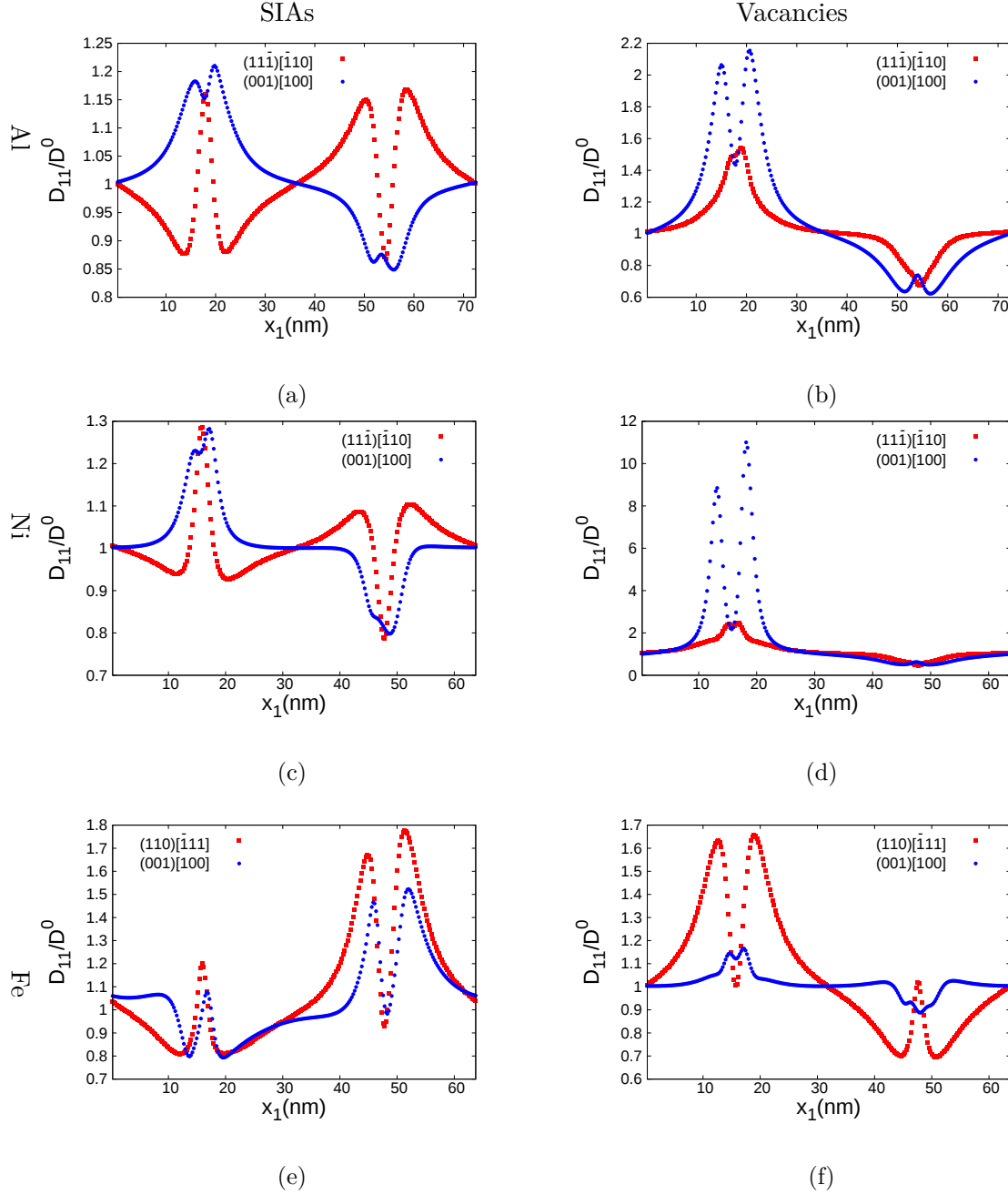


Figure 2.25: Profiles of the normalized diffusion coefficients D_{11}/D^0 along L_1 (see Fig. 2.21-a)) respectively for SIAs a) Al, c) Ni and e) Fe, and for vacancies b) Al, d) Ni and f) Fe with full elastodiffusion for different Burgers vector orientations.

2.3.3.2 Grain boundary

A STGB with low misorientation is considered as illustrated in Fig. 2.7. Each dislocation has the same characteristics listed in the case of straight dislocations (Burgers vector, line

vector and vector normal to the glide plane). The interspacing between dislocations h was set to $6b$ which corresponds to a misorientation of $\theta = 9.55^\circ (h \simeq b/\theta)$. The radius r_0 of the capture zone is still equal to $4b$ for each dislocation. The STGB in Al and Ni corresponds to the $(\bar{1}10)[\bar{1}\bar{1}2]$ GB and in Fe to the $(\bar{1}11)[\bar{1}\bar{1}2]$ GB.

The PD fluxes towards the GB are plotted in Fig. 2.26. As in the case of isolated

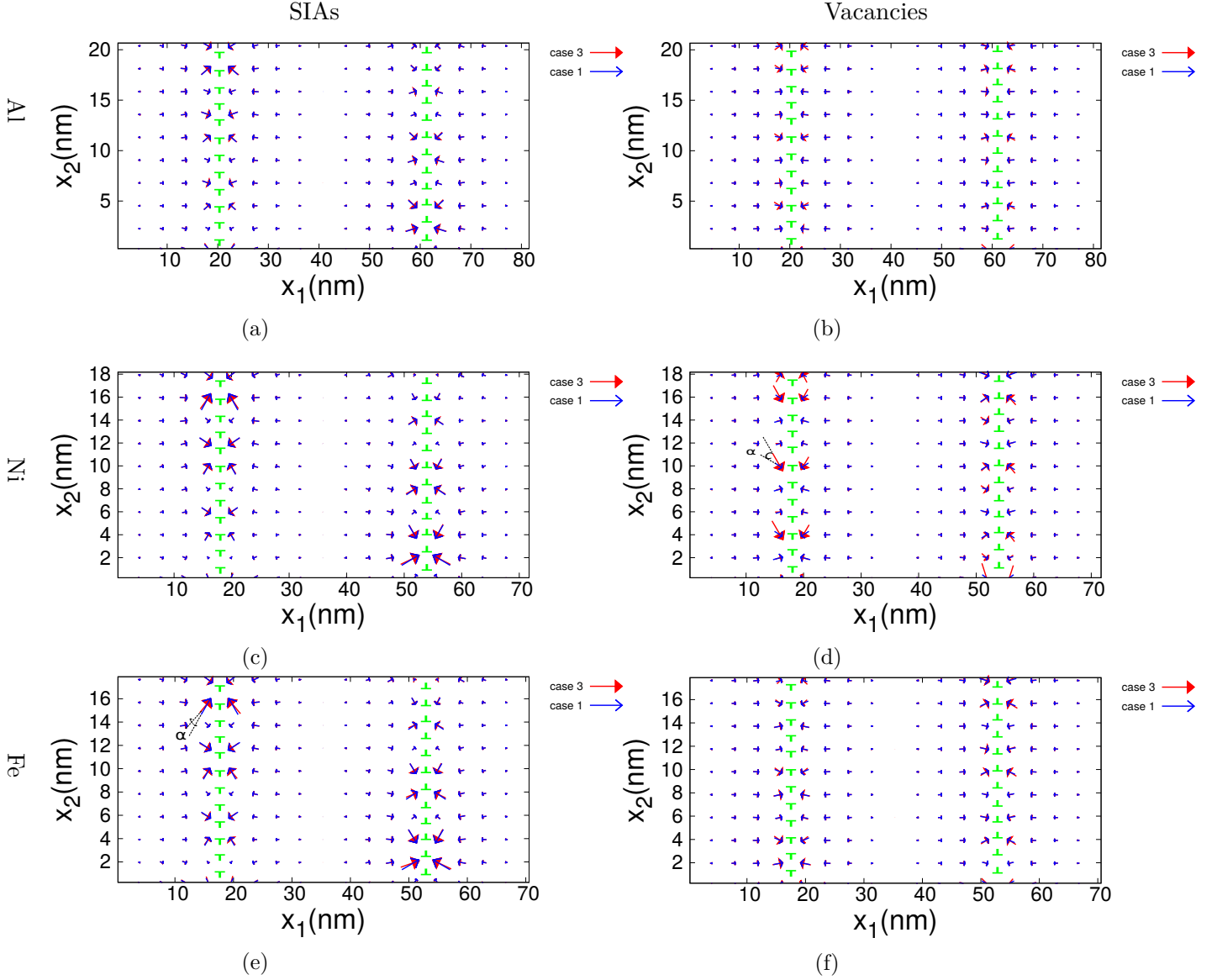


Figure 2.26: Fluxes of a) SIAs and b) vacancies in Al, c) SIAs and d) vacancies in Ni, e) SIAs and f) vacancies in Fe, without elastodiffusion (case 1) and with full elastodiffusion (case 3) for low angle STGB. The length of the vector is proportional to the norm of the flux $\|\mathbf{J}\| = \sqrt{J_1^2 + J_2^2}$.

straight dislocations ($\theta \rightarrow 0^\circ$), SIAs migrate preferentially in the tension region of each

dislocation for each case of simulation and material. Contrariwise, vacancies migrate preferentially to the compression zone. The SIA trajectory changes very little in Al and Ni when full elastodiffusion is taken into account (case 3) compared to the case without (case 1). The same result is obtained for vacancies in Fe. However, the vacancy trajectory is strongly affected near the low angle STGB with full elastodiffusion in Ni, which is also the case for SIAs in Fe.

In Figs. 2.27, 2.28 and 2.29 are represented the PD atomic fraction maps respectively in Al, Ni and Fe without (case 1) and with full elastodiffusion (case 3). There are no

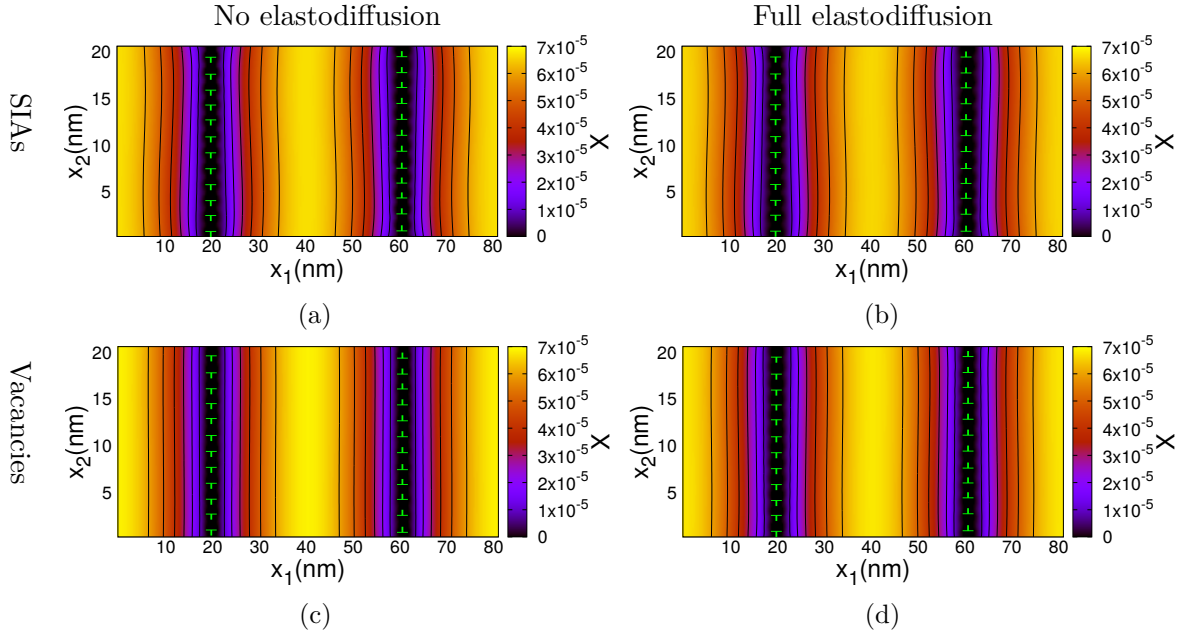


Figure 2.27: Atomic fraction maps of SIAs and vacancies respectively without elastodiffusion (case 1) a) and c), and with full elastodiffusion (case 3) b) and d) in Al for low angle STGB.

remarkable differences in the shape and size of the PD depletion regions between the two cases of simulations in Al for both PDs, in Ni for SIAs and in Fe for vacancies. A noticeable difference is observed for vacancies in Ni and for SIAs in Fe as predicted by the PD flow plots.

The sink strength for SIAs and vacancies, and the sink bias are given in Figs. 2.30, 2.31 and 2.32. The analytical solution of the sink strength of a continuous planar sink (no elastic interactions) given by $k^2 = 12/(d - e)^2$ [62] is also plotted. e is the width of the planar sink which corresponds to the width of the capture region $2r_0$ in our simulations, d is the interplanar spacing. The sink strengths for both PDs, in all the cases of simulations and in all the materials are very close to the analytical solution for large STGB inter-spacing ($d > 30$ nm). The bias for these STGB inter-spacings is less than 10 %. For low STGB inter-spacings ($d < 30$ nm), the elastic effects become significant which leads to a strongly biased STGB. Especially for $d \simeq 5$ nm, the sink strength for vacancies is approximately two times greater than the analytical solution for all the simulation cases, while the increase of the sink strength for SIAs is more significant than that of vacancies. The sink strength is

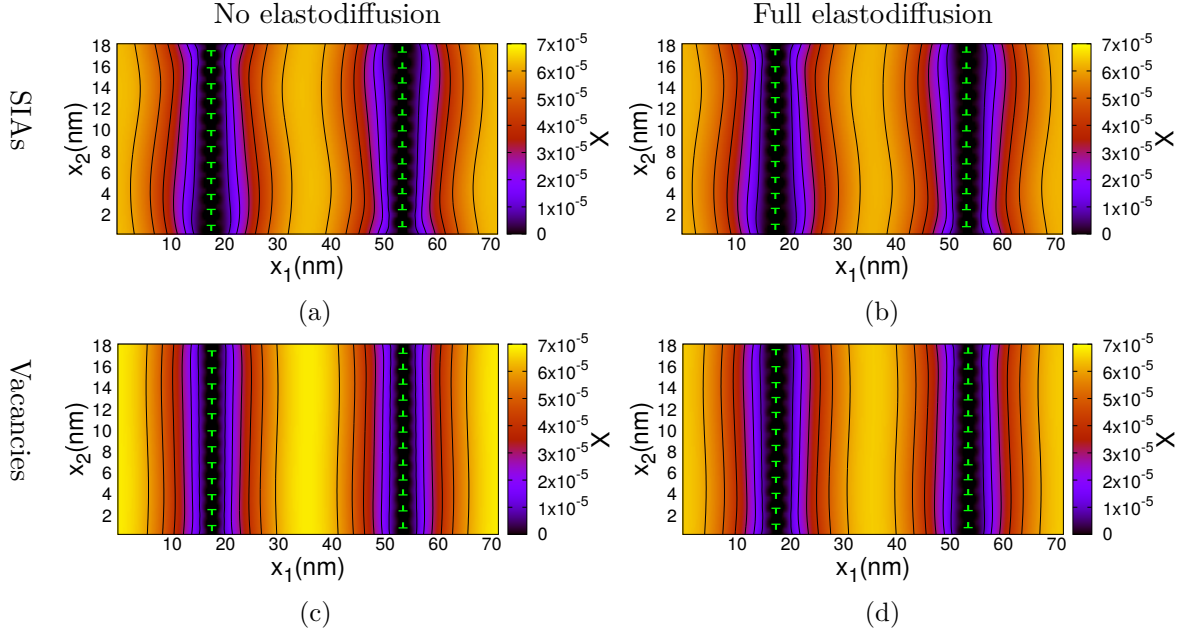


Figure 2.28: Atomic fraction maps of SIAs and vacancies respectively without elastodiffusion (case 1) a) and c), and with full elastodiffusion (case 3) b) and d) in Ni for low angle STGB.

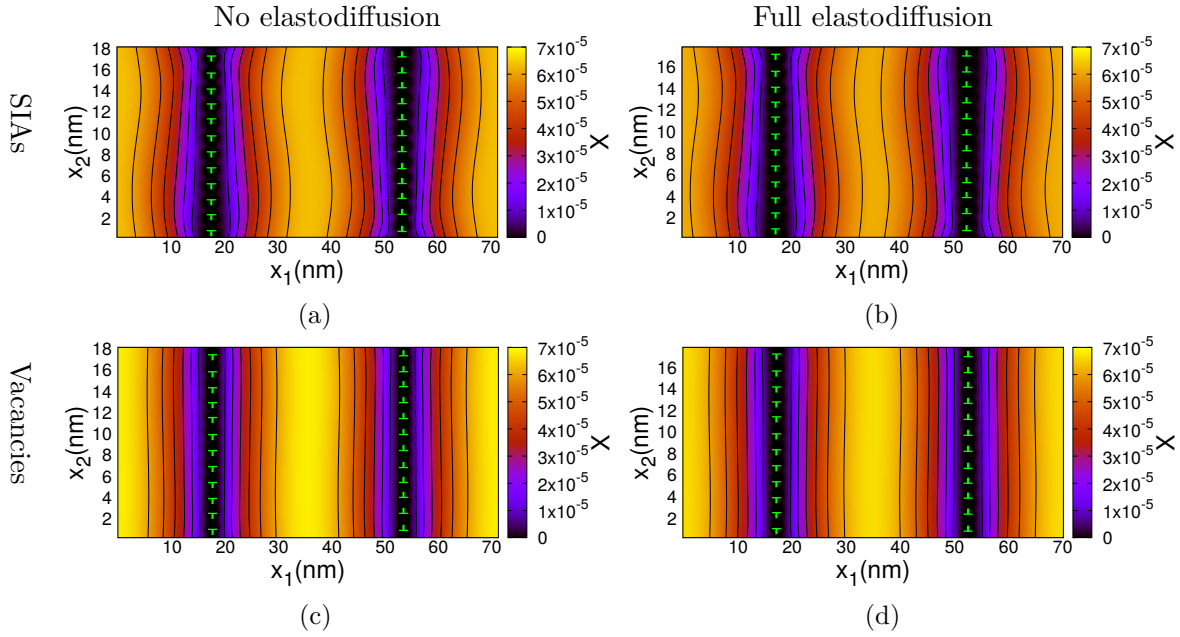


Figure 2.29: Atomic fraction maps of SIAs and vacancies respectively without elastodiffusion (case 1) a) and c), and with elastodiffusion (case 3) b) and d) in Fe for low angle STGB.

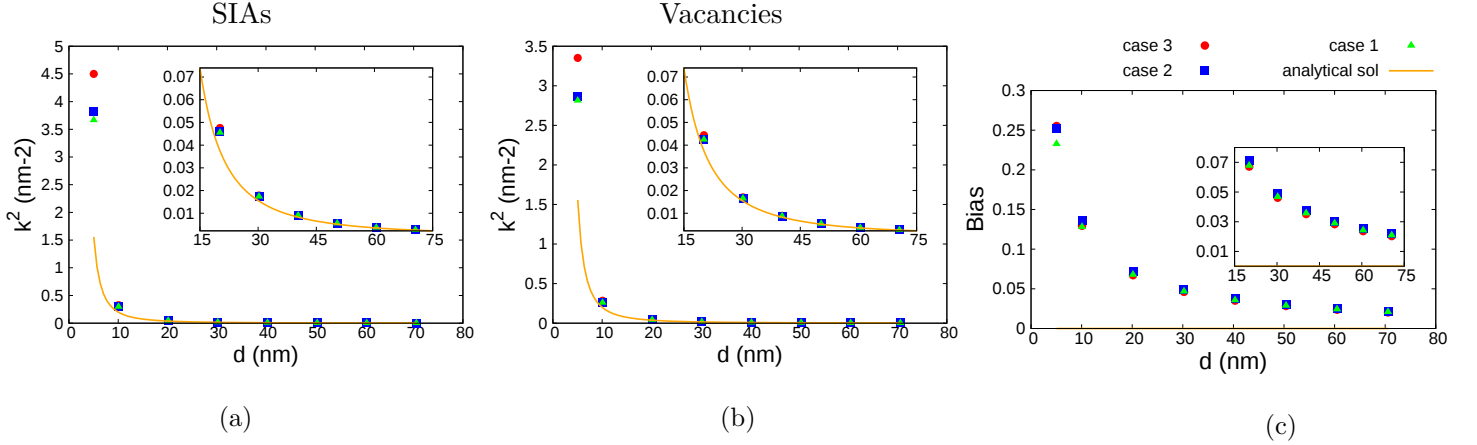


Figure 2.30: Sink strength as a function of STGB inter-spacing for a) SIAs and b) vacancies, and c) bias in Al. Case 1: no elastodiffusion, case 2: elastodiffusion with isotropic PD at saddle point, case 3: full elastodiffusion.

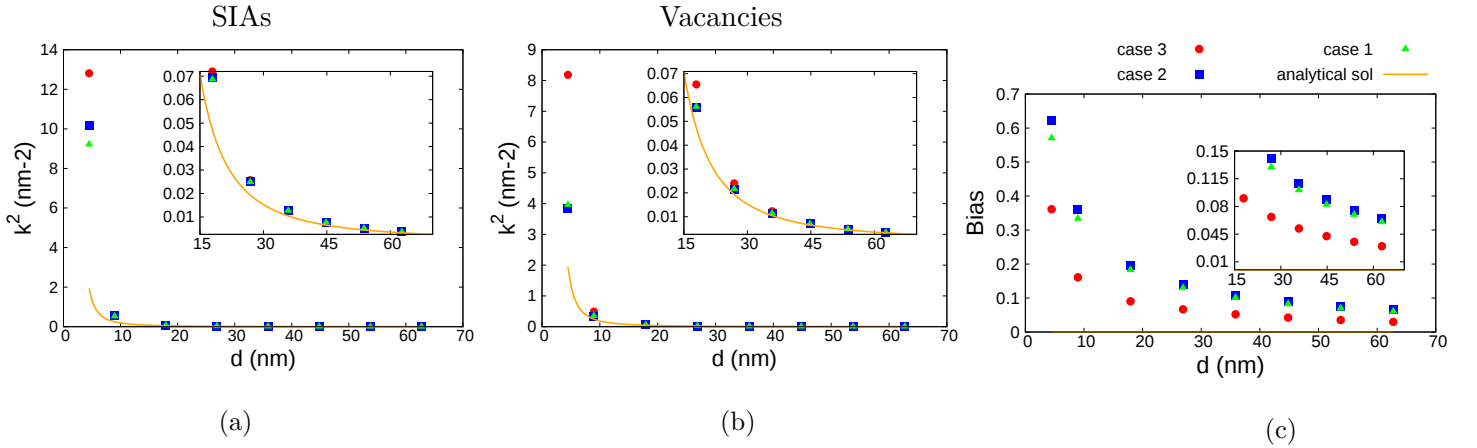


Figure 2.31: Sink strength as a function of STGB inter-spacing for a) SIAs and b) vacancies, and c) bias in Ni. Case 1: no elastodiffusion, case 2: elastodiffusion with isotropic PD at saddle point, case 3: full elastodiffusion.

higher when full elastodiffusion (case 3) is taken into account compared to the cases where PD is isotropic at saddle point (case 2) and where there is no elastodiffusion (case 1), like in the case of isolated dislocations. In Al, the sink strengths calculated in cases 1 to 3 are close for both PDs and the biases are almost the same for all the simulations. In the case of Ni, full elastodiffusion effects are more significant especially for vacancies and induce a strong decrease of the bias compared to the other cases. In Fe, elastodiffusion in cases 2 has no effects on the sink strength for vacancies, in case 3 an increase is observed for small STGB inter-spacings. For SIAs elastodiffusion does not change the sink strengths when SIAs are considered isotropic at saddle point. However, with full elastodiffusion, the sink strength increases strongly for small STGB inter-spacings and leads to strong variations of the STGB bias as shown in Fig. 2.32-c) (bias $\simeq 70$ % for $d \simeq 5$ nm).

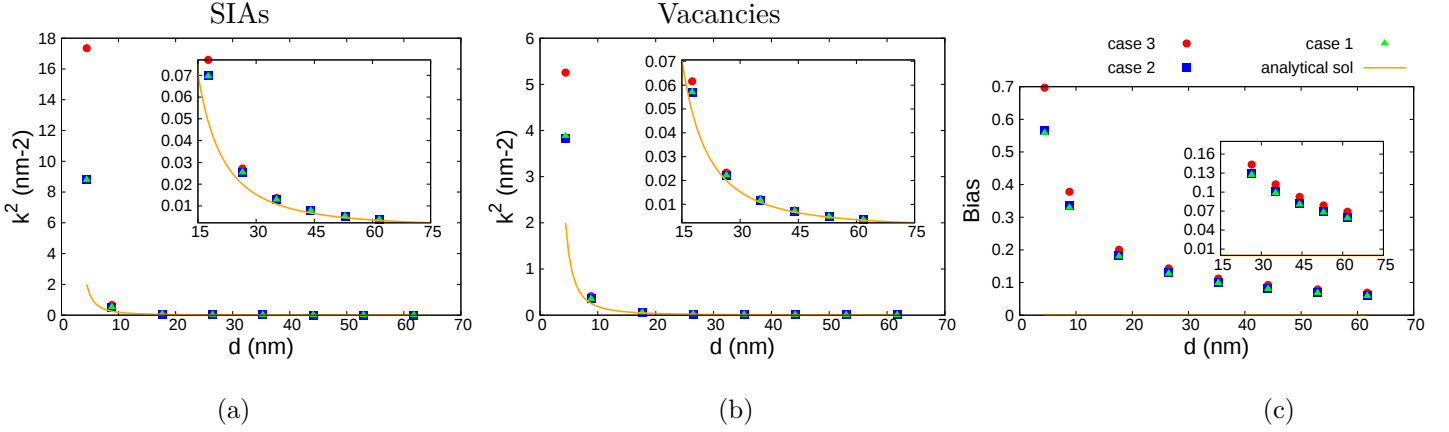


Figure 2.32: Sink strength as a function of the STGB inter-spacing for a) SIA and b) vacancies, and c) bias in Fe. Case 1: no elastodiffusion, case 2: elastodiffusion with isotropic PD at saddle point, case 3: full elastodiffusion.

Discussion

The elastodiffusion effects on the sink strength and bias have been investigated near a low angle STGB. The results obtained show that for high STGB inter-spacings, the sink strengths for both PDs are weakly affected by elastodiffusion compared to the case without elastodiffusion (case 1) and without any elastic interactions (analytical solution). As a consequence the STGB can be considered as a neutral sink for high inter-spacings. GBs are usually considered as neutral sinks in the literature [10], but for low GB inter-spacings, this consideration is no longer valid and GBs act as biased sinks (see Figs. 2.30-c), 2.31-c) and 2.32-c)). The stress field generated by a low angle STGB decays exponentially far from the STGB [52]. Thus, there are no long-range stresses which allows to explain why there are no effect of the elastic interactions on the sink strength for high STGB inter-spacings. The normalized PD diffusion coefficients D_{ij}/D^0 obtained with full elastodiffusion are plotted in Figs. 2.33, 2.34 and 2.35. As the STGB does not produce any long-range stress, the diffusion coefficients change only in the vicinity of the STGB. In Al and Ni, the variations of the ratio D_{ij}/D^0 are more important for vacancies than SIA as in the case of isolated dislocations. But these variations of the ratio D_{ij}/D^0 are small and remain comparable for both PDs in Al which explains the small change of the sink strength and bias (see Fig. 2.30). In Ni, the variations are more remarkable for vacancies compared to SIA and this explains the strong effects of full elastodiffusion on sink strength for vacancies in this case. The ratio D_{ij}/D^0 in Fe varies strongly for both PD (see Fig. 2.35). The variations are more pronounced for SIA which leads to the more noticeable effects of full elastodiffusion on sink strength for SIA in Fe. The contribution of each possible jump direction on the diffusion coefficients has also been studied. Table 2.5 shows that in Al and Ni, all jump directions bring on average the same contribution. In Fe, there are some directions which contribute more remarkably than the others to the diffusion coefficients.

The misorientation angle effects on the sink strength have been investigated by performing simulations with various values of the dislocation spacing h . Figure 2.36 shows the sink strength and bias for all the materials as a function of the misorientation angle,

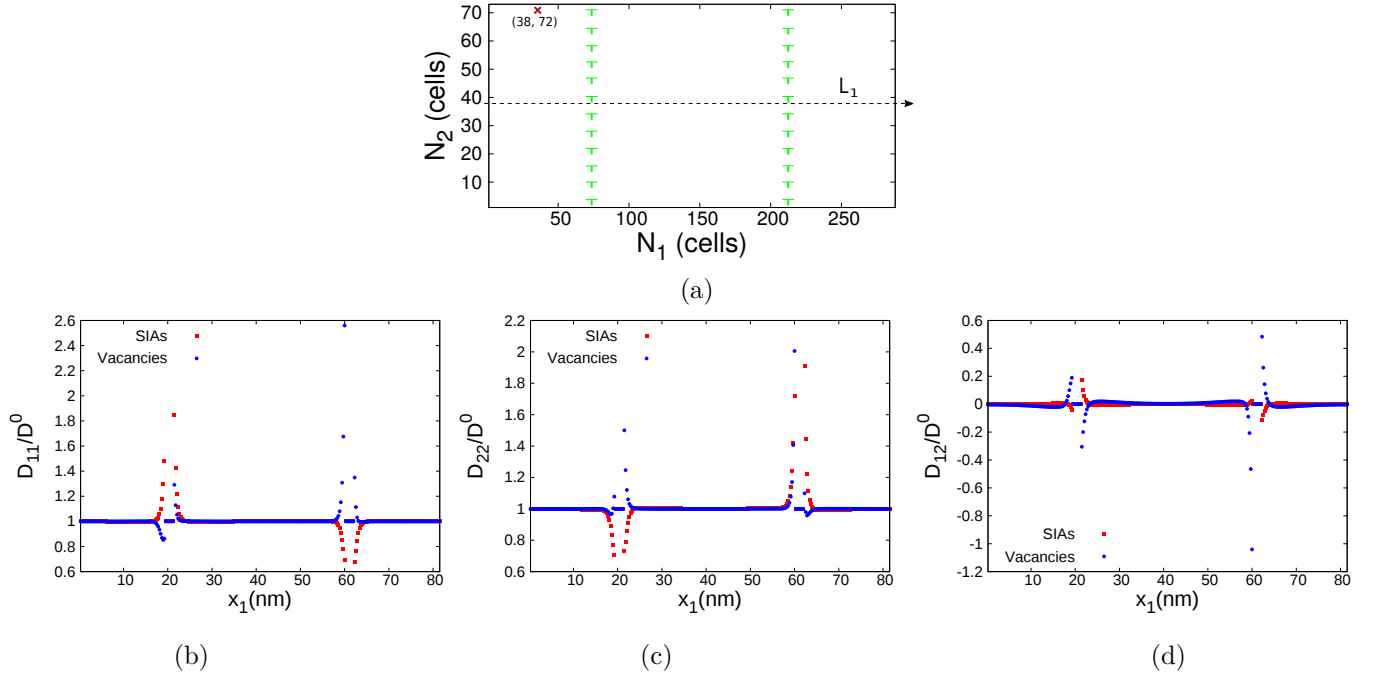


Figure 2.33: Profiles of the normalized diffusion coefficients along $\mathbf{L}_1$ (at $x_2 = 10.75$ nm) a) D_{11}/D^0 , b) D_{22}/D^0 and c) D_{12}/D^0 with full elastodiffusion (case 3) in Al for a low angle STGB.

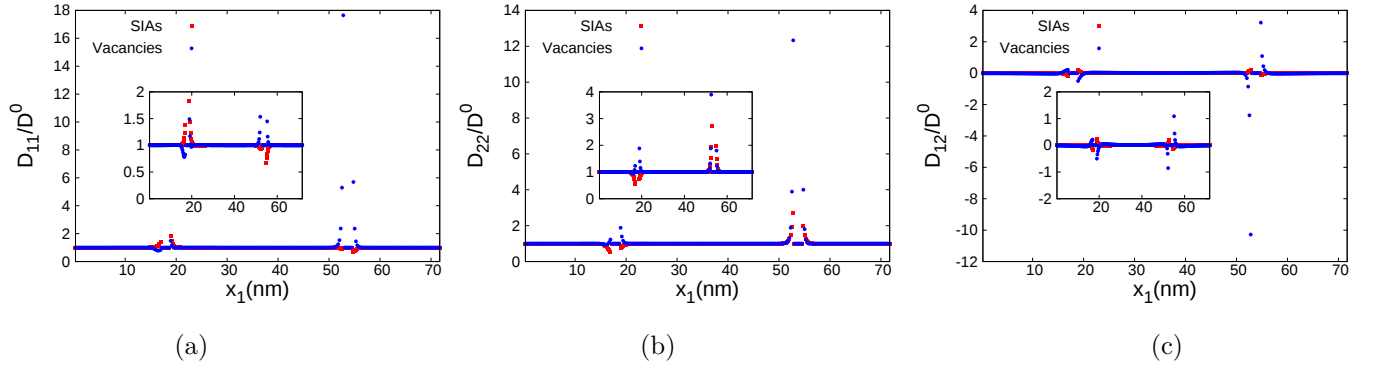


Figure 2.34: Profiles of the normalized diffusion coefficients along $\mathbf{L}_1$ (at $x_2 = 9.462$ nm, see Fig. 2.33-a)) for $\mathbf{L}_1$ axis a) D_{11}/D^0 , b) D_{22}/D^0 and c) D_{12}/D^0 with full elastodiffusion (case 3) in Ni for a low angle STGB.

for a chosen GB inter-spacing. The results are qualitatively the same in Al, Ni and Fe. For vacancies in Al and Fe, the sink strength increases with the misorientation angle and tends towards a constant value when θ becomes greater than approximately 3° . In the case of SIAs for all the materials, there is an increase followed by a decrease of the sink strength with θ , the maximum is obtained for $\theta \simeq 3^\circ$, which is also the case for vacancies in Ni. The representation of the bias given in Fig. 2.36-c) shows a decrease with the misorientation angle. These results are very similar to those obtained by Jiang et al. [62] in

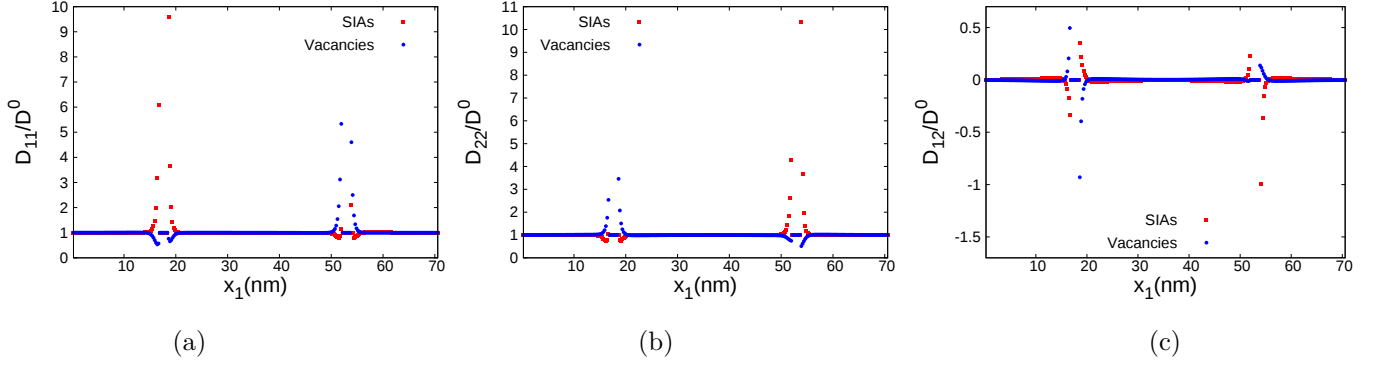


Figure 2.35: Profiles of the normalized diffusion coefficients along $\mathbf{L}_1$ (at $x_2 = 9.31$ nm, see Fig. 2.33-a)) for $\mathbf{L}_1$ axis a) D_{11}/D^0 , b) D_{22}/D^0 and c) D_{12}/D^0 with full elastodiffusion (case 3) in Fe for a low angle STGB.

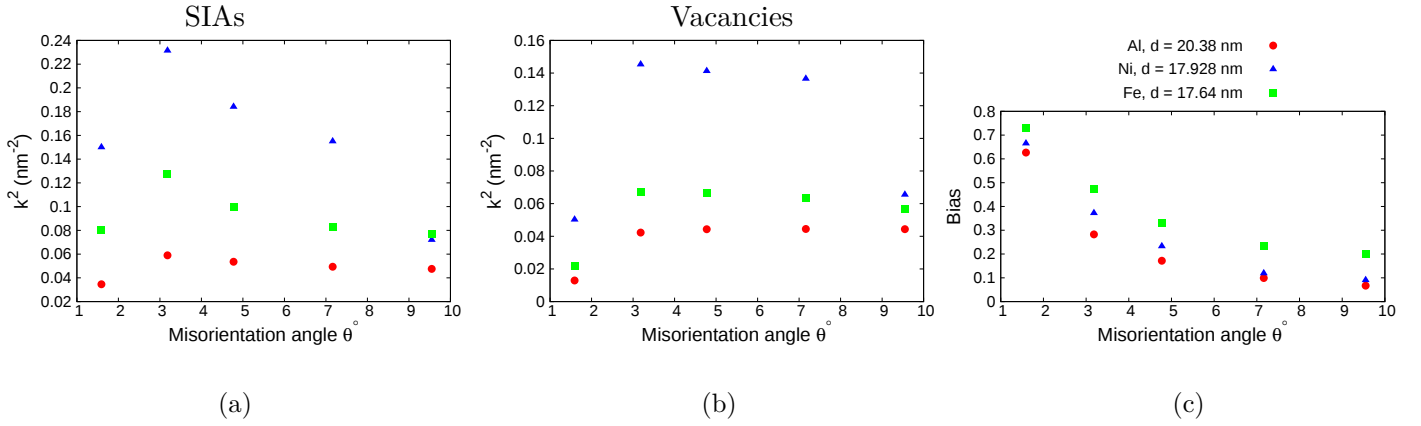


Figure 2.36: Sink strength and bias as a function of the misorientation angle at a given STGB inter-spacing d .

fcc Cu. In the study of Jiang, the maximum of the sink strength for SIAs is around $\theta = 2^\circ$. As explained by Jiang, the maxima in the GB sink strength is the result of 2 antagonistic effects: the sink strength increases with the dislocation density ($\rho_{dislo} = 1/hd = \theta/bd$) and consequently with θ as obtained in the case of straight dislocation. Contrariwise, for high dislocation densities (small h or high θ), the stress fields of neighboring GB dislocations overlap more strongly which leads to a mutual cancellation. Thus, the GB tends to act as a neutral planar sink for high dislocation densities (high misorientation angles). The maximum is less visible for vacancies due to their small relaxation volume compared to the one of SIAs which implies weak elastic interactions [62].

Crystal anisotropy effects have also been studied by changing the plane orientation i.e. its normal $\mathbf{n}$ which is parallel to the Burgers vector $\mathbf{b}$. The results of the GB bias calculations with full elastodiffusion are given in Fig. 2.37. In Al, the bias does not change a lot with the GB orientation. In Ni and Fe the bias changes strongly with the GB orientation, especially in Ni the bias changes its sign for low GB inter-spacings. To better understand these results, the profile of the normalized diffusion coefficient D_{11}/D^0

Table 2.5: Contribution of the possible jump direction $\mathbf{h}$ to the diffusion coefficients (Eq. 2.16) for a low angle STGB. $(x_{p1}, x_{p2}) = (38, 72)a_0$ (see Fig. 2.33-a)) with a_0 the size of the corresponding unit PF cell.

$\mathbf{h}$	$\beta \sum_{kl} (P_{kl}^{sad} - \bar{P}_{kl}^e) \varepsilon_{kl}(x_{p1}, x_{p2})$	$\exp(\beta \sum_{kl} (P_{kl}^{sad} - \bar{P}_{kl}^e) \varepsilon_{kl}(x_{p1}, x_{p2}))$
Al; Ni		
Vacancies		
[110] $[\bar{1}\bar{1}0]$	$-1.0963 \times 10^{-2}; -1.5552 \times 10^{-3}$	0.9891; 0.9984
[1 $\bar{1}0$] $[\bar{1}10]$	$-7.0822 \times 10^{-3}; 7.6614 \times 10^{-5}$	0.9929; 1.0000
[011] $[0\bar{1}\bar{1}]$ $[01\bar{1}]$ $[0\bar{1}\bar{1}]$		
[101] $[\bar{1}01]$ $[10\bar{1}]$ $[\bar{1}0\bar{1}]$	$-5.5906 \times 10^{-2}; -1.5696 \times 10^{-2}$	0.9456; 0.9844
Dumbbell [100]		
[110] $[\bar{1}\bar{1}0]$	$1.7463 \times 10^{-2}; 3.1794 \times 10^{-3}$	1.0176; 1.0031
[1 $\bar{1}0$] $[\bar{1}10]$	$-3.7497 \times 10^{-2}; -8.2513 \times 10^{-3}$	0.9632; 0.9917
[101] $[\bar{1}0\bar{1}]$	$-4.3900 \times 10^{-3}; -2.0245 \times 10^{-3}$	0.9956; 0.9979
$[\bar{1}01]$ $[10\bar{1}]$	$-1.8142 \times 10^{-2}; -2.4842 \times 10^{-3}$	0.9820; 0.9975
Fe		
Vacancies		
[111] $[\bar{1}\bar{1}\bar{1}]$ $[\bar{1}\bar{1}1]$ $[\bar{1}\bar{1}\bar{1}]$	1.9830×10^{-2}	1.0200
$[\bar{1}\bar{1}\bar{1}]$ $[\bar{1}\bar{1}1]$ $[\bar{1}\bar{1}\bar{1}]$ $[\bar{1}\bar{1}\bar{1}]$	-3.2637×10^{-2}	0.9678
Dumbbell [110]		
[111] $[\bar{1}\bar{1}\bar{1}]$ $[\bar{1}\bar{1}1]$ $[\bar{1}\bar{1}\bar{1}]$	-4.2570×10^{-2}	0.9583
$[\bar{1}\bar{1}\bar{1}]$ $[\bar{1}\bar{1}1]$ $[\bar{1}\bar{1}\bar{1}]$ $[\bar{1}\bar{1}\bar{1}]$	4.9653×10^{-2}	1.0509

is plotted for each GB orientation in Fig. 2.38. It can be seen that, in Al the ratio D_{11}/D^0 changes slowly with the GB orientation for both PDs which leads to the slow bias change. In Ni, D_{11}/D^0 is higher for the (100)[001] than for the $(\bar{1}10)[\bar{1}\bar{1}2]$ GB in the case of vacancies while the variations are comparable for SIAs. Then the sink strength of vacancies increases strongly for the (100)[001] GB which leads to a significant decrease of the bias as shown in Fig. 2.37-b). In Fe, the D_{11}/D^0 decreases for both PDs in the (100) orientation compared to the $(\bar{1}10)$ orientation. Thus the bias decrease in the (100) compared to the $(\bar{1}10)$ GB orientation as illustrated in Fig. 2.37-c).

In conclusion of this section, like in the case of straight dislocations, the sink strength of low angle STGB is higher with full elastodiffusion compared to the case where elastodiffusion is not considered. The full elastodiffusion effects on sink strength are more important for vacancies in Al and Ni like for straight dislocations, which leads to

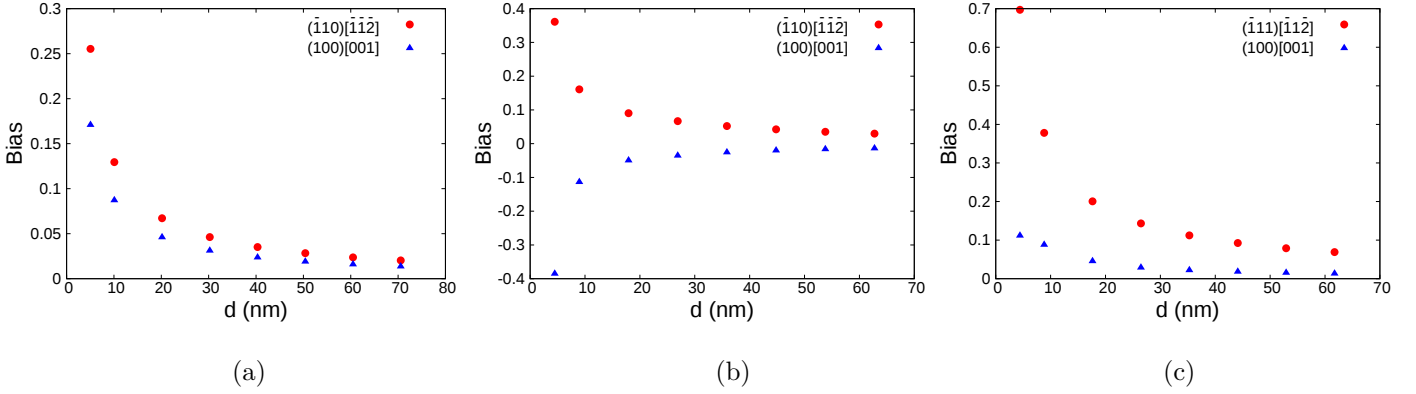


Figure 2.37: Sink bias as a function of STGB inter-spacing for different STGB orientations with full elastodiffusion in a) Al, b) Ni and c) Fe.

the sink bias decrease compared to the case without. This sink bias decrease with full elastodiffusion is more visible in Ni. In Fe, an increase of the STGB bias is obtained with full elastodiffusion compared to the case without, while a sink bias decrease has been obtained for straight dislocations. This difference in the sink bias modifications with full elastodiffusion can be explained by the following argument. As shown by the diffusion coefficients profiles, the full elastodiffusion effects on the ratio D_{11}/D^0 are comparable for SIAs and vacancies in the case of isolated dislocations, whereas in the case of STGB, D_{11}/D^0 for SIAs is affected more strongly than for vacancies when full elastodiffusion is considered. The misorientation angle effects on STGB sink strength and bias have also been studied. The results show the existence of two regimes: a regime at low θ ($\theta < 3^\circ$) where the sink strength increases with θ and a second regime $\theta > 3^\circ$ where the sink strength decreases with θ . Lastly, the effects of the STGB orientation have been investigated. It emerged that the STGB bias is slightly modified when the STGB changes from the orientation $(\bar{1}10)[\bar{1}\bar{1}\bar{2}]$ to $(100)[001]$ in Al. But in Ni and Fe, the bias is highly modified when the STGB changes from the orientation $(\bar{1}10)[\bar{1}\bar{1}\bar{2}]$ to $(100)[001]$ and from $(\bar{1}11)[\bar{1}\bar{1}\bar{2}]$ to $(100)[001]$ in Ni and Fe respectively. In the section below 2.3.3.3, the case of a spherical cavity is treated.

2.3.3.3 Spherical cavity

A spherical cavity is located at the center of a cubic PF simulation domain as illustrated in Fig. 2.9. The cavity radius was set to $R_{cav} = 1$ nm ($4a_0$). The cavity surface was modelled as a diffuse interface with a width of 1 nm ($w = 4a_0$). The radius of the capture region thus corresponds to $r_0 = 2$ nm ($r_0 = R_{cav} + w$). The PF basis is given by:

$$\begin{cases} \mathbf{e}_1 = [100] \\ \mathbf{e}_2 = [010] \\ \mathbf{e}_3 = [001] \end{cases} \quad (2.74)$$

The PD flows towards the cavity are represented on Fig. 2.39 in the x_1x_2 -plane for a given cavity density. The trajectories of both PDs are normal to the cavity in all the cases of

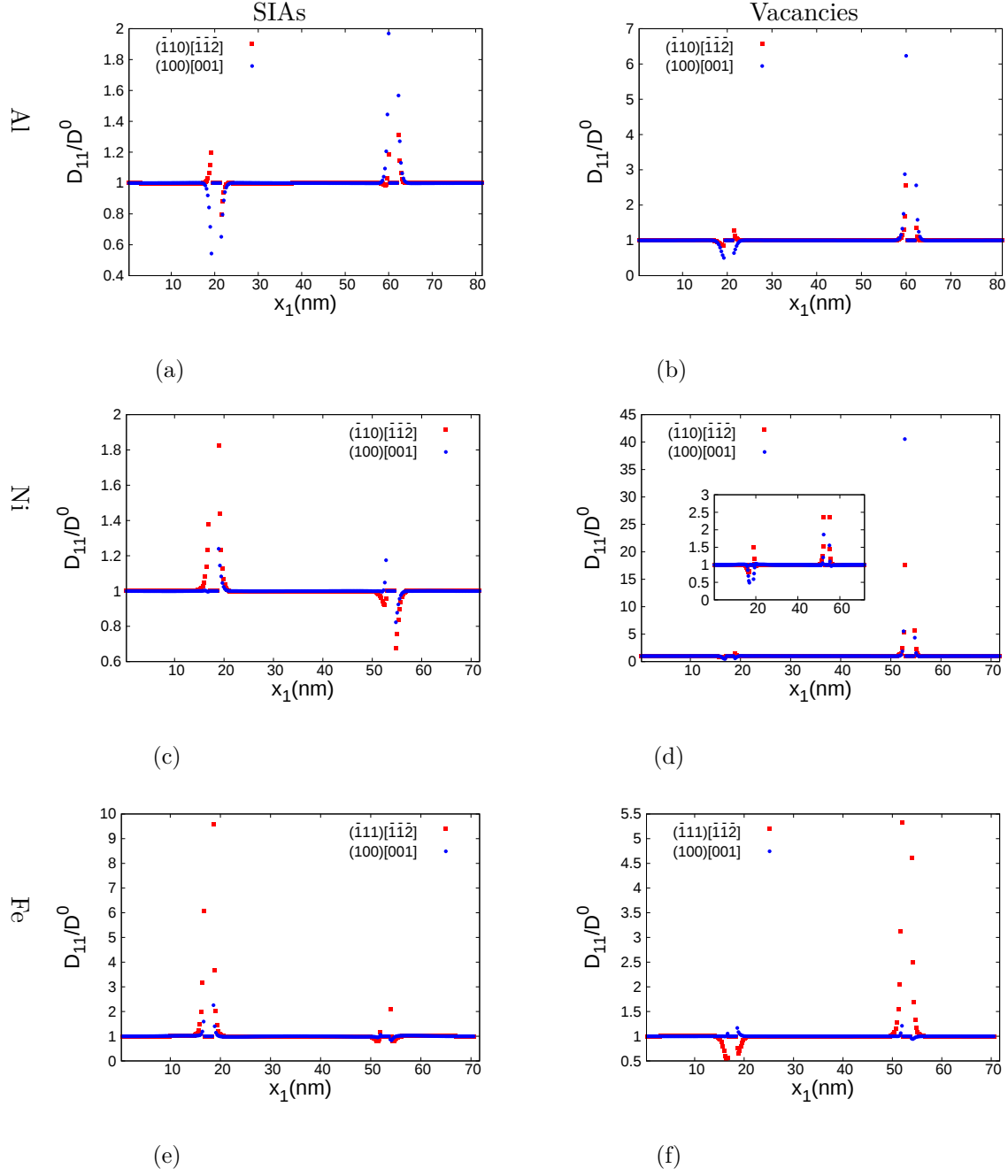


Figure 2.38: Normalized diffusion coefficients D_{11}/D^0 along L_1 (see Fig. 2.33-a)) respectively for SIAs a) (at $x_2 = 10.75$ nm) Al, c) (at $x_2 = 9.462$ nm) Ni and e) (at $x_2 = 9.31$ nm) Fe, and for vacancies b) Al, d) Ni and f) Fe with full elastodiffusion for different GB orientations.

simulations and for all the materials. The SIA trajectory does not change remarkably with the saddle point anisotropy in all the systems, the same behavior is observed in

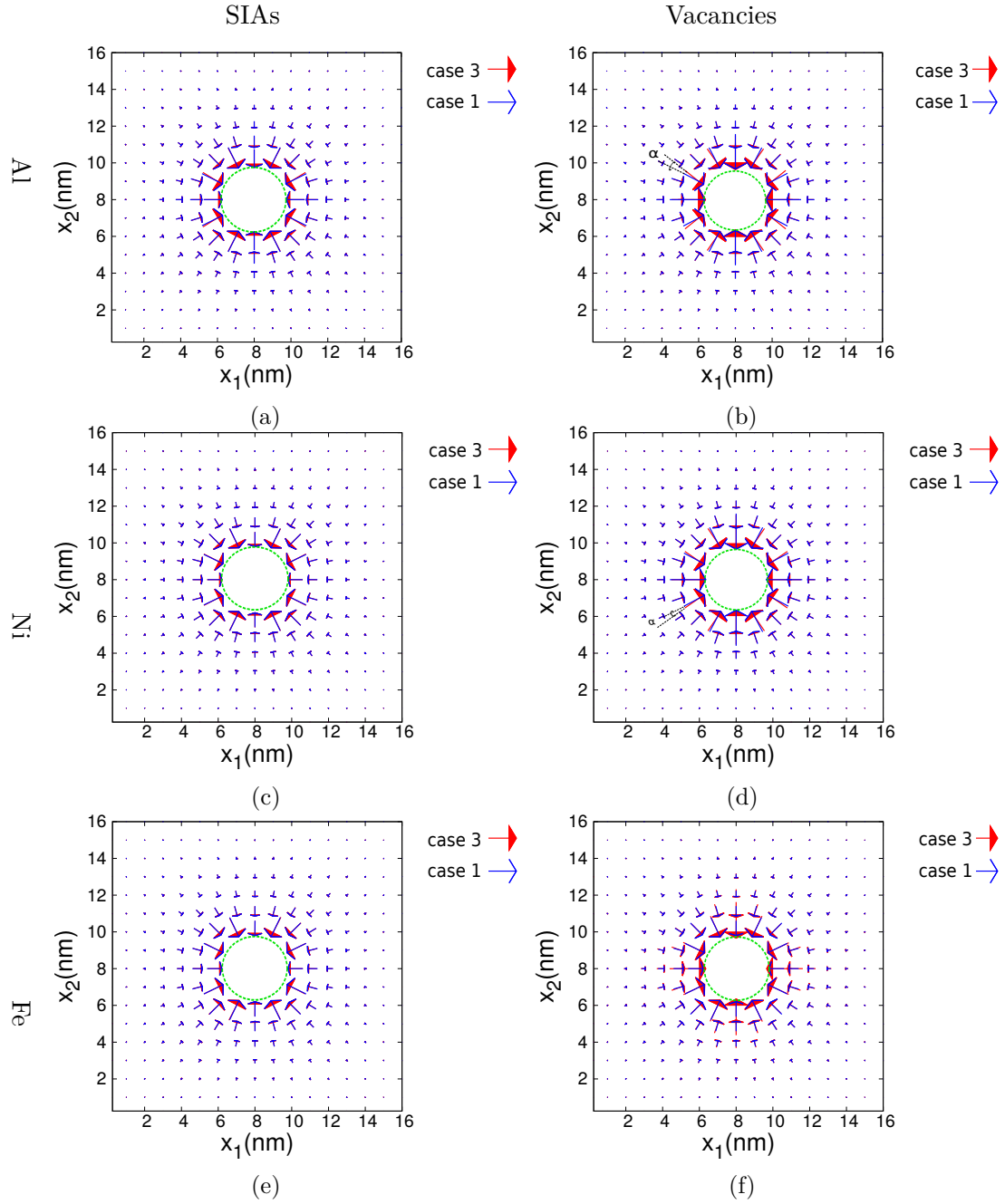


Figure 2.39: Fluxes in the x_1x_2 -plane of a) SIAs and b) vacancies in Al, c) SIAs and d) vacancies in Ni, e) SIAs and f) vacancies in Fe, without elastodiffusion (case 1) and with full elastodiffusion (case 3) for a spherical cavity according to the x_1x_2 -plane passing through the center of cavity. The length of the vector is proportional to the norm of the flux $\|\mathbf{J}\| = \sqrt{J_1^2 + J_2^2}$.

the trajectory of vacancies in Fe. On the other hand, a significant change is noted in the vacancy flow near the cavity in Al and Ni. As shown in Figs. 2.39-b) and 2.39-d) the vacancy trajectory is deflected in the vicinity of the cavity with the PD anisotropy at saddle point. Carpentier et al. [34] have obtained the same effects of the P_{ij} -tensor anisotropy at saddle point on the PD trajectories near a spherical cavity in Al.

Figs. 2.40, 2.41 and 2.42 show the atomic fraction maps of PD around the cavity in the x_1x_2 -plane. In case 1, the shape of the vacancy depletion region is almost the same when

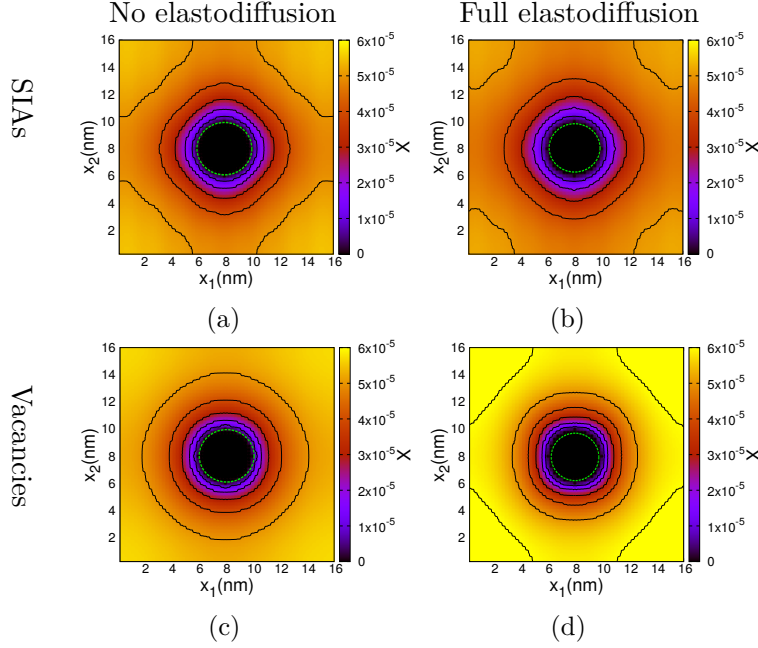


Figure 2.40: Atomic fraction maps of SIAs and vacancies respectively without elastodiffusion (case 1) a) and c), and with full elastodiffusion (case 3) b) and d) in Al for a spherical according to the x_1x_2 -plane passing through the center of cavity.

there is no elastic interactions (spherical symmetry) in all the materials. On the contrary, the shape of the depletion zone for SIAs is different from that without elastic interactions, especially for Ni and Fe. This difference is due to the elastic constant anisotropy and the magnitude of this change depends on the PD relaxation volume. The relaxation volume of vacancies is smaller than the one of SIAs and thus the shape of the vacancy depletion region is less affected by the elastic interactions. Moreover, the shape of the depletion region of SIAs in Al has almost a spherical symmetry around the cavity. This is due to the lower anisotropy factor of Al compared to Ni and Fe (see table 2.3 for anisotropy factors). The shape of the depletion region does not change significantly with the saddle point anisotropy (case 3) for both PDs in all the systems. The size of the depletion region for vacancies decreases with full elastodiffusion which means a slower absorption, whereas the size of the depletion zone of SIAs is practically unchanged.

The sink strengths and biases are plotted in Figs. 2.43, 2.44 and 2.45. The sink strengths obtained for both PDs in cases 1 and 2 are close to the Wiedersich solution for all the systems. The bias in these cases is less than 5% and the cavity can be considered

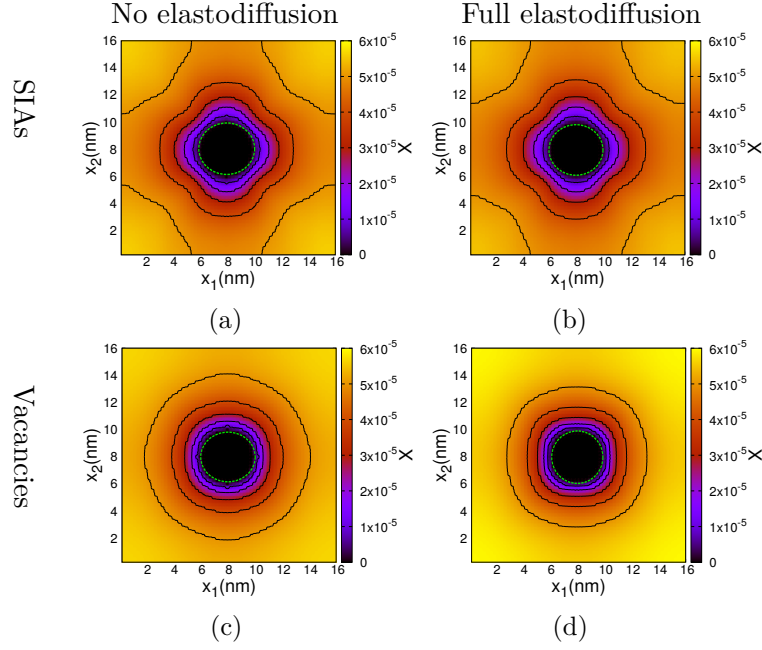


Figure 2.41: Atomic fraction maps of SIAs and vacancies respectively without elastodiffusion (case 1) a) and c), and with full elastodiffusion (case 3) b) and d) in Ni for a spherical according to the x_1x_2 -plane passing through the center of cavity.

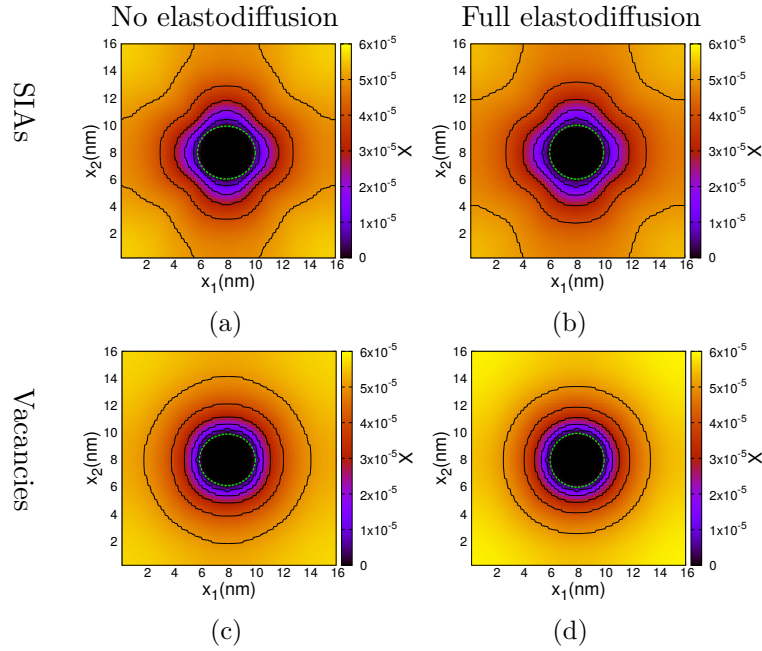


Figure 2.42: Atomic fraction maps of SIAs and vacancies respectively without elastodiffusion (case 1) a) and c), and with full elastodiffusion (case 3) b) and d) in Fe for a spherical according to the x_1x_2 -plane passing through the center of cavity.

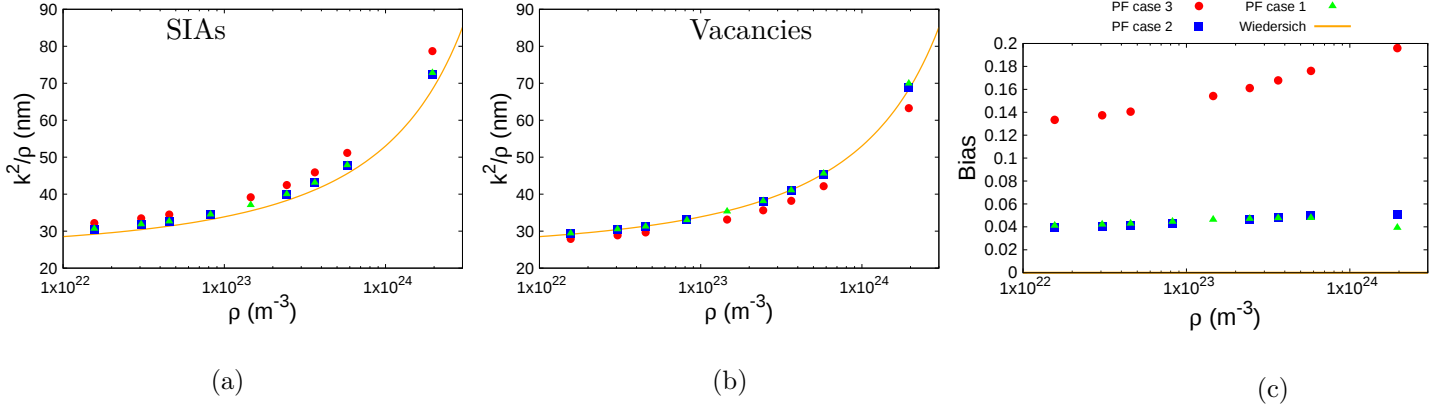


Figure 2.43: Sink strength as a function of the cavity density for a) SIAs and b) vacancies, and bias c) in Al. Case 1: no elastodiffusion, Case 2: isotropic PD at stable and saddle points, Case 3: full elastodiffusion (real P_{ij} -tensors).

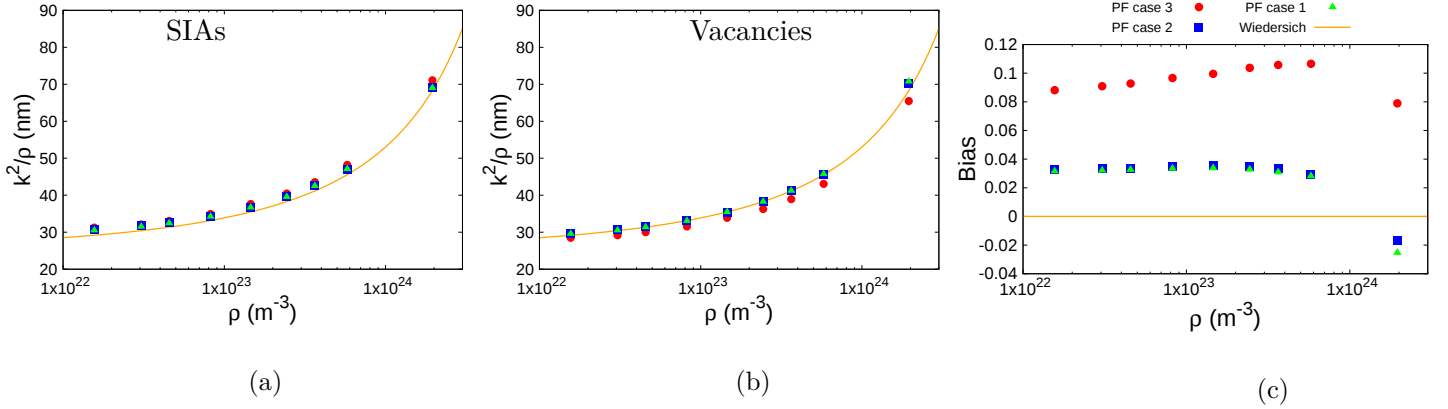


Figure 2.44: Sink strength as a function of cavity density for a) SIAs and b) vacancies, and bias c) in Ni. Case 1: no elastodiffusion, Case 2: isotropic PD at stable and saddle points, Case 3: full elastodiffusion (real P_{ij} -tensors).

as a neutral sink [10]. The results in the case of full elastodiffusion (case 3) show an increase of the sink strength for SIAs and a decrease for vacancies compared to the cases 1 and 2. The sink bias increases and is around 20% in Al and 10% in Ni and Fe for the corresponding cavity radius. Thus, a cavity cannot be considered again as a neutral sink when all the elastic effects are taken into account (full elastodiffusion). It should also be noted that the bias varies slightly with the cavity density because a cavity produces a strain with a short range (see Eq. 2.71).

Discussion

The results of the sink strength and bias computations of cavity with elastodiffusion show that the PD anisotropy at saddle point leads to a significant change of the sink strength and bias. Therefore cavity can no longer be considered as a neutral sink. In cases 1 and 2 the bias is modified but remains less than 5 %. The normalized diffusion coefficients

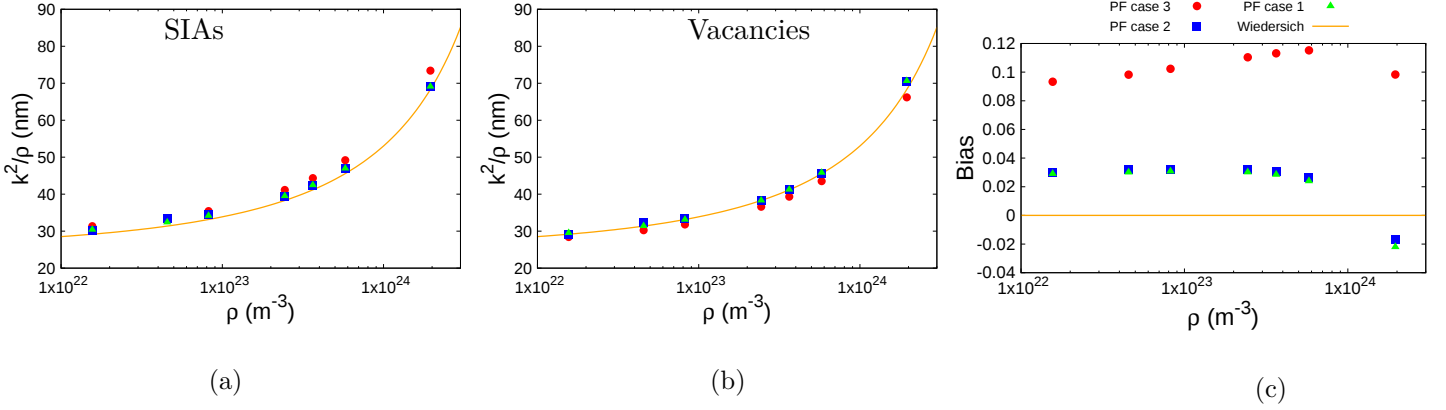


Figure 2.45: Sink strength as a function of cavity density for a) SIA and b) vacancies, and bias c) in Fe. Case 1: no elastodiffusion, Case 2: isotropic PD at stable and saddle points, Case 3: full elastodiffusion (real P_{ij} -tensors).

D_{ij}/D^0 are plotted in Figs. 2.46, 2.47 and 2.48 in the case of full elastodiffusion. The ratios D_{ij}/D^0 are very close to 1 for diagonal terms ($i = j$) and to 0 for off-diagonal terms ($i \neq j$) in all the systems. These small changes of the diffusion coefficients are due to the small strain field generated by the cavity.

The bias evolution with the cavity radius R_{cav} has been investigated. The results of Carpentier et al. [34] and the analytical solution of Borodin et al. [39] are also reported in Fig. 2.49. In the Borodin solution, the radius of the capture region corresponds to the radius of the cavity ($r_0 = R_{cav}$). In the study of Carpentier, r_0 stays close to R_{cav} , $r_0 = R_{cav} + R_{PD}$ where R_{PD} is the point defect radius ($R_{PD} = 0.16$ nm). In our study, the capture radius of cavity is $r_0 = R_{cav} + w$ where w is the width of the cavity surface. The width of the cavity surface then was set to $4a_0$ ($a_0 = 0.25$ nm) and the capture radius corresponds to $r_0 = R_{cav} + 1$ nm. The bias is represented in function of the sink capture radius r_0 in Fig. 2.49. The results show a decrease of the cavity bias with its radius. This can be explained by the fact that the eigenstrain of the cavity is proportional to $1/R_{cav}$ (see Eq. 2.67) and the corresponding strain field decreases with R_{cav} . As a consequence the bias decreases with the cavity radius, since the elastic interactions decrease. In the cases of Al and Ni, we have a good agreement with the Borodin solution for large cavities. For small cavities, the elastic strain field becomes stronger and the differences in the results are growing. The results of Carpentier in Al are very close to the analytical solution of Borodin for large cavities and differ for small cavities. In Fe, there is a large difference between our results and the analytical solution. Several reasons may explain these discrepancies with the solution of Borodin:

- The Borodin solution depends only on the elastic dipole tensor at saddle point and varies as $1/R_{cav}$.
- SIA and vacancies are assumed to have the same P_{ij} -tensor symmetry at saddle point in the Borodin solution. In our simulations, this is not the case for vacancies and dumbbells in Fe.
- The strain field around the cavity given in the Borodin solution corresponds to the

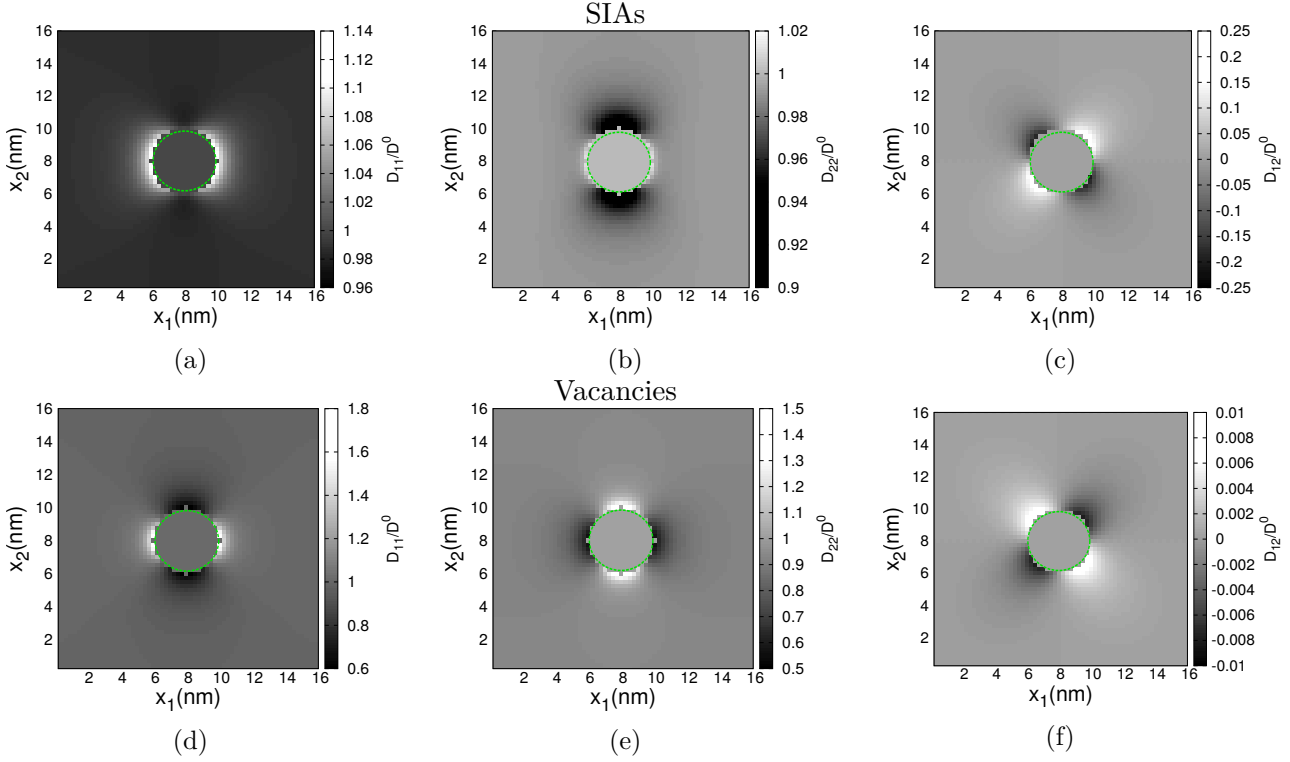


Figure 2.46: Normalized diffusion coefficients D_{11}/D^0 , D_{22}/D^0 and D_{12}/D^0 respectively for SIAs a), b) and c), and for vacancies d), e) and f) in Al in the x_1x_2 -plane passing through the center of the cavity.

one obtained considering an infinite isotropic medium and is assumed small.

The discrepancies observed with the results of Carpentier are may be due to the fact that like in the Borodin solution, the strain field is given for the cavity in an infinite isotropic medium.

In summary of this section, the sink bias of a spherical cavity is low ($< 5\%$) without elastodiffusion, but when full elastodiffusion is taken into account, the sink strength for SIAs increases while it decreases for vacancies in all the materials which leads to a significant sink bias increase (close to 10%). It has also been shown that the cavity bias decreases when the cavity radius increases. This is due to the fact that the eigenstrain of a spherical cavity is inversely proportional to its radius and then the strain field that it generates decays with R_{cav} . Thus for large cavity radius, the cavity tends to act as a neutral sink.

2.4 Conclusion

In this chapter, a systematic study of PD diffusion modified by a stress field due to microstructural defects, including elastodiffusion, has been done in fcc (Al, Ni) and bcc

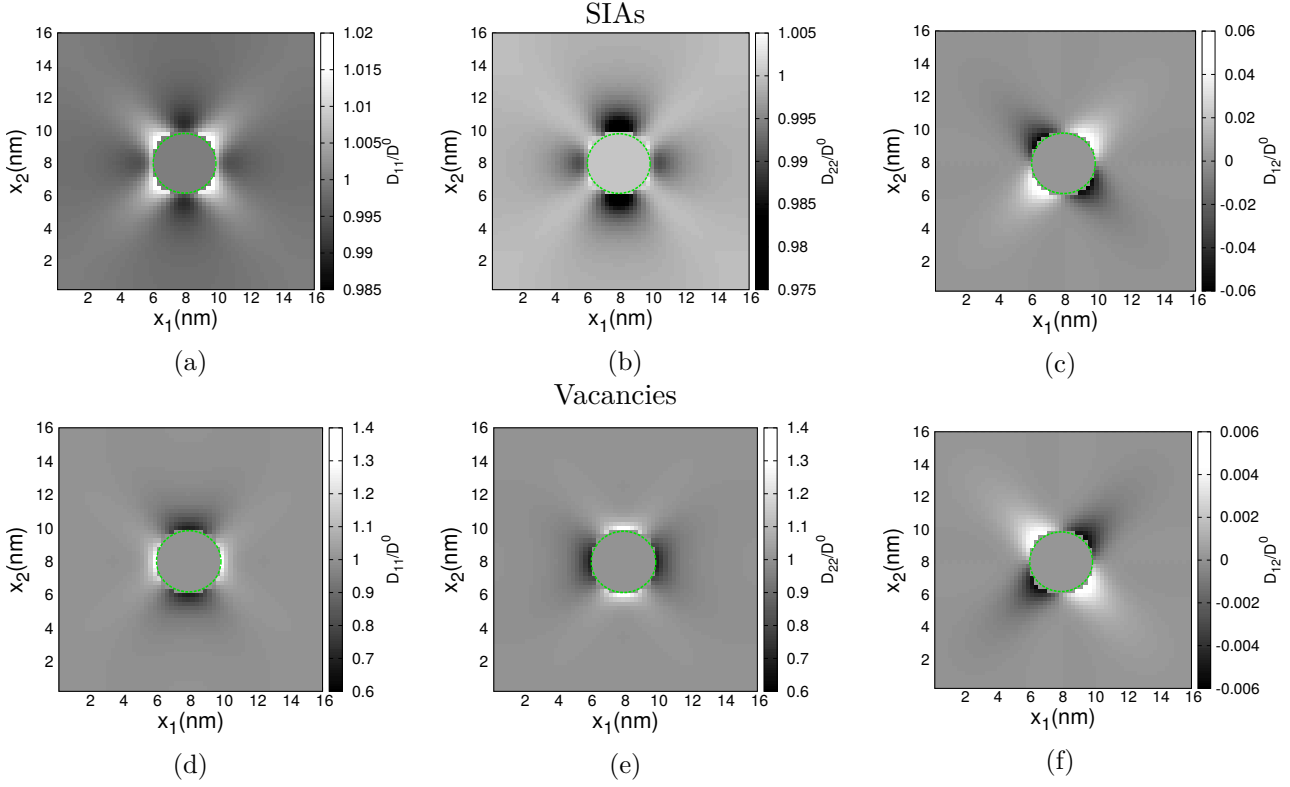


Figure 2.47: Normalized diffusion coefficients D_{11}/D^0 , D_{22}/D^0 and D_{12}/D^0 respectively for SIAs a), b) and c), and for vacancies d), e) and f) in Ni in the x_1x_2 -plane passing through the center of the cavity.

(Fe) metals. PD was described by its elastic dipole tensor at stable and saddle point. Many cases of simulations have been performed to investigate the role of the PD anisotropy at saddle point. The PD trajectory, atomic fraction map towards the sink, the sink strength and bias have been represented in the case of straight dislocations, low-angle STGB and spherical cavities. The results show a change in the PD trajectory, PD depletion region (size and shape) and sink strength. Globally, the sink strength of straight dislocations and STGB increases for both PD with the PD anisotropy at saddle point. In the case of a spherical cavity, the sink strength increases for SIAs but decreases for vacancies with full elastodiffusion. The PD anisotropy at saddle point has strong effects on sink strength of straight dislocations and STGB for vacancies compared to SIAs in fcc metals Al and Ni. In bcc Fe, the same result as in Al and Ni has been obtained for straight dislocations, but not for STGB. This leads to a decrease of the sink bias of straight dislocations in all the metals. The sink bias of STGB decreases significantly in Ni, while in Al and Fe the bias change slightly. As with full elastodiffusion the sink strength of cavity increases for SIAs and decreases for vacancies, the cavity bias increases in all the metals. An important point to emphasize is that, STGBs and cavities are biased sinks when all the elastic interactions are taken into account. In particular, the STGB bias increases strongly for low GB inter-spacings (high densities). Finally, these results indicate that the PD

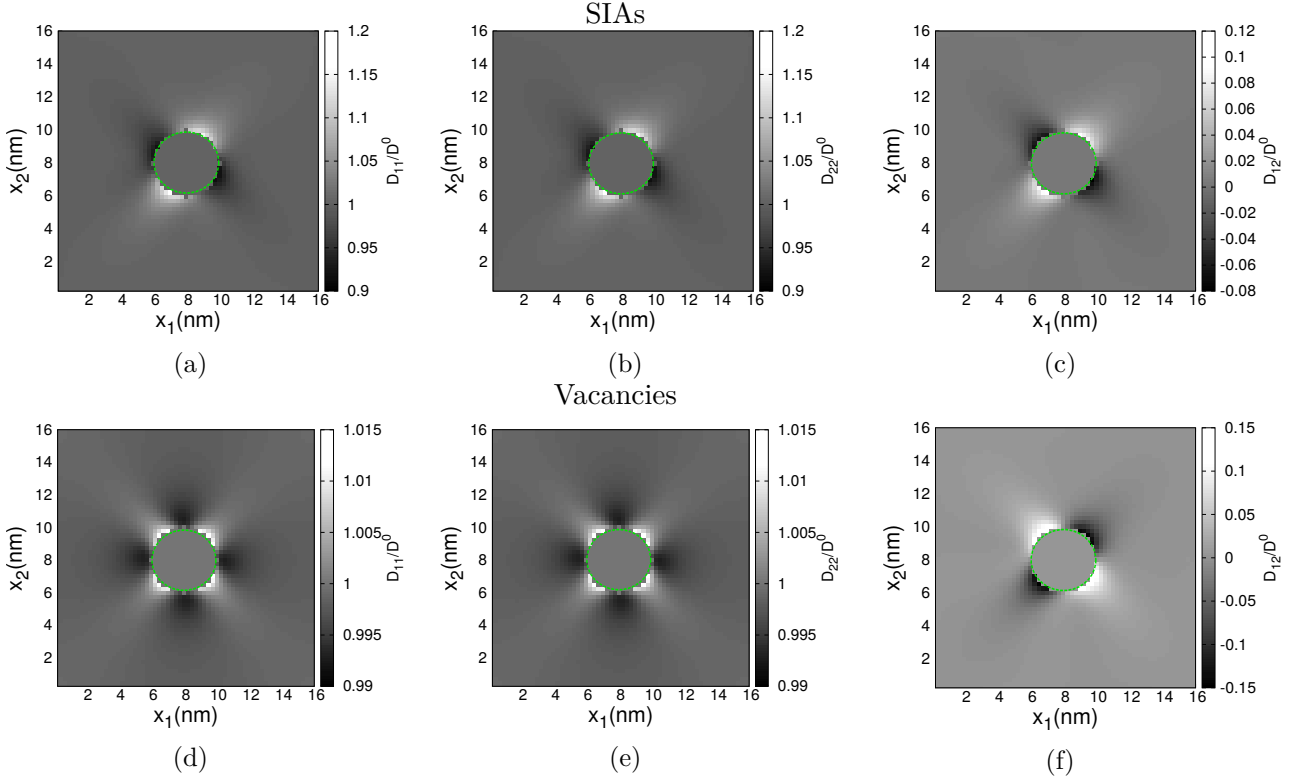


Figure 2.48: Normalized diffusion coefficients D_{11}/D^0 , D_{22}/D^0 and D_{12}/D^0 respectively for SIAs a), b) and c), and for vacancies d), e) and f) in Fe in the x_1x_2 -plane passing through the center of the cavity.

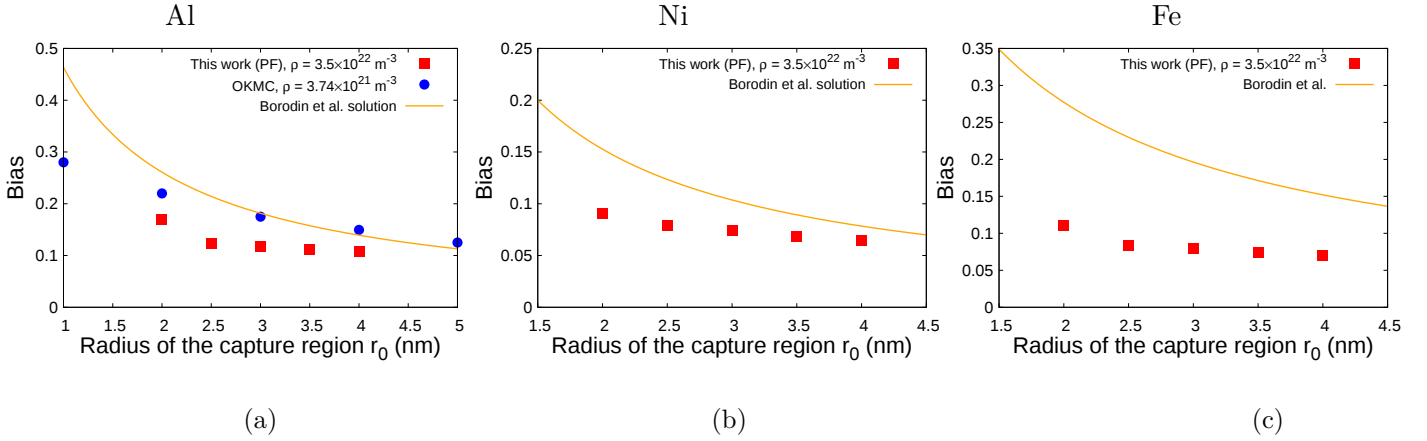


Figure 2.49: Sink bias as a function of the cavity capture radius r_0 with full elasto diffusion in a) Al, b) Ni and c) Fe.

anisotropy at saddle point plays an important role in the sink strength calculations when all the elastic interactions are taken into account. Another important factor is the system anisotropy. As shown by the results of the bias calculations in cases of straight dislocations

and STGB, the bias can vary strongly with the glide system of the dislocation like in the case of Ni, and with the STGB orientation like in the case of Ni and Fe.

Chapter 3

Phase field model of dislocation climb generalized to vacancies and SIAs: application to dislocation loop evolution under irradiation

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In chapter 2, the effects of elastic interactions between PDs and microstructural defects on the sink strengths have been investigated. However, the sink strengths has been calculated assuming immobile sinks. But the sink evolution due to the PD absorption is also known to be responsible for many observed phenomena such as irradiation creep [63, 64, 65, 66]. In this chapter, we propose a new PF model of dislocation climb and we apply it to describe the dislocation loop evolution under irradiation.

3.1 Bibliography

Dislocation climb is a mechanism which allows to better understand the plastic deformation of materials. The climb process occurs by absorption or emission of PDs at the dislocation cores. This process is more common at high temperature due to the high PD concentration especially the one of vacancies and becomes an essential part of high temperature creep [67, 68]. The PD absorption/emission by the dislocation takes place at specific defects along the dislocation line called **jogs**. In the case of high jog density, the kinetic of attachment/detachment of PD at dislocation cores is instantaneous compared to the PD diffusion towards dislocation cores. The **local equilibrium** of PD around the dislocation core is maintained along the dislocation line [9, 69, 70] and dislocations act as **perfect sinks/sources**. The climb process is then limited by the PD diffusion. For low jog density, the assumption of local equilibrium of PD along the dislocation line is no longer verified. PD will migrate along the dislocation line which is so called **pipe diffusion**. The PD diffusion towards the dislocation is no longer invariant along the dislocation line due to the PD flux along this line. The climb process is then limited by the mechanism of PD absorption/emission. To quantify the climb process, the dislocation climb velocity is generally calculated. The climb rate can be determined analytically, by experiments or by performing simulations.

In the analytical models [69, 71], the climb rate is determined by solving the vacancy diffusion equation around an infinite straight dislocation of Burgers vector $\mathbf{b}$ as illustrated in Fig. 3.1:

$$\frac{\partial X}{\partial t} = \nabla \cdot M(X) \nabla \mu \quad (3.1)$$

where μ is the chemical potential of vacancies and $M(X)$ their mobility given by:

$$M(X) = \frac{D}{k_B T} X \quad (3.2)$$

In the assumption that there is no elastic interaction between dislocation and vacancies, μ can be written as:

$$\mu = \ln(X/X_{eq})/\beta \quad (3.3)$$

with $\beta = 1/k_B T$ and X_{eq} the atomic fraction of vacancies at equilibrium. The vacancy diffusion towards the dislocations is assumed to be a faster process than the dislocation motion. Thus, the vacancy profile around the dislocations is not modified by the dislocation motion in the stationary state where $\frac{\partial X}{\partial t} = 0$. Eq. 3.1 becomes:

$$\Delta X = 0 \quad (3.4)$$

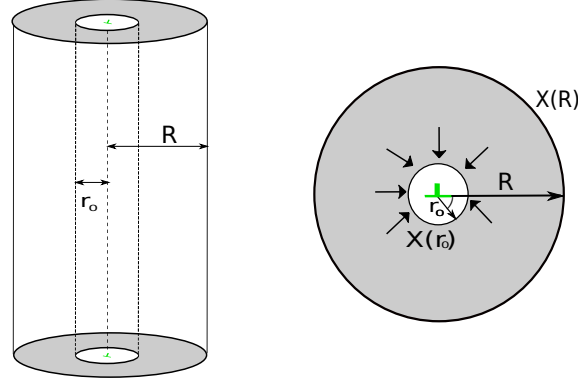


Figure 3.1: Geometry of straight dislocation used to determine the analytical expression of the climb velocity.

To solve Eq. 3.4, the vacancy fraction at the domain boundaries is fixed $X(r = R) = X(R)$. The vacancy fraction in the vicinity of dislocations is determined in the assumption of local equilibrium (perfect sink/source): $X(r_0)$ is chosen such as the chemical potential of vacancies is equal to the work due to the Peach and Koehler force:

$$\begin{aligned} \ln(X(r_0)/X_{eq})/\beta &= F_{Pk}V_{at}/b \\ \implies X(r_0) &= X_{eq} \exp(\beta F_{Pk}V_{at}/b) \end{aligned} \quad (3.5)$$

where

$$F_{Pk} = ((\sigma \mathbf{b}) \wedge \mathbf{l}) \cdot \mathbf{n} \quad (3.6)$$

with σ the local stress, $\mathbf{l}$ the line vector and $\mathbf{n}$ the vector normal to the glide plane of the dislocation. The vacancy fraction is then given by [10, 72]:

$$X(r) = X(R) + (X(R) - X(r_0)) \frac{\ln(r/R)}{\ln(R/r_0)} \quad (3.7)$$

The climb velocity is obtained by integrating the vacancy flow arriving on dislocation and is given by [72, 1]:

$$v = \frac{2\pi X_{eq} D}{b \ln(R/r_0)} \left[\frac{X(R)}{X_{eq}} - \exp(\beta F_{Pk}V_{at}/b) \right] \quad (3.8)$$

Eq. 3.8 shows that the dislocation climb can occur if:

- The vacancy atomic fraction in the bulk is different from its equilibrium value (supersaturation). The driving force is chemical and given in term of $X(R)/X_{eq}$.
- The system is constrained by an external/internal stress σ . The driving force is mechanical and given in terms of F_{Pk} .

The experimental measure of dislocation climb rate has been done in several studies [73, 74, 75]. Tartour and Washburn [74] have studied the climb kinetics of prismatic dislocation loops annealing in Al using transmission electron microscopy techniques. The

climb rate was deduced from the linear evolution of the dislocation loop area with time. Tartour and Washburn have observed that the perfect loops shrink by conserving their circular shape. They have suggested a rapid diffusion of vacancies along the dislocation line to explain the shape conservation of dislocation loops during the shrinkage. The rapid diffusion of vacancies along the dislocation line implies high jog densities. The kinetics measured is in good agreement with the analytical solution obtained under the assumption of local equilibrium of vacancies along the dislocation.

Dislocation climb is extensively studied using numerical simulations which are based on the diffusion theory. Among the simulation methods used, the most popular are discrete dislocation dynamics (DDD) [72, 76, 77] and more recently PF approaches [2, 1, 3]. Mordehai et al. [72] have introduced dislocation climb model by bulk diffusion (Eq. 3.8) in DDD simulations in the case of perfect sinks. Through their implementation, Mordehai et al. have modelled the shrinkage and expansion of circular prismatic dislocation loops in Al. The results obtained have shown the shrinkage of vacancy loop with a constant surface shrinkage rate. They have compared their results to the experimental ones and they obtained a good agreement. Yulan Li et al. [23] have simulated interstitial loop growth in bcc iron under irradiation using PF approach. The evolution equations describing the vacancy and SIA diffusion, and the dislocation motion through climbing are written and solved simultaneously. They obtained a linear loop growth with time which is in good agreement with experimental observations. Moreover, Li et al. have investigated the effects of elastic interaction and it appears that elastic interaction speeds up the loop growth kinetics and also causes anisotropic growth rates. However, the model of Li et al. does not ensure the balance between the PD fluxes in the bulk and the dislocation loop evolution. They also have assimilated the interstitial loop as a platelet-shaped precipitate with a composition of 100% of SIAs. This choice may introduce artificial SIA composition at the interface between the loop and the matrix and also influence the climb rate calculation.

In the PF models [2, 1, 3], the balance between the quantity of vacancies absorbed or emitted by the dislocation and the dislocation motion is explicitly guaranteed through a coupling term between the evolution equations. The PF approach is particularly suitable to study the dislocation climb because the diffusion process and the elastic interactions are incorporated in its formalism. In the PF studies [2, 1, 3], the dislocation climb is only due to the vacancy diffusion and high temperatures are considered. The role of SIAs on climb is neglected compared to vacancies, since the atomic fraction of SIAs at high temperature remains low compared to the one of vacancies. Under irradiation, vacancies and SIAs are created in higher quantities and both contribute to the dislocation climb. Dislocation climb can occur at low temperatures and allows to understand irradiation creep [63, 64, 65, 66]. In section 3.2 we present a new PF method based on the previous ones [2, 1, 3] to describe the dislocation climb in a single crystal. This new model includes the effects of both PDs (vacancies and SIAs) on climb and is adapted to deal with low PD atomic fractions which are common at low temperatures. The model allows to simulate the evolution of interstitial/vacancy dislocation loops under irradiation.

3.2 PF methodology

The evolution of one dislocation loop by the absorption/emission of PDs as shown in Fig. 3.2 is investigated in a single crystal. The system is assumed free of any applied stress. As done in section 2.2, we define successively the order parameters, the total free energy and the evolution equations.

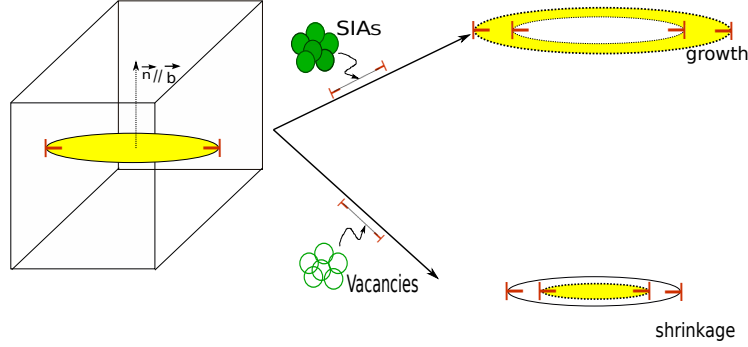


Figure 3.2: Schematics illustrating the evolution of an interstitial dislocation loop by absorption of PD.

3.2.1 Order parameters

The necessary order parameters to describe the system evolution are the following:

- The atomic fraction of vacancies X_v and SIAs X_i inside the matrix.
- The fields η_v^l and η_i^l which are related respectively to the atomic fraction of vacancies and SIAs absorbed or emitted by the loop.
- The order parameter η^l : classically, in PF methods a dislocation loop is identified on the boundary between a platelet of thickness d (see Fig. 2.2), within which the plastic field $\eta^l = 1$ and the matrix within which $\eta^l = 0$. Dislocation loops according to their types (interstitial or vacancy) grow or shrink through the net absorption or emission of SIAs or vacancies. Then, the order parameter η^l defined as follows:

$$\eta^l = \frac{1}{X^*} sg(l)(\eta_i^l - \eta_v^l) \quad (3.9)$$

is the [plastic field](#) associated with the loop. $sg(l) = 1$ for interstitial loop and -1 for vacancy loop, and $X^* = b/d$ is the number of PDs required for a unitary climb process, b is the length of the Burgers vector.

3.2.2 Energy of the system

The total free energy of the system F is given by the sum of three contributions, namely the chemical energy of PDs F_{chem} , the dislocation core energy F_{core} and the elastic energy F_{el} :

$$F(X_d, \eta^l) = F_{chem}(X_d) + F_{core}(\eta^l) + F_{el}(X_d, \eta^l) \quad (3.10)$$

Chemical free energy

The chemical free energy is determined in the limit of [dilute solution](#) as in section [2.2](#) and is given by [\[10\]](#):

$$F_{chem}(X_d) = \frac{1}{V_{at}} \sum_d \int_V E_f^d X_d + k_B T [X_d \ln X_d + (1 - X_d) \ln(1 - X_d)] dV \quad (3.11)$$

Dislocation core energy

The dislocation core energy is expressed as the sum of a crystalline and a gradient energy term, a simple double-well function is used for the crystalline energy:

$$F_{core}(\eta^l) = F_{cry} + F_{grad} = \int_V H(\eta^l)^2 (1 - \eta^l)^2 + \frac{\gamma}{2} |\mathbf{n} \wedge \nabla \eta^l|^2 dV \quad (3.12)$$

with $\mathbf{n}$ the normal to the habit plane of the loop. The coefficients H (J/m³) and γ (J/m) allow to control the dislocation core energy E_{core} and width w through the following expressions:

$$w = \sqrt{\frac{8\gamma}{H}}, \quad E_{core} = b \sqrt{\frac{H\gamma}{12}} \quad (3.13)$$

The gradient of η^l is projected on the habit plane of the loop to eliminate any energy contribution along $\mathbf{n}$. This expression of the dislocation core energy is limited to a [single loop](#) and a [single slip plane](#). To simulate a system with multiple dislocations and slip planes, the formulation proposed by Wang et al. [\[49\]](#) and successfully applied can be used.

Elastic energy

The elastic energy is calculated in the same way as in section [2.2](#):

$$F_{el}(X_d, \eta^l) = \frac{1}{2} \int_V C_{ijkl} [\varepsilon_{ij}(\mathbf{r}) - \varepsilon_{ij}^{0,tot}(\mathbf{r})] [\varepsilon_{kl}(\mathbf{r}) - \varepsilon_{kl}^{0,tot}(\mathbf{r})] dV \quad (3.14)$$

The total eigenstrain $\varepsilon_{ij}^{0,tot}$ is given by:

$$\varepsilon_{ij}^{0,tot}(\mathbf{r}) = \sum_d \varepsilon_{ij}^{0,X_d} X_d(\mathbf{r}) + \varepsilon_{ij}^{0,\eta^l} f(\eta^l(\mathbf{r})) \quad (3.15)$$

where ε_{ij}^{0,X_d} is the tensor of the Vegard's coefficients of PD d and $\varepsilon_{ij}^{0,\eta^l}$ the eigenstrain of the loop given by (Eq. [2.52](#)):

$$\varepsilon_{ij}^{0,\eta^l} = \frac{b_i n_j + b_j n_i}{2d} \quad (3.16)$$

Instead of η in Eq. [2.24](#), an [interpolation function](#) $f(\eta^l)$ defined as $f(\eta^l) = \eta^l$ and $f'(\eta^l) = 0$ if η^l is an integer i.e. in the bulk and inside the loop, is used in Eq. [3.15](#). The derivative of $f(\eta^l)$ must be zero in the bulk and inside the loop to ensure that the elastic contribution does not modify the energy minima in these regions [\[1, 3\]](#). A non-linear function which verifies the properties listed above is given by [\[78, 79\]](#):

$$f(\eta^l) = \eta^l - \frac{1}{2\pi} \sin(2\pi\eta^l) \quad (3.17)$$

The calculation of the total strain $\varepsilon_{ij}(\mathbf{r})$ remains the same as in section 2.2. The Fourier space is used to solve the mechanical equilibrium (Eq. 2.31) and to compute the elastic energy (Eq. 3.14).

3.2.3 Kinetic equations

As described in the existing models [1, 3], during the exchange of PD between the loop and the matrix, the fields X_d and η_d^l are not conserved, but the system evolves such that the total PD atomic fraction in the matrix and absorbed/emitted by the loop $\phi_d = X_d + \eta_d^l$ is conserved. The field ϕ_d is then a **conserved** parameter and is governed by a **Cahn-Hilliard**-type equation. Moreover, η_d^l is a **non-conserved** order parameter and follows the **Allen-Cahn** equation usually used in PF models to simulate dislocation dynamics. The evolution equations are written according to the driving forces deriving from the total energy $F(\phi_I, \phi_V, \eta_I^l, \eta_V^l)$:

$$\frac{\partial \phi_I}{\partial t} = \nabla \cdot [M^I \nabla \frac{\delta F(\phi_I, \phi_V, \eta_I^l, \eta_V^l)}{\delta \phi_I}] \quad (3.18)$$

$$\frac{\partial \phi_V}{\partial t} = \nabla \cdot [M^V \nabla \frac{\delta F(\phi_I, \phi_V, \eta_I^l, \eta_V^l)}{\delta \phi_V}] \quad (3.19)$$

$$\frac{\partial \eta_I}{\partial t} = -L_{\eta^I}^I \frac{\delta F(\phi_I, \phi_V, \eta_I^l, \eta_V^l)}{\delta \eta_I} \quad (3.20)$$

$$\frac{\partial \eta_V}{\partial t} = -L_{\eta^I}^V \frac{\delta F(\phi_I, \phi_V, \eta_I^l, \eta_V^l)}{\delta \eta_V} \quad (3.21)$$

where M^d is the mobility of the PD defined as:

$$M^d = \beta D^d X_d \quad (3.22)$$

$L_{\eta^I}^d$ denotes the coefficient that accounts for the kinetics of PD absorption/emission by the dislocation cores and can be chosen to reproduce quantitatively the climb rate of a jogged dislocation [3] as discussed in section 3.2.3.1. In our simulations, $L_{\eta^I}^d$ is **assumed proportional** to M^d in order to ensure numerical stability:

$$L_{\eta^I}^d = \zeta_{\eta^I}^d M^d \quad (3.23)$$

The link between the PF parameter $\zeta_{\eta^I}^d$ (consequently $L_{\eta^I}^d$) and the jog inter-spacing d_j (dislocation atomic scale property) is established in section 3.2.3.1. To write the evolution equations in function of the natural parameters $(X_I, X_V, \eta_I^l, \eta_V^l)$, it is necessary to make a variable change $F(\phi_I, \phi_V, \eta_I^l, \eta_V^l)$ to $F(X_I, X_V, \eta_I^l, \eta_V^l)$. The calculations are detailed in appendix B and allow to obtain the following contracted evolution equations:

$$\frac{\partial X_d}{\partial t} = \nabla \cdot [M^d \nabla (\mu_{chem}^d + \mu_{el}^d)] - \frac{\partial \eta_d^l}{\partial t} \quad (3.24)$$

$$\frac{\partial \eta_d^l}{\partial t} = -L_{\eta^I}^d \left[\frac{1}{X^*} sg(l) sg(d) (\mu_{core}^{\eta^I} + \mu_{el}^{\eta^I}) - (\mu_{chem}^d + \mu_{el}^d) \right] \quad (3.25)$$

where $sg(d) = 1$ for SIAs and -1 for vacancies. The expression of the driving forces μ_{chem}^d , μ_{el}^d , $\mu_{el}^{\eta^l}$ and $\mu_{core}^{\eta^l}$ are given in appendix B. The evolution equations 3.24 and 3.25 show the coupling between the PD diffusion and the dislocation motion through the absorption/emission term $\frac{\partial \eta_d^l}{\partial t}$.

The loop growth/shrinkage given by $\frac{\partial \eta_d^l}{\partial t}$ is then the result of the competition between the driving forces due to the dislocation core and the elastic energies ($\mu_{core}^{\eta^l} + \mu_{el}^{\eta^l}$) and the driving force ($\mu_{chem}^d + \mu_{el}^d$) so called osmotic force.

3.2.3.1 Determination of the coefficient $L_{\eta^l}^d$

As mentioned above, $L_{\eta^l}^d$ is a coefficient which controls the kinetics of PD absorption/emission by the dislocation cores. To access the coefficient $L_{\eta^l}^d$, Geslin et al. [3] proposed to compare the climb velocity established analytically and the one obtained by the PF method. The analytical solution of the climb rate is obtained by solving the vacancy diffusion for the bulk and dislocation core (cylindrical geometry see Fig. 3.1) [3]:

$$v = \frac{\frac{2\pi X_{eq} D_B^V}{b} \left[\frac{X(R)}{X_{eq}} - \exp(\beta V_{at}\sigma) \right]}{\ln(R/r_0) + \frac{l_B^2}{r_0^2} [1 + 2\alpha^2 (\frac{d_j}{2\alpha l_C} \coth \frac{d_j}{2\alpha l_C} - 1)]} \quad (3.26)$$

with

$$l_C^2 = \frac{D_C^V r_0}{a\nu} \exp(\beta E_{C-B}), \quad l_B^2 = \frac{D_B^V r_0}{a\nu} \exp(\beta E_{B-C}), \quad \alpha^2 = \frac{l_B^2 + r_0^2 \ln(R/r_0)}{2l_B^2} \quad (3.27)$$

where D_B^V and D_C^V are respectively the vacancy diffusion coefficient in the bulk and in the core, E_{B-C} and E_{C-B} are respectively the exchange energy barriers from the bulk to the core and from the core to the bulk. ν is the Debye frequency, a the interatomic distance and d_j the average distance between jogs. The climb rate in the PF model can be determined by two methods. The vacancy fraction is considered quasistatic and the field η^l is assumed to conserve its shape during climb. The first method consists in multiplying Eq. B.13 by the derivative of η^l and integrating this equation in the vicinity of the dislocation core ($\mathcal{D} = w \times b$) where the vacancy fraction X_V is assumed constant and equal to $X(r_0)$. This leads to the following climb rate [3]:

$$v_{PF} = \frac{3w}{2} L_{\eta^l}^d \left[\frac{1}{V_{at}\beta} \ln\left(\frac{X(r_0)}{X_{eq}}\right) - \sigma \right] \quad (3.28)$$

The second PF expression of the climb rate is obtained by integrating the vacancy flow arriving on dislocation as described in section 3.1:

$$v_{PF} = \frac{2\pi X_{eq} D_B^V}{b \ln(R/r_0)} \left[\frac{X(R)}{X_{eq}} - \frac{X(r_0)}{X_{eq}} \right] \quad (3.29)$$

Expressions 3.28 and 3.29 are equal and allow to fix $X(r_0)$:

$$\frac{X(r_0)}{X_{eq}} = \frac{\exp[W(\frac{\Gamma}{\zeta_{\eta^l}^V b^2} \frac{X(R)}{X_{eq}} \exp[\frac{\Gamma}{\zeta_{\eta^l}^V b^2} - \beta V_{at} \sigma])]}{\exp[\frac{\Gamma}{\zeta_{\eta^l}^V b^2} - \beta V_{at} \sigma]} \quad (3.30)$$

with

$$\Gamma = \frac{4\pi b}{3w \ln(R/r_0)} \quad (3.31)$$

$\zeta_{\eta^l}^V$ is related to $L_{\eta^l}^V$ through the relation (see Eq. 3.23 for $X_V = X(r_0)$):

$$L_{\eta^l}^V = \beta V_{at} D_B^V \zeta_{\eta^l}^V X(r_0) \quad (3.32)$$

W is the Lambert function which is the reciprocal function of $f(x) = xe^x$ ($W(xe^x)=x$). The PF climb velocity is then given by:

$$v_{PF} = \frac{2\pi X_{eq} D_B^V}{b \ln(R/r_0)} \left[\frac{X(R)}{X_{eq}} - \frac{\exp[W(\frac{\Gamma}{\zeta_{\eta^l}^V b^2} \frac{X(R)}{X_{eq}} \exp[\frac{\Gamma}{\zeta_{\eta^l}^V b^2} - \beta V_{at} \sigma])]}{\exp[\frac{\Gamma}{\zeta_{\eta^l}^V b^2} - \beta V_{at} \sigma]} \right] \quad (3.33)$$

Identification of Eqs. 3.26 and 3.33 allows to give a link between the coefficient $\zeta_{\eta^l}^V$ (respectively the coefficient $L_{\eta^l}^V$) and the jog inter-spacing d_j . The expression of Eq. 3.33 differs from that of [80] due to the assumption that $L_{\eta^l}^V$ is proportional to X_d in our approach.

3.2.3.2 Irradiation conditions

The irradiation conditions are reproduced by adding an effective source term of PD K_0^d in the evolution equation of X_d . The PDs recombination is neglected. Edge dislocations are known to be biased sinks (see section 2.3.3.1). Thus in the stationary state, a net flow of one type of PD is obtained near the dislocation cores as shown in section 3.2.5 which leads to the loop evolution. To simulate the presence of [another sink](#) noted s , we introduce in the PD diffusion equation an additional absorption term. The sink is assumed perfect, not evolving by the absorption of PD and immobile. The absorption term is thus defined using the expression of Eq. 2.39:

$$J_{s,d}^{abs}(\mathbf{r}, t) = \lambda_s(\mathbf{r}) \lambda_{eff} (X_d(\mathbf{r}, t) - X_d^s) \quad (3.34)$$

Eqs. 3.24 and 3.25 are solved in their dimensionless form using the following dimensionless parameters (noted with $*$):

$$\left\{ \begin{array}{l} F^* = F/H, \quad \mu^* = \mu/V_{at}H \\ D^{d,*} = D^d/D^0, \quad \zeta_{\eta^l}^{d,*} = \beta H V_{at} a_0^2 \zeta_{\eta^l}^d \\ \nabla^* = a_0 \nabla, \quad \gamma^* = \gamma/(H a_0^2) \\ t^{d,*} = t^d/t_0 \\ K_0^{d,*} = K_0^d t_0^d, \quad J_{s,d}^{abs,*} = t_0^d J_{s,d}^{abs} \end{array} \right. \quad (3.35)$$

where t_0 is the reference time which corresponds to the minimum of t_0^d , t_0^d is the characteristic time associated to the PD diffusion defined in section 3.2.4. The dimensionless evolution equations are then the following:

$$\frac{\partial X_d}{\partial t^{d,*}} = \beta H V_{at} \nabla^* \cdot [D^{d,*} X_d \nabla^* (\mu_{chem}^{d,*} + \mu_{el}^{d,*})] - \frac{\partial \eta_d^l}{\partial t^{d,*}} + K_0^{d,*} - J_{s,d}^{abs,*} \quad (3.36)$$

$$\frac{\partial \eta_d^l}{\partial t^{d,*}} = -\zeta_{\eta^l}^{d,*} D^{d,*} X_d \left[\frac{1}{X^*} sg(l) sg(d) (\mu_{core}^{\eta^l,*} + \mu_{el}^{\eta^l,*}) - (\mu_{chem}^{d,*} + \mu_{el}^{d,*}) \right] \quad (3.37)$$

3.2.4 Numerical scheme and multi-time step algorithm

A finite difference scheme is used for the spatial discretization of equations 3.36 and 3.37. For the temporal discretization, an explicit Euler scheme is used as defined in section A. Generally, the PD diffusion is much faster than the climb process. In bcc iron for example, Duparc et al. [81] have measured experimentally the dislocation loop growth rate under irradiation. At 700 K, the loop growth rate is of the order of $v_{\eta^l} \simeq 10^{-10}$ m/s. The diffusion coefficients of PDs are $D_I = 1.1 \times 10^{-8}$ m²/s and $D_V = 7.2 \times 10^{-11}$ m²/s. For a given time of $t = 100$ s, we have the diffusion length $l^I = \sqrt{D_I t} = 1.04 \times 10^{-3}$ m, $l^V = \sqrt{D_V t} = 8.48 \times 10^{-5}$ m and $v_{\eta^l} t = 10^{-8}$ m. These values show that $\sqrt{D_I t} > \sqrt{D_V t} \gg v_{\eta^l} t$ which means both PDs diffuse faster than the loop growth process and SIAs diffuse faster than vacancies. Usually, the evolution equations 3.36 and 3.37 are solved simultaneously using a single time step δt chosen such as $\delta t = \min(\delta t^I, \delta t^V, \delta t^{\eta^l})$. δt^d and δt^{η^l} are determined such that the following stability criteria are verified:

$$\frac{\delta t^d}{t_0^d} < \frac{1}{2N_{dim}} \quad (3.38)$$

$$\frac{\delta t^{\eta^l}}{t_0^{\eta^l}} < 1 \quad (3.39)$$

where N_{dim} is the system dimension, t_0^d and $t_0^{\eta^l}$ the characteristic time associated respectively to the PD diffusion and the dislocation motion:

$$t_0^d = a_0^2 / D^d, \quad t_0^{\eta^l} = a_0 / v_{\eta^l} \quad (3.40)$$

These stability criteria are based on the fact that the PD diffusion length l^d and the length of a climb process l^{η^l} ($= v_{\eta^l} \delta t^{\eta^l}$) must be smaller than the grid spacing a_0 during one time step. With the Fe parameters given above, it can be seen that $\delta t^I < \delta t^V \ll \delta t^{\eta^l}$ for a grid spacing comparable to the nanometer. Thus, to reach the steady state and observe the loop evolution, a huge number of iterations at δt^I would be required. A similar problem has been encountered by Piochaud et al. [82] in the study of radiation induced segregation (RIS) near a planar sink. In this study, PD diffusion is much faster than solute diffusion. A multi-time step algorithm has been proposed in [82] to accelerate the convergence towards the steady state. This multi-time step algorithm is adapted to our study and can be described as follows. At a time t^* , all the system variables are supposed to be known. First, the PD evolution equations are integrated with $\delta t^{d,*}$ to reach the quasi-steady state,

for some given value of $\eta^l(t^*)$ (which is not at steady state). The convergence criterion on the PD evolution equations is given by:

$$\left| 1 - \frac{\bar{X}_d^{t^* + n_d \delta t^{d,*}}}{\bar{X}_d^{t^* + (n_d - 1) \delta t^{d,*}}} \right| < \epsilon \quad (3.41)$$

where n_d is the number of iterations needed to reach the quasi-steady state, $\bar{X}_d$ the average value of the PD atomic fraction in the system and ϵ a constant set at 10^{-7} . During this stage, all the properties depending on X_d are reevaluated at each time step $\delta t^{d,*}$. In the second stage, the evolution equation of η^l is integrated with the time step $\delta t^{\eta^l,*}$. The field $X_d^{t^* + \delta t^{\eta^l,*}}$ is simply equal to $X_d^{t^* + n_d \delta t^{d,*}}$ at the end of the second stage. These stages are then repeated. Fig. 3.3 illustrates the multi-time step algorithm.

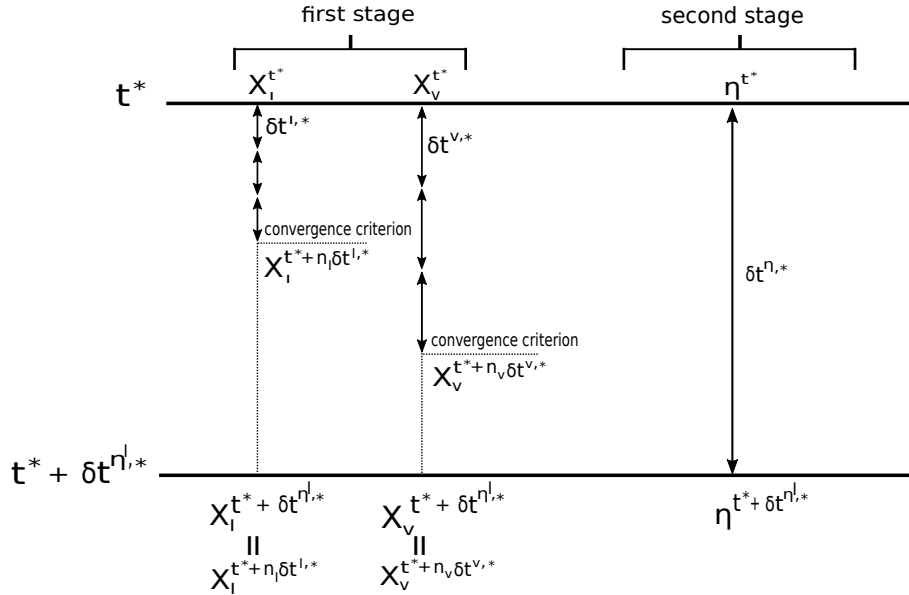


Figure 3.3: Schematic representation of the multi-time step algorithm.

3.2.5 Analytical expressions of the climb velocity

The determination of the dislocation climb velocity in the case of supersaturation or under applied stress requires the resolution of the PD diffusion equation as mentioned in section 3.1. Under irradiation, the climb rate can be calculated easily. At steady state, we have:

$$\frac{\partial \bar{X}_d}{\partial t} = -\frac{\partial \bar{\eta}_d^l}{\partial t} - \bar{J}_{s,d}^{abs} + K_0^d = 0 \quad (3.42)$$

which implies:

$$\frac{\partial \bar{\eta}_d^l}{\partial t} = -\bar{J}_{s,d}^{abs} + K_0^d \quad (3.43)$$

$\bar{J}_{s,d}^{abs}$ can be written as (see Eq. 2.48):

$$\overline{J_{s,d}^{abs}} = k_{s,d}^2 D^d (\bar{X}_d - X_d^s) \quad (3.44)$$

where $k_{s,d}^2$ is the sink strength of the sink s for PD d , X_d^s the atomic fraction of PD at the sink s and $\bar{X}_d$ the average atomic fraction of PD in the system. The loop evolution is given by η^l which is related to η_d^l through Eq. 3.9. Then:

$$\frac{\partial \bar{\eta}^l}{\partial t} = \frac{1}{X^*} sg(l) [(k_{s,v}^2 D^v (\bar{X}_v - X_v^s) - k_{s,i}^2 D^i (\bar{X}_i - X_i^s)) + (K_0^I - K_0^V)] \quad (3.45)$$

For a given 2D edge dislocation dipole, the average value of η^l can be seen as the dipole volume fraction in the system:

$$\bar{\eta}^l_{dipole} = \frac{V_{dipole}}{V} \quad (3.46)$$

where V_{dipole} and V are respectively the representative volume of the dipole and the system volume. V_{dipole} is given by:

$$V_{dipole} = 2Ra_0^2 \quad (3.47)$$

with R the half of the distance between the dislocations. Then we have:

$$\frac{\partial \bar{\eta}^l}{\partial t} = \frac{2a_0^2}{V} \frac{\partial R}{\partial t} \quad (3.48)$$

By combining Eq. 3.48 and Eq. 3.45 we obtain:

$$\frac{2a_0^2}{V} \frac{\partial R}{\partial t} = \frac{1}{X^*} sg(l) [(k_{s,v}^2 D^v (\bar{X}_v - X_v^s) - k_{s,i}^2 D^i (\bar{X}_i - X_i^s)) + (K_0^I - K_0^V)] \quad (3.49)$$

The dislocation climb velocity $v_{\eta^l} = \frac{\partial R}{\partial t}$ is then given by:

$$v_{\eta^l} = \frac{V}{2X^*a_0^2} sg(l) [(k_{s,v}^2 D^v (\bar{X}_v - X_v^s) - k_{s,i}^2 D^i (\bar{X}_i - X_i^s)) + (K_0^I - K_0^V)] \quad (3.50)$$

Eq. 3.50 shows that, to obtain a loop evolution at steady state, two types of simulation are possible:

- Simulation type 1: the system is assumed to be free of any other sinks ($\overline{J_{s,d}^{abs}} = 0$) and the PD effective generation rates are chosen non equal $K_0^I \neq K_0^V$:

$$v_{\eta^l} = \frac{V}{2X^*a_0^2} sg(l) (K_0^I - K_0^V) \quad (3.51)$$

In this case, the climb rate is simply controlled by the PD effective generation rates for a given system volume V .

- Simulation type 2: PDs are created at the same generation rate K_0 and the presence of another sink allows to obtain a loop evolution (which is more realistic):

$$v_{\eta^I} = \frac{V}{2X^*a_0^2} sg(l) [(k_{s,v}^2 D^V (\bar{X}_V - X_V^s) - k_{s,I}^2 D^I (\bar{X}_I - X_I^s))] \quad (3.52)$$

It can be seen that the climb rate depends on the PD diffusion coefficients, the PD average atomic fraction in the system and the sink strength of the sink s , for a given system volume V . The average atomic fraction $\bar{X}_d$ can be estimated assuming that $\bar{X}_d$ is not modified by the dislocation motion. The approximation of static sink can be used for dislocations in comparison to the PD diffusion:

$$\frac{\partial \bar{\eta}_d^I}{\partial t} = k_{dislo,d}^2 D^d (\bar{X}_d - X_d^{dislo}) \quad (3.53)$$

with $k_{dislo,d}^2$ the sink strength of dislocations and X_d^{dislo} the atomic fraction of PD at the dislocation cores. Eq. 3.42 becomes:

$$k_{dislo,d}^2 D^d (\bar{X}_d - X_d^{dislo}) + k_{s,d}^2 D^d (\bar{X}_d - X_d^s) = K_0 \quad (3.54)$$

$\bar{X}_d$ is then given as follows:

$$\bar{X}_d = \frac{K_0 + D^d (k_{dislo,d}^2 X_d^{dislo} + k_{s,d}^2 X_d^s)}{D^d (k_{dislo,d}^2 + k_{s,d}^2)} \quad (3.55)$$

Thus, the dislocation climb rate at the stationary state will depend also on the sink strength of dislocations. For X_d^{dislo} and X_d^s close to zero, $\bar{X}_d$ is reduced to:

$$\bar{X}_d = \frac{K_0}{D^d (k_{dislo,d}^2 + k_{s,d}^2)} \quad (3.56)$$

The climb rate is then given by the following simplified expression:

$$v_{\eta^I} = \frac{VK_0}{2X^*a_0^2} sg(l) \left[\frac{k_{s,v}^2}{k_{dislo,v}^2 + k_{s,v}^2} - \frac{k_{s,I}^2}{k_{dislo,I}^2 + k_{s,I}^2} \right] \quad (3.57)$$

Usually, dislocations absorb more SIAs than vacancies ($k_{dislo,I}^2 > k_{dislo,v}^2$). In the case where s is a neutral sink ($k_{s,I}^2 = k_{s,v}^2 = k_s^2$), Eq. 3.57 becomes:

$$v_{\eta} = \frac{VK_0}{2X^*a_0^2} sg(l) \left[\frac{k_s^2}{k_{dislo,v}^2 + k_s^2} - \frac{k_s^2}{k_{dislo,I}^2 + k_s^2} \right] \quad (3.58)$$

Eq. 3.58 shows that a growth is obtained in the case of an interstitial loop. In figure 3.4 the evolution of the climb rate given by Eq. 3.58 is illustrated for a given system volume V of $256 \times 512 a_0^3$ with $a_0 = 0.283\text{nm}$ (bcc iron lattice parameter) which corresponds to a dislocation density of $\rho_{dislo} = 1.905 \times 10^{14} \text{m}^{-2}$ ($\rho_{dislo} = \frac{2a_0}{V}$). K_0 was set at $10^{-5} \text{dpa.s}^{-1}$ and the temperature at 700 K. The sink strength of dislocations was calculated using the solution of Rauh and Simon [32] (see table 2.1) and the one of planar sink by $k_s^2 = 12/d^2$ where d the interplanar spacing. Fig. 3.4 shows an increase of the climb rate with the interplanar spacing d .

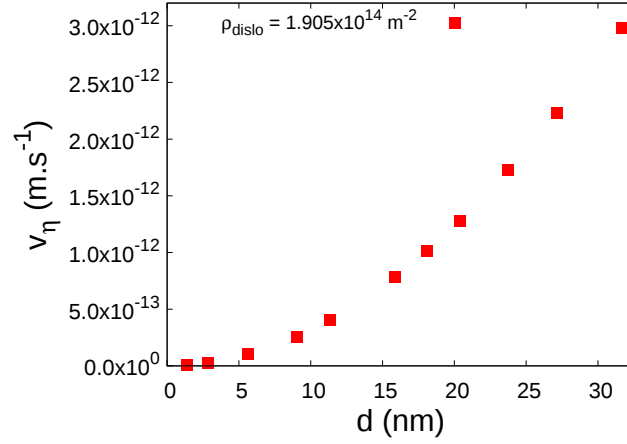


Figure 3.4: Evolution of the climb rate of dislocations (see Eq. 3.58) as a function of the interplanar spacing d in the case of system containing a dipole of edge dislocations and a planar sink (simulation type 2) for a dislocation density of $\rho_{dislo} = 1.905 \times 10^{14} \text{m}^{-2}$. ρ_{dislo} is related to the system volume by the relation $\rho_{dislo} = \frac{2a_0}{V}$.

3.3 Validation and limitations of the model

The model was tested before the application to a real material to verify its validity and limitations. For simplicity, subscript l has been suppressed in the notation of η . The growth of a prismatic interstitial loop by a net absorption of SIAs is simulated. The loop is represented by a dipole of edge dislocations as illustrated in Fig. 3.5-a). The dislocations

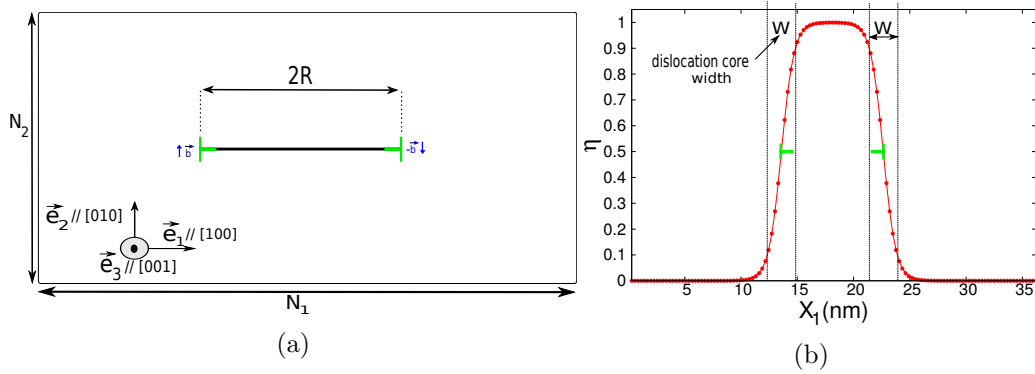


Figure 3.5: a) 2D simulation mimicking an interstitial dislocation loop and b) initial profile of η along the dipole.

are located initially at (17.4 nm, 9.6 nm) and (24 nm, 9.6 nm). The necessary parameters for the simulations are given in table 3.1. The order parameter η was initialized using Eq. 2.53 and schematized in Fig. 3.5-b). The equilibrium atomic fraction of PD was set close to zero ($X_d^{eq} = 0$). The grid spacing a_0 and the platelet thickness d were taken equal to

the length of the Burgers vector b .

Table 3.1: Necessary parameters for the PF climb model validation.

T	700 K
b, a_0	0.3 nm
dislocation core energy	$[1:10]$ eV.Å ⁻¹
dislocation core width	2.4 nm
domain size	38.4×19.2 nm ² (128×64 cells)
initial loop radius R_0	4.8 nm
Shear modulus μ	33 GPa
Poisson ratio ν	0.33
Atomic volume V_{at}	2.3×10^{-29} m ³
D_I, D_V	10^{-15} m ² .s ⁻¹

We first tested the model without elastic interactions.

3.3.1 Without elastic interactions

The simulations of type 1 ($K_0^I > K_0^V$) were performed firstly using the parameters of table 3.1 with $\zeta_\eta^{d,*} = 1$. The PD effective generation rates were $K_0^I = 4.45 \times 10^{-4}$ s⁻¹ and $K_0^V = 3.45 \times 10^{-4}$ s⁻¹ which corresponds to an analytical climb rate of $v_\eta = 1.23 \times 10^{-10}$ m.s⁻¹ (see Eq. 3.51). The average atomic fractions of PDs are plotted in Fig. 3.6 and do not reach any steady-state value, contrary to what is expected. The PD atomic fraction

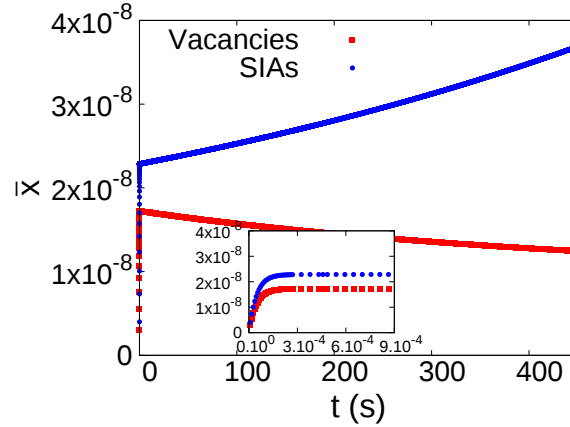


Figure 3.6: Evolution of the average atomic fraction $\bar{X}$ of PD during simulation type 1 without elastic interactions.

maps and the profile of η at $t = 450$ s are represented in Fig. 3.7. The PD atomic fraction maps show a bad sink behavior of dislocation cores. Especially, an enrichment is observed at dislocation cores for vacancies (see Fig. 3.7-b). Moreover, there is a non physical enrichment (respectively depletion) of SIAs (respectively vacancies) in the habit

plane of the loop. The field η varies in the bulk and inside the loop as shown in Fig. 3.7-c) and adopts values different from 0 in the bulk and 1 inside the loop which explains the bad sink behavior. The examination of the evolution equation of η (see Eq. 3.25) shows that

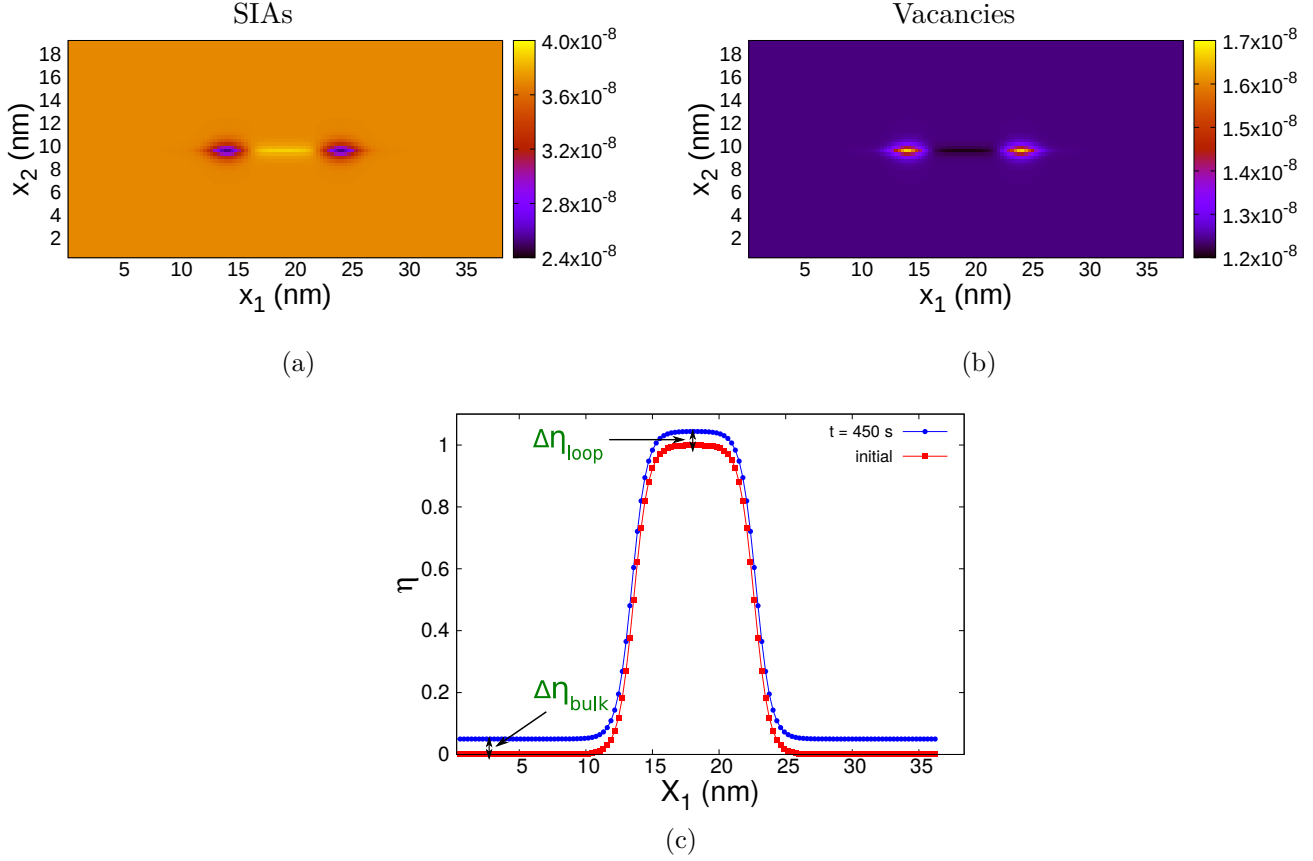


Figure 3.7: Atomic fraction maps of a) SIAs and b) vacancies, and c) profile of η in the habit plane ($x_2 = 9.6$ nm) at $t = 450$ s in the case of simulation type 1 without elastic interactions.

this particular evolution of η is due to an [unphysical osmotic force](#) contribution far from the dislocation cores. Thus, the field η does not remain at its value 0 or 1 in the bulk and inside the loop. To overcome this undesired effect, we introduce a [shape function](#) $\lambda(\eta)$ in front of the osmotic force to ensure its value is zero outside the dislocation cores:

$$\lambda(\eta) = \begin{cases} 1 & \text{inside the core region} \\ 0 & \text{outside} \end{cases} \quad (3.59)$$

We made the choice to delimit the dislocation core region by $0.1 \leq \eta \leq 0.9$ as illustrated in Fig. 3.8. The evolution equations are rewritten as follows:

$$\frac{\partial X_d}{\partial t} = \nabla \cdot [M^d \nabla (\mu_{chem}^d + \mu_{el}^d)] - \frac{\partial \eta_d}{\partial t} + K_0^d - J_{s,d}^{abs} \quad (3.60)$$

$$\frac{\partial \eta_d}{\partial t} = -L_\eta^d \left[\frac{1}{X^*} sg(l) sg(d) (\mu_{core}^\eta + \mu_{el}^\eta) - \lambda(\eta) (\mu_{chem}^d + \mu_{el}^d) \right] \quad (3.61)$$

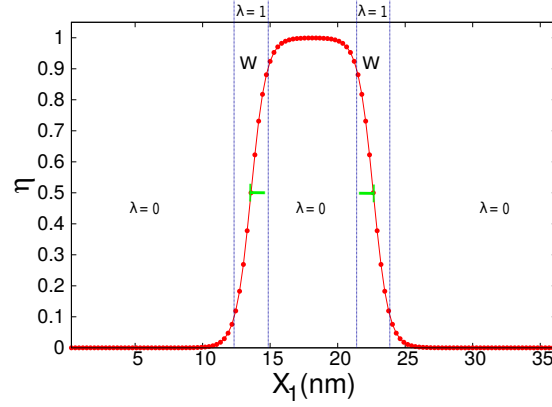


Figure 3.8: Profile of η and delimitation of the dislocation core region given by the shape function λ .

The simulations were performed with this new formulation by keeping the same parameters. The atomic fraction maps of PD and the profile of η at steady state are plotted in Fig. 3.9. No shift from the values 0 and 1 in the bulk and inside the loop is observed on

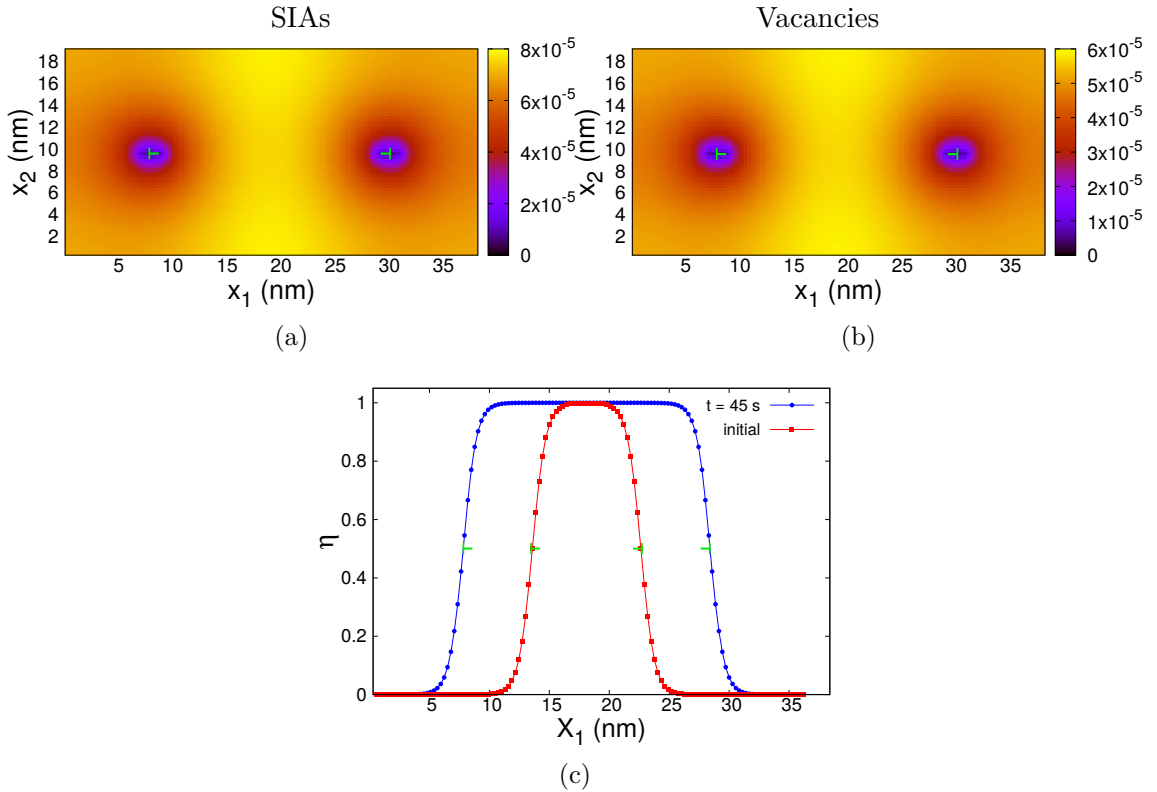


Figure 3.9: Atomic fraction maps of a) SIAs and b) vacancies, and c) profile of η in the habit plane ($x_2 = 9.6$ nm) at $t = 45$ s, with the shape function $\lambda(\eta)$ in front of the osmotic force $(\mu_{chem}^d + \mu_{el}^d)$ (simulation type 1 without elastic interactions).

the profile of η and the atomic fraction maps show a good sink behavior of the dislocation cores. The average value of η is represented in Fig. 3.10 and its evolution is linear with time. The climb rate v_η is deduced from the slope of the linear curve of Fig. 3.10 and

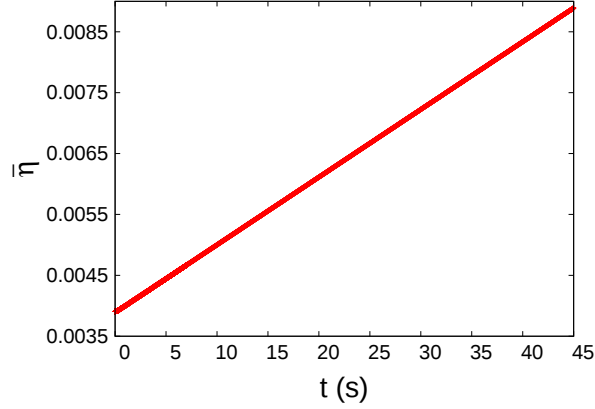


Figure 3.10: Evolution of $\bar{\eta}$ (simulation type 1, no elasticity) as a function of time.

is equal to $1.33 \times 10^{-10} \text{m.s}^{-1}$. This value is in good agreement with the one predicted analytically $v_\eta = 1.23 \times 10^{-10} \text{m.s}^{-1}$ and allows to validate our model.

A shape function in front of the osmotic force (see Eq. 3.61) is then necessary to ensure that the dislocation climb occurs due to the osmotic force only at dislocation cores. It must be noticed that this shape function is an ad hoc function introduced in the model, and does not come from the variational derivation of the PF model described in section 3.2.3. A more physical approach could focus on an alternative formulation of the free energy F allowing to introduce a counterpart of this shape function in the kinetic equations.

3.3.1.1 Influence of the coefficient ζ_η^d (simulation type 1)

The influence of the coefficient ζ_η^d (respectively L_η^d , see Eq. 3.23) has been investigated by varying the dimensionless coefficient $\zeta_\eta^{d,*}$. The average atomic fraction of PD is plotted in Fig. 3.11 as a function of time for different values of $\zeta_\eta^{d,*}$. This figure shows a decrease of the average atomic fraction when the dimensionless coefficient $\zeta_\eta^{d,*}$ that accounts for the kinetics of PD absorption increases. Periodic oscillations are also observed on the evolution of the average atomic fraction of PD given in Fig. 3.11. These oscillations occur after each unitary climb process.

The profiles of the PD atomic fraction along the dipole given in Fig. 3.12 show that X_d tends to stay close to the equilibrium value ($X_d^{eq} \simeq 0$) in the vicinity of the dislocation cores when $\zeta_\eta^{d,*}$ is high. The analytical expression of the climb rate as a function of the jog inter-spacing d_j (see Eq. 3.26) has been plotted for different values of $\zeta_\eta^{d,*}$ in Fig. 3.13. To compute the climb rate given by Eq. 3.26, the value of $X(R)$ was necessary. $X(R)$ has

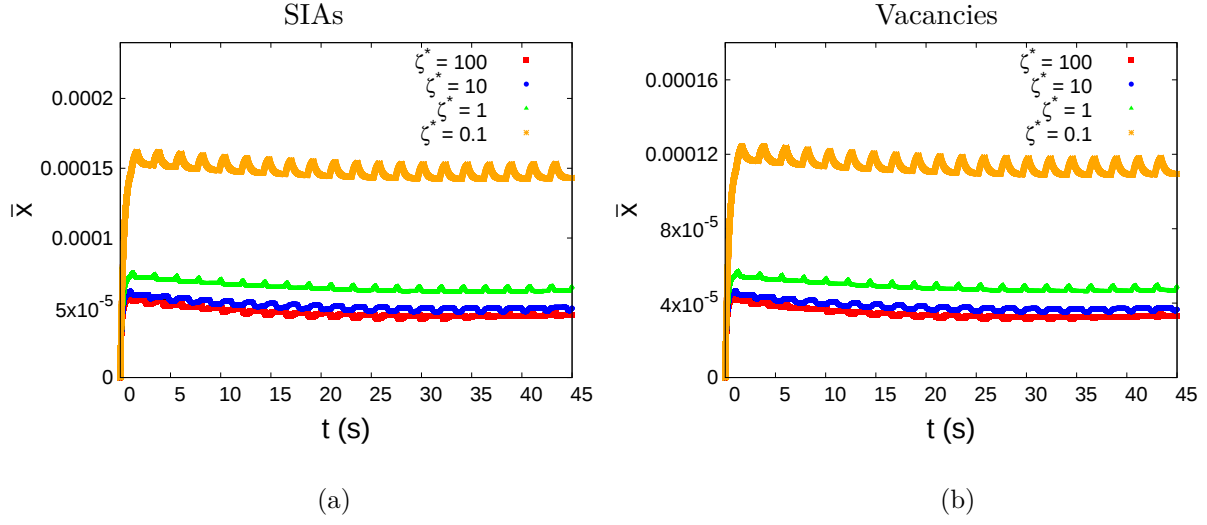


Figure 3.11: Average atomic fraction of a) SIA and b) vacancy as a function of time, without elastic interactions for different values of $\zeta_{\eta}^{d,*}$ in the case of simulation type 1.

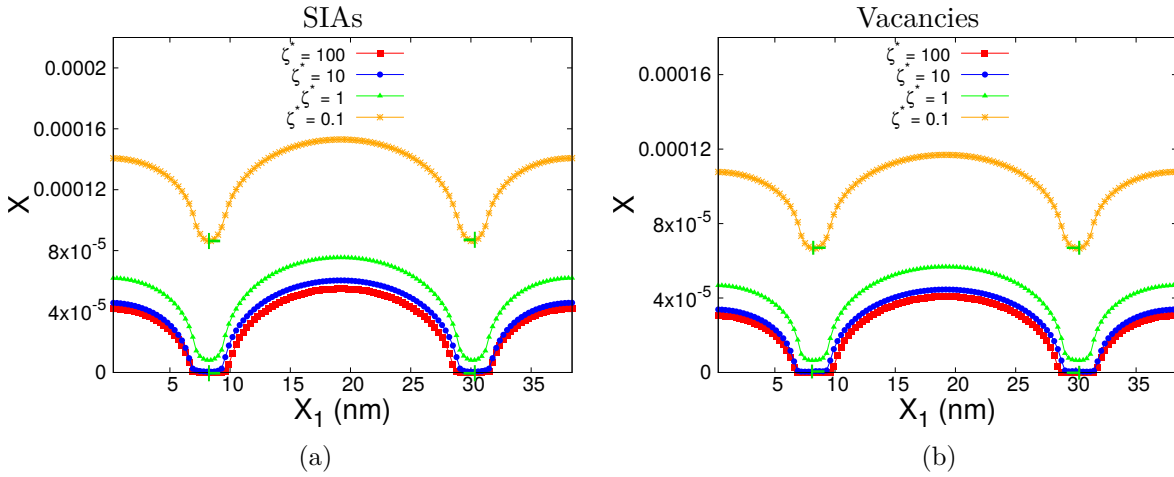


Figure 3.12: Atomic fraction profile in the habit plane ($x_2 = 9.6$ nm) of a) SIA b) vacancy at $t = 45$ s, without elastic interactions for different values of $\zeta_{\eta}^{d,*}$ in the case of simulation type 1.

been calculated using the solution of the PD fraction at steady state for cylindrical sinks given by [10]:

$$X_d(\mathbf{r}) = X_d(r_0) + \frac{K_0^d R^2}{2D^d} \left[\ln(r/r_0) - \frac{r^2 - r_0^2}{2R^2} \right] \quad (3.62)$$

As expressions 3.28 and 3.29 are equal, $X_d(r_0)$ has been determined using the solution of

$X(R)$:

$$X_d(r_0) = X_{eq}^d \frac{\exp[W(\frac{V_{at}\beta H\Gamma}{X_{eq}^d \zeta_\eta^{d,*}} \frac{K_0^d R^2}{2D^d} [\ln(R/r_0) - \frac{R^2 - r_0^2}{2R^2}] \exp(-\beta V_{at}\sigma))]}{\exp(-\beta V_{at}\sigma)} \quad (3.63)$$

where Γ is given by Eq. 3.31 and L_η^d (see Eq. 3.23) was substituted by $D^d \zeta_\eta^{d,*} X_d(r_0) / Hb^2$ in Eq. 3.28. The parameters $E_{C-B} = 0.4$ eV, $\nu = 9.3 \times 10^{13}$ s⁻¹ given in [3] have been considered to perform calculations. These parameters were necessary for the calculations and make it possible to get an idea of the climb rate value as a function of a given jog inter-spacing d_j . The core diffusion coefficient D_V^C was chosen higher than the bulk diffusion coefficient as in [3], $D_V^C = 100D_V^B$. Fig. 3.13 shows that, for each value of $\zeta_\eta^{d,*}$ is associated

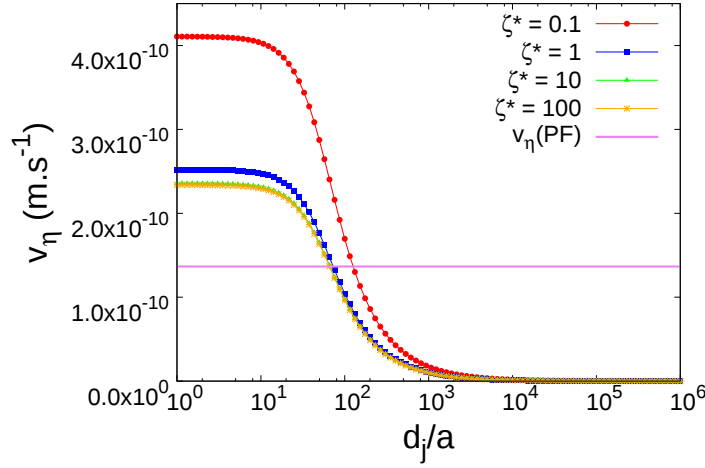


Figure 3.13: Climb rate v_η as a function of jog inter-spacing d_j (see Eq. 3.26) for different values of $\zeta_\eta^{d,*}$ ($E_{C-B} = 0.4$ eV, $\nu = 9.3 \times 10^{13}$ s⁻¹, $D_V^C = 100D_V^B$).

a jog inter-spacing d_j (respectively a jog density $\rho_j = 1/d_j$) by identification of the climb rate obtained by the PF simulations and given by the analytical solution (see Eq. 3.26). It can be seen that when $\zeta_\eta^{d,*}$ increases, the jog inter-spacing d_j decreases for the chosen PF climb rate. Thus, our model verifies that, for high values of $\zeta_\eta^{d,*}$ (consequently L_η^d) which is equivalent to a high jog density, the local equilibrium of PD around the dislocation cores is maintained [9, 69, 70]. The dislocation cores act as perfect sinks for $\zeta_\eta^{d,*} \gg 1$ ($L_\eta^d \gg 1$). The average value of η and the η profiles along the dipole are also represented in Fig. 3.14. It can be seen that the climb rate at quasi-steady state is the same for all the values of $\zeta_\eta^{d,*}$ used. Indeed the climb rate, in the case of a system free of any other sink (simulation type 1), depends only on the PD effective generation rates (see Eq. 3.51).

The effects of $\zeta_\eta^{d,*}$ (respectively jog inter-spacing) on the PD atomic fraction have been studied in the case of simulation type 1 (climb rate fixed). The results have shown the perfect sink behavior of dislocation cores when $\zeta_\eta^{d,*}$ increases (as equivalently when

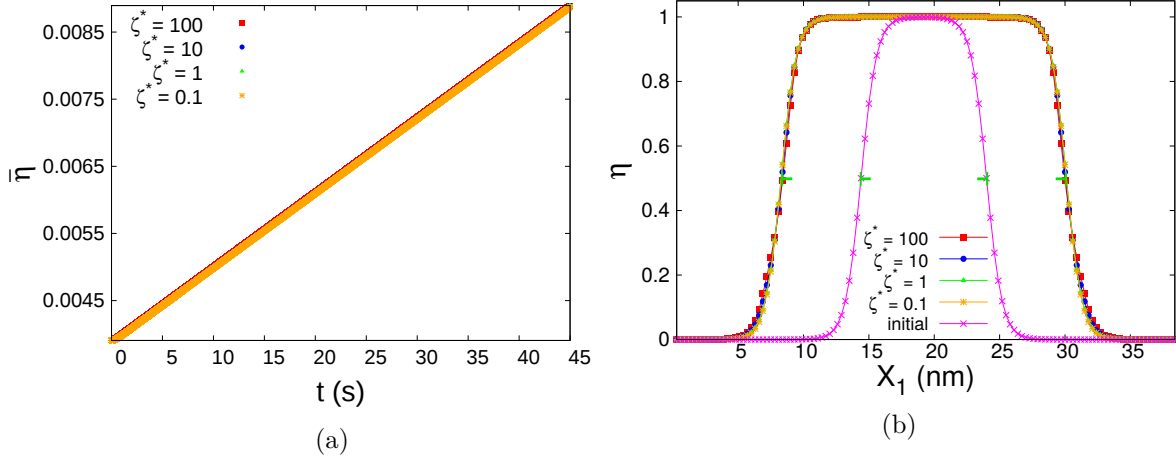


Figure 3.14: a) Average value of η and b) profile of η along the dipole ($x_2 = 9.6$ nm) at $t = 45$ s without elastic interactions for different values of ζ_η^* in the case of simulation type 1.

the jog density increase). To investigate the effects of the coefficient $\zeta_\eta^{d,*}$ on the climb velocity, simulations of type 2 have also been performed and are analyzed in section 3.3.2.

3.3.2 With elastic interactions

The simulations of type 1 described in section 3.3.1 are now performed by taking into account the elastic interactions with $\zeta_\eta^{d,*} = 100$ (perfect sink). The PD relaxation volumes are $\Omega_I = 1.2V_{at}$ and $\Omega_V = -0.6V_{at}$. The temporal evolution of $\bar{X}_d$ is plotted in Fig. 3.15 and the maps of X_d and the profile of η along the dipole are represented in Fig. 3.16 at $t = 31.5$ s. The PD atomic fraction map of SIAs shows an enrichment in the tension region of the dislocations and depletion in the compression region, which is expected, while the opposite behavior is observed in the case of vacancies. The absorption of SIAs by an interstitial loop leads to the loop growth while the vacancies absorption leads to the loop shrinkage. As the local distribution of X_d around the dislocation cores is heterogeneous due to elasticity, the evolution of η is also heterogeneous along the interface as shown in Fig. 3.16-c) due to the dependence of L_η^d with X_d (see Eqs. 3.22 and 3.23). The part of the interface located in the tension zone moves faster than the other one located in the compression zone. To conserve the shape of η during loop evolution, the average value of X_d is considered inside the core region to compute L_η^d (see Eq. 3.23) during the temporal integration of the evolution equation of η_d :

$$\eta_d(t + \delta t) = \eta_d(t) + \left[\frac{\partial \eta_d}{\partial t} \right]^{corr} \delta t + \tau \quad (3.64)$$

with

$$\left[\frac{\partial \eta_d}{\partial t} \right]^{corr} = -\zeta_\eta^{d,*} D^{d,*} X_d^{corr} \left[\frac{1}{X^*} sg(l) sg(d) (\mu_{core}^{\eta,*} + \mu_{el}^{\eta,*}) - \lambda (\mu_{chem}^{d,*} + \mu_{el}^{d,*}) \right] \quad (3.65)$$

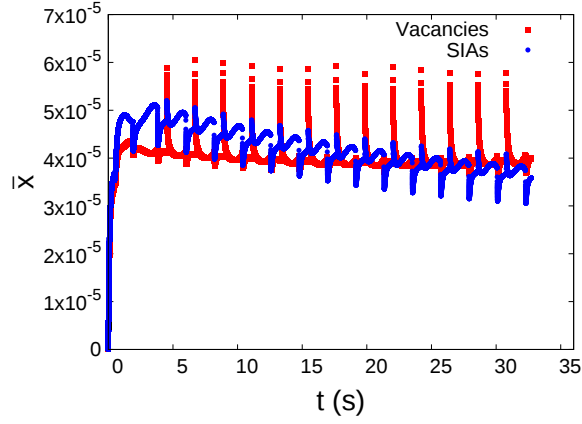


Figure 3.15: Evolution of the average atomic fraction $\bar{X}$ of PD during simulation of type 1 with elastic interactions.

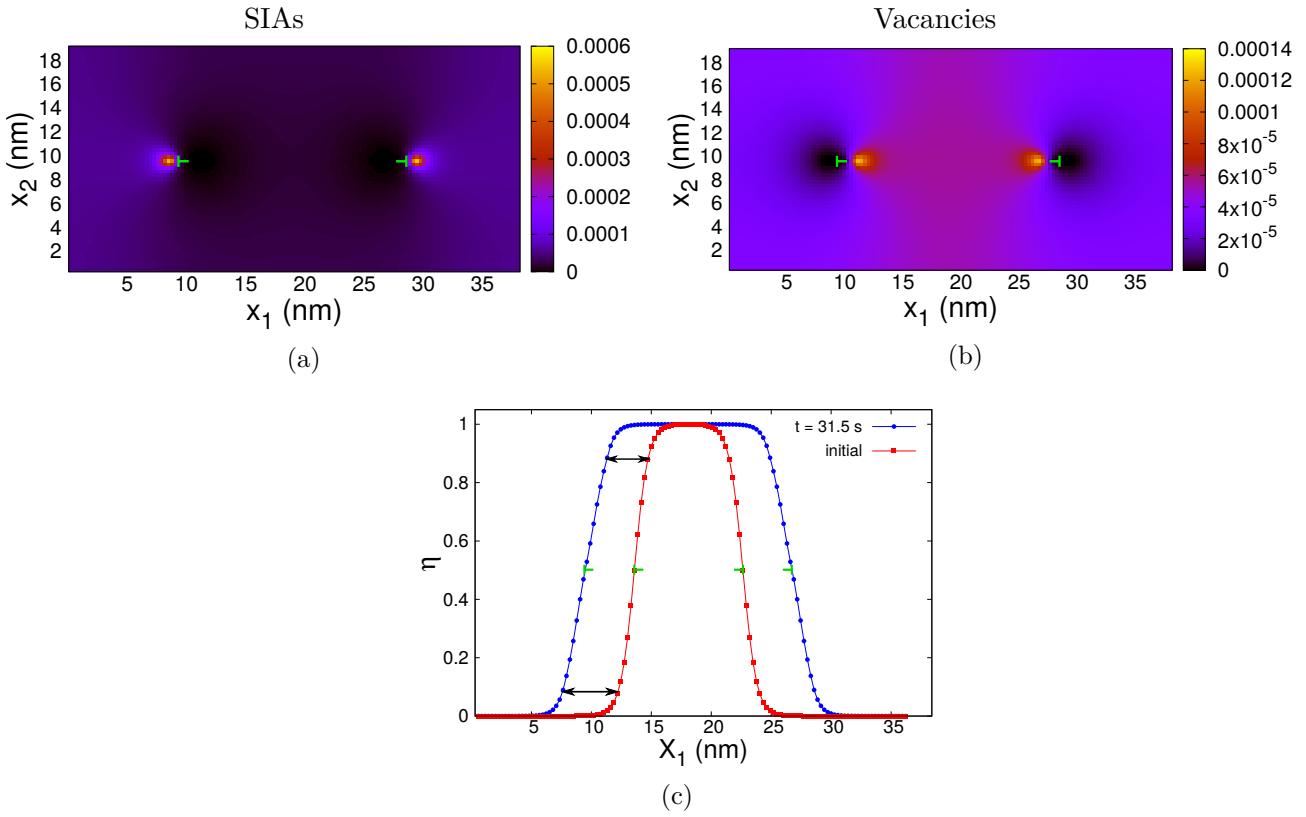


Figure 3.16: Atomic fraction maps of a) SIA and b) vacancies, and c) profile of η along the dipole ($x_2 = 9.6$ nm) at $t = 31.5$ s with elastic interactions in the case of simulation type 1.

$$X_d^{corr} = \begin{cases} \frac{\int_V \lambda X_d dV}{\int_V \lambda dV} & \text{inside the core region} \\ X_d & \text{outside} \end{cases} \quad (3.66)$$

τ is a corrective term to ensure the conservation of the field $X_d + \eta_d$:

$$\tau = (\lambda/\bar{\lambda}) \left(\overline{\left[\frac{\partial \eta_d}{\partial t} \right]^{corr}} - \overline{\frac{\partial \eta_d}{\partial t}} \right) \delta t \quad (3.67)$$

The dislocation core energy E_{core} can be also artificially increased to conserve the shape of η as suggested by Geslin [80]. The dislocation core structure which is modelled as a diffuse interface is modified due to the elastic interactions. Typically, the dislocation core energy is increased in our simulations by a factor within the range of values 1-10. After the application of Eq. 3.64 to conserve the shape of η , $\bar{X}_d$, the maps of X_d and the profile of η along the dipole are plotted in Figs. 3.17 and 3.18 with the effective dislocation core energy $E_{core}^{eff} = 8E_{core}$. The interface width w was conserved. Practically, only the value of H was increased by a factor 8 in the PF code. The profile of η (see Fig. 3.18-c) shows

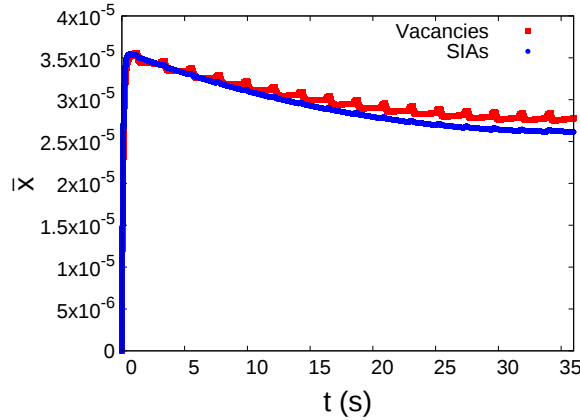


Figure 3.17: Evolution of the average atomic fraction $\bar{X}$ of PD during simulation type 1 as a function of time, with elastic interactions after application of Eq. 3.64 to conserve the shape of η .

its shape conservation during dislocation climb. The PD atomic fraction maps are also different from that of Fig. 3.16. The evolution of $\bar{\eta}$ is linear with time as shown in Fig. 3.19. The climb rate obtained is the same as the one obtained without elastic interactions, which is expected (simulation type 1, see Eq. 3.51).

To summarize, the shape of η (or equivalently the dislocation core structure) is modified when the elastic interactions are taken into account. To conserve the shape of η during climb, Eq. 3.64 is applied and the dislocation core energy is artificially increased.

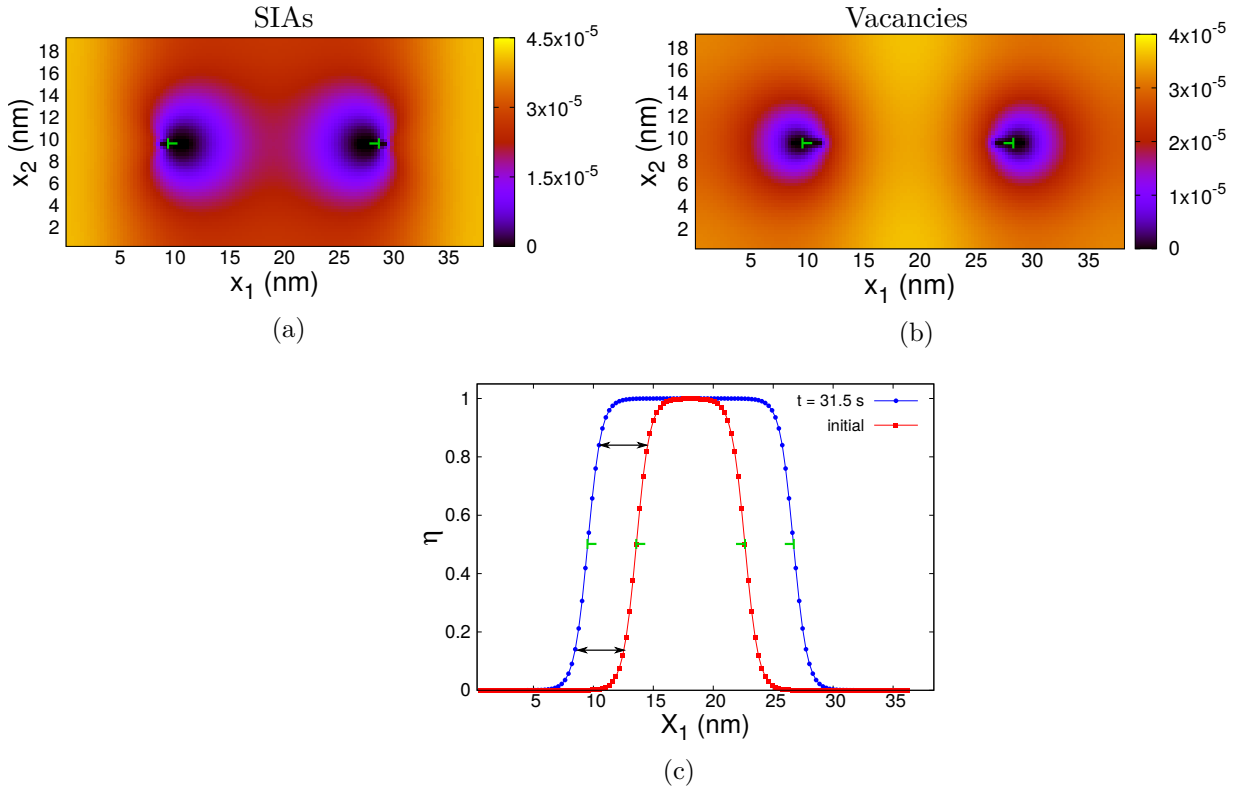


Figure 3.18: Atomic fraction maps of a) SIAs and b) vacancies, and c) profile of η along the dipole ($x_2 = 9.6$ nm) at $t = 31.5$ s, with elastic interactions after application of Eq. 3.64 to conserve the shape of η (simulation type 1).

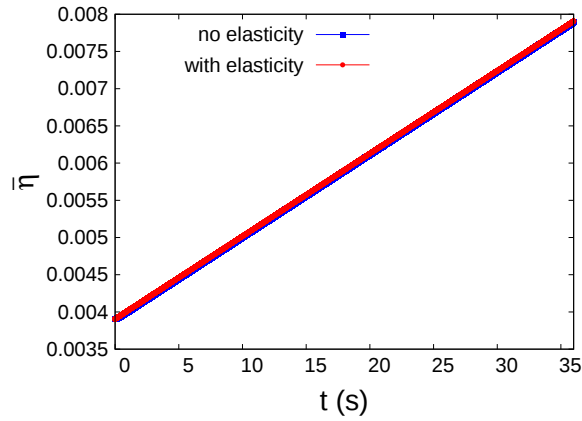


Figure 3.19: Evolution of $\bar{\eta}$ without elasticity a) and with elasticity b) (simulation type 1).

In the preliminary study presented above, the growth of an interstitial dislocation loop has been simulated. Another test to validate our model is the simulation of the loop shrinkage. Simulation of type 1 was performed by using the parameters of table 3.1 and $\zeta_{\eta}^{d,*} = 100$. The effective generation rate of vacancies was chosen higher than the one of SIAs in order to obtain an interstitial loop shrinkage at steady state, $K_0^I = 3.45 \times 10^{-4} \text{s}^{-1}$ and $K_0^V = 4.45 \times 10^{-4} \text{s}^{-1}$. These generation rates correspond to an analytical climb rate of $v_{\eta} = -1.23 \times 10^{-10} \text{m.s}^{-1}$ (see Eq. 3.51). The evolution of the profile of η along the dipole as a function of time is plotted in Fig. 3.20 and shows the shrinkage of the loop until the dipole annihilation. The PF climb rate obtained at steady state is of $-1.36 \times 10^{-10} \text{m.s}^{-1}$ which is in a good agreement with the analytical solution.

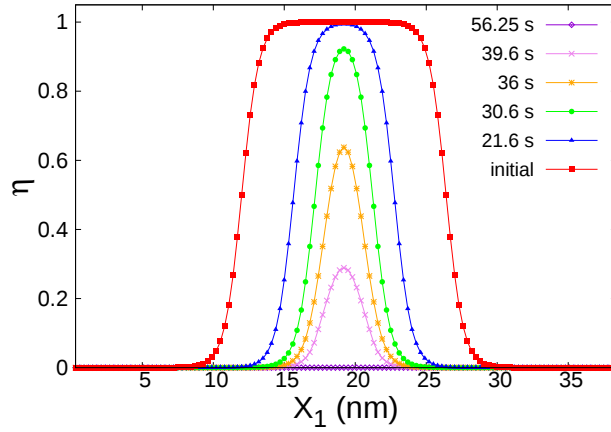


Figure 3.20: Profile of η as a function of time along the dipole ($x_2 = 9.6 \text{ nm}$) in the case of interstitial loop shrinkage (simulation type 1).

3.3.2.1 Influence of the coefficient ζ_{η}^d on the climb rate (simulation type 2)

To investigate the effects of ζ_{η}^d and Ω_d on the climb rate, simulations of type 2 were performed. PDs are created at the same effective generation rate $K_0 = 3.45 \times 10^{-4} \text{s}^{-1}$. As edge dislocations absorb more SIAs than vacancies, the presence of a neutral sink like a low-angle STGB (see section 2.3.3.2) should lead to the interstitial loop growth (see Eq. 3.58). The low-angle STGB is modeled as a planar sink as illustrated on Fig 3.21. Parameters of table 3.1 have been used. The simulations were performed for different values of $\zeta_{\eta}^{d,*}$ ($\zeta_{\eta}^{V,*} = \zeta_{\eta}^{I,*}$) with $\Omega_I = 1.2V_{at}$, $\Omega_V = -0.6V_{at}$. Figs. 3.22-a) and 3.22-b) show a decrease of the average atomic fraction at the stationary state when $\zeta_{\eta}^{d,*}$ increases like in the case of simulation type 1 (see Fig. 3.11). The average value of η decreases also when $\zeta_{\eta}^{d,*}$ increases as illustrated on Fig. 3.22-c). Thus the climb rate decreases when $\zeta_{\eta}^{d,*}$ increases (i.e. when d_j decreases) in this type of simulations as shown in Fig. 3.22-d). The decrease of the climb rate with the coefficient $\zeta_{\eta}^{d,*}$ ($\zeta_{\eta}^{V,*} = \zeta_{\eta}^{I,*}$) can be explained as follows. When $\zeta_{\eta}^{d,*}$ increases, the kinetics of PD attachment at dislocation cores increases also. Thus, the

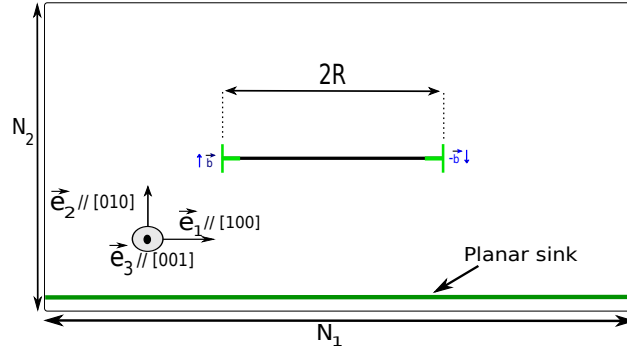


Figure 3.21: 2D simulation cell mimicking an interstitial dislocation loop near a planar sink (low-angle STGB).

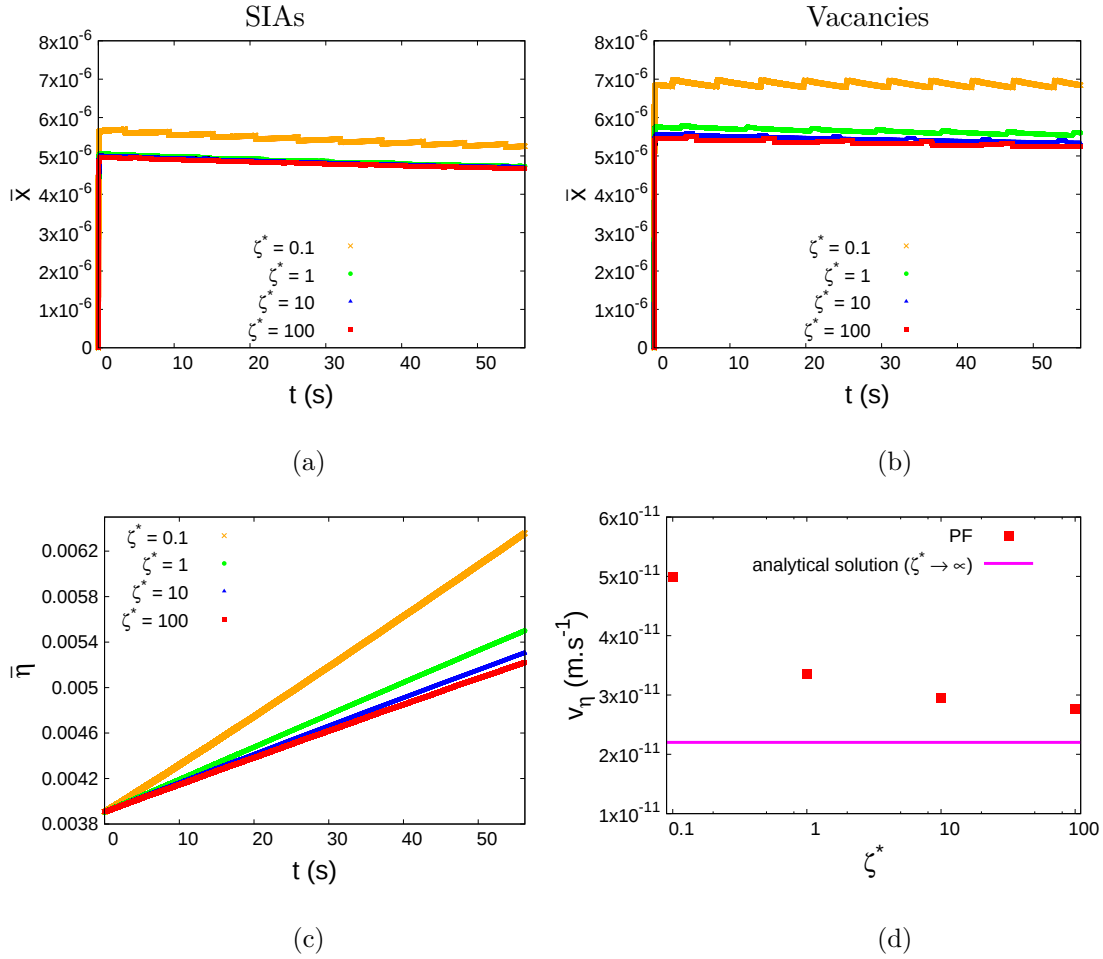


Figure 3.22: Average atomic fractions of a) SIAs and b) vacancies, c) the average value of η and d) the climb rate as a function of ζ^* in the case of simulation type 2 (dipole of edge dislocations + planar sink).

rate absorption of PD at steady state increases with $\zeta_\eta^{d,*}$ which leads to the increase of the climb rate through vacancy and SIA absorption as shown in Fig. 3.23. Moreover, the increase of the climb rate with $\zeta_\eta^{d,*}$ via the vacancy absorption is more important than via the SIA absorption. Indeed, as SIAs are more attracted towards the dislocation cores than vacancies due to the elastic drift term ($|\Omega_i| > |\Omega_v|$), the absorption rate of SIAs is therefore less affected by the variations of $\zeta_\eta^{d,*}$ than the absorption rate of vacancies, since the absorption rate depends also on the PD flow towards the sinks. Finally, the net climb rate (difference between the climb rate via SIA diffusion and vacancy diffusion) decreases when $\zeta_\eta^{d,*}$ increases.

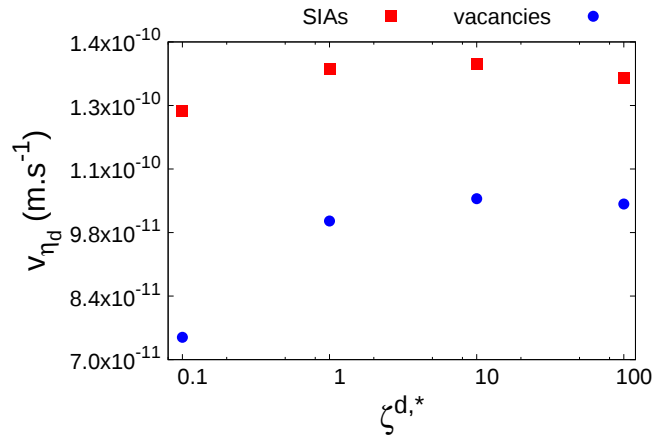


Figure 3.23: Climb rate through SIA and vacancy diffusion as a function of $\zeta_\eta^{d,*}$ in the case of simulation type 2 (dipole of edge dislocations + planar sink), $v_{\eta_d} = \frac{V}{2a_0^2} \frac{\partial \bar{\eta}_d}{\partial t}$ (see Eq. 3.48).

The analytical solution of the climb rate of Eq. 3.58 corresponds to the case of perfect sinks ($\zeta_d^* \rightarrow \infty$) since the sink strength used to calculate it were established under this assumption, and is represented in Fig. 3.22-d). This figure shows that the good order of magnitude of the climb rate is obtained, but a discrepancy is observed between the PF solution for $\zeta_\eta^{d,*} = 100$ and the analytical solution. This discrepancy may be due to the fact that the solution of Rauh and Simon for dislocation sink strength calculations [32] (see table 2.1) deviates from the PF solution. Several reasons mentioned by Rouchette et al. [4] and listed in section 2.3.3.1 allow to explain this difference.

3.3.2.2 Influence of the PD relaxation volume Ω_d on the climb rate (simulation type 2)

The effects of the PD relaxation volume Ω_d on the climb velocity were investigated by performing simulations for different values of Ω_v with Ω_i fixed at $1.2V_{at}$ and $\zeta_\eta^{d,*} = 100$. Fig. 3.24 represents the average atomic fraction of vacancies which decreases at steady state with $|\Omega_v|$. This result is expected knowing that the sink strength (inversely proportional to $\bar{X}$, Eq. 2.48) of edge dislocations increases with $|\Omega|$ as obtained in section 2.3.3.1.

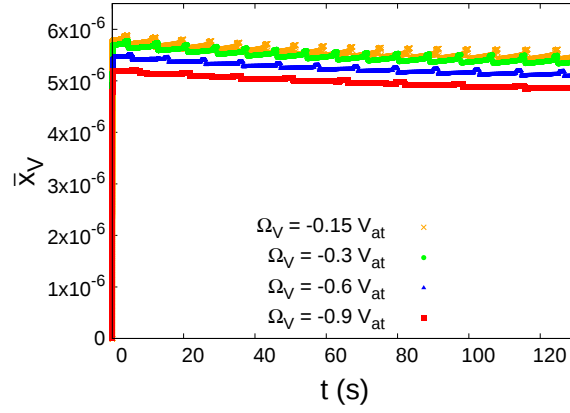


Figure 3.24: Average atomic fraction of vacancies as a function of time for different values of Ω_V in the case of simulation type 2 (dipole of edge dislocations + planar sink).

It means that at higher values of $|\Omega_V|$, more vacancies are absorbed by the dislocations, which induces a lower climb rate of the loop as illustrated in Fig. 3.25. This tendency is in qualitative accordance with the analytical solution given by Eq. 3.58, but significant differences between PF and analytical results especially for higher values of $|\Omega_V|$ can be noticed (see Fig. 3.25-b)). As mentioned in section 3.3.2.1, these differences may be due to the solution of Rauh and Simon for dislocation sink strength which deviates from the PF solution, used to compute the analytical climb rate.

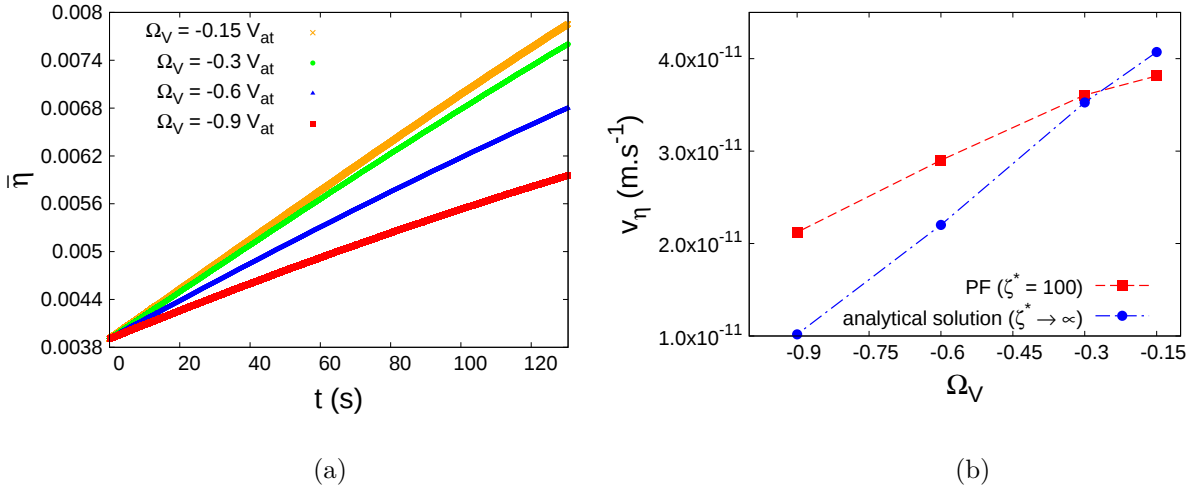


Figure 3.25: a) Average value of η as a function of time and b) climb rate for different values of Ω_V in the case of simulation type 2 (dipole of edge dislocations + planar sink).

In summary of this section, several tests were carried out with the PF model of dislocation climb under irradiation. They showed the limits of existing models and adjustments were therefore necessary. In particular, a shape function to ensure the existence of the osmotic force only at the dislocation cores was introduced in the model. Taking into account the elastic effects destabilizes the dislocation core structure (modification of the shape of the η profile). To overcome this difficulty, Eq. 3.64 was applied and the dislocation core energy was also increased artificially. The influence of the parameters $\zeta_{\eta}^{d,*}$ (related to the jog inter-spacing) and Ω_d on the climb rate has been studied by performing simulations of type 2. The results showed that, when the coefficient $\zeta_{\eta}^{d,*}$ which refers to the kinetics of PD absorption increases, the climb rate through each PD increases also. This increase is more significant for vacancies which leads to the decrease of the net climb rate with $\zeta_{\eta}^{d,*}$. The results also showed that as the sink strength increases with $|\Omega_d|$, the climb rate via each PD increases also and then for $|\Omega_i|$ fixed the net climb rate of the interstitial loop decreases with $|\Omega_v|$. In section 3.4, the PF model of dislocation climb is applied to simulate the evolution of interstitial loops in bcc pure iron.

3.4 Application to bcc iron

Experimental studies [83, 84, 11] have shown that under neutron irradiation, more interstitial loops are observed than vacancy loops in α -Fe. Edge dislocations are biased sinks (see section 2.3.3.1), SIAs being more absorbed than vacancies. Thus the growth (respectively shrinkage) of interstitial (respectively vacancy) loops is favored, which allows to explain the experimental observations. Two types of interstitial loops have been observed at low temperatures [84]: $\langle 100 \rangle$ -type ($\mathbf{b} = a\langle 100 \rangle$) and $\langle 111 \rangle$ -type ($\mathbf{b} = \frac{a}{2}\langle 111 \rangle$) interstitial loops, a being the lattice parameter, but at high temperatures ($T > 573$ K), only $\langle 100 \rangle$ -type loops are present [83, 11].

In this section, the PF model of dislocation climb under irradiation is applied to study the interstitial loop evolution in pure α -Fe. First, the growth of $\langle 100 \rangle$ -type interstitial loop is considered with and without any surrounding microstructure corresponding respectively to simulation type 1 and 2 (see section 3.2.5). The dislocation density, temperature, loop orientation and elastodiffusion effects on the climb rate are then investigated.

3.4.1 Growth of a $\langle 100 \rangle$ -type interstitial loop in a system free of any other sink (simulation type 1)

A dipole of edge dislocations was used to mimic an interstitial dislocation loop as illustrated on Fig. 3.5-a). The growth of the loop is simulated by choosing K_0^d such as $K_0^d > K_0^v$ (see Eq. 3.51). The order of magnitude chosen for K_0^d corresponds to electron irradiation conditions. The physical parameters for simulations are given in table 3.2. $\zeta_{\eta}^{d,*}$ was set to 400 for both PDs to reproduce a perfect sink i.e. a high jog density. The analytical climb rate at the stationary state given by Eq. 3.51 is $v_{\eta} = 1.16 \times 10^{-11} \text{m.s}^{-1}$ for these corresponding conditions.

The average atomic fractions of PD and the average value of the field η as a function of

Table 3.2: Physical parameters for the simulations

T	700 K
b	2.83 Å
dislocation core energy	8 eV.Å ⁻¹
dislocation core width	2.264 nm
domain size	36.2 nm × 18.1 nm
initial loop radius R ₀	4.528 nm
K ₀ ^I , K ₀ ^V	2 × 10 ⁻⁵ , 10 ⁻⁵ dpa.s ⁻¹
D ^I , D ^V	1.1 × 10 ⁻⁸ , 7.2 × 10 ⁻¹¹ m ² .s ⁻¹ [82]
C ₁₁ , C ₁₂ , C ₄₄	243, 145, 116 GPa [59, 60]
Ω _i , Ω _v	1.86V _{at} , -0.3V _{at} [55]
V _{at}	1.13 × 10 ⁻²⁹ m ³
X _{eq} ^I , X _{eq} ^V	3.28 × 10 ⁻²⁹ , 1.21 × 10 ⁻¹⁴ [82]

time are plotted in Fig. 3.26 and there is linear evolution of $\bar{\eta}$. The atomic fraction maps

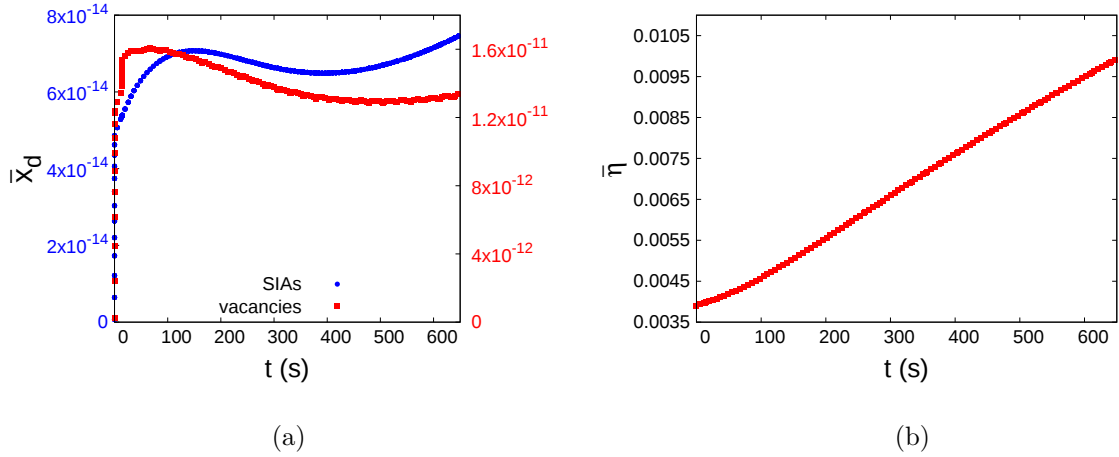


Figure 3.26: a) Average atomic fraction of PD and b) average value of η as a function of time (simulation type 1).

of PDs are plotted in Fig. 3.27 at the time $t = 596$ s. These maps show a depletion of SIAs in the compression region of dislocations which is expected, while the opposite behavior is observed for vacancies. The angular dependence of the profiles of the PD atomic fraction around the dislocation and visible in Fig. 3.27 is due to the elastic constant anisotropy. The system anisotropy effects are not remarkable in the case of vacancies due to their low relaxation volume. The evolution of the PD atomic fraction profiles and the profile of η along the dipole as a function of time are represented in Fig. 3.28. During the loop growth, the PD atomic fractions increase inside the loop and decrease in the bulk (see Figs. 3.28-a) and 3.28-b)) at the same time as the dislocations move away as shown in Fig. 3.28-c).

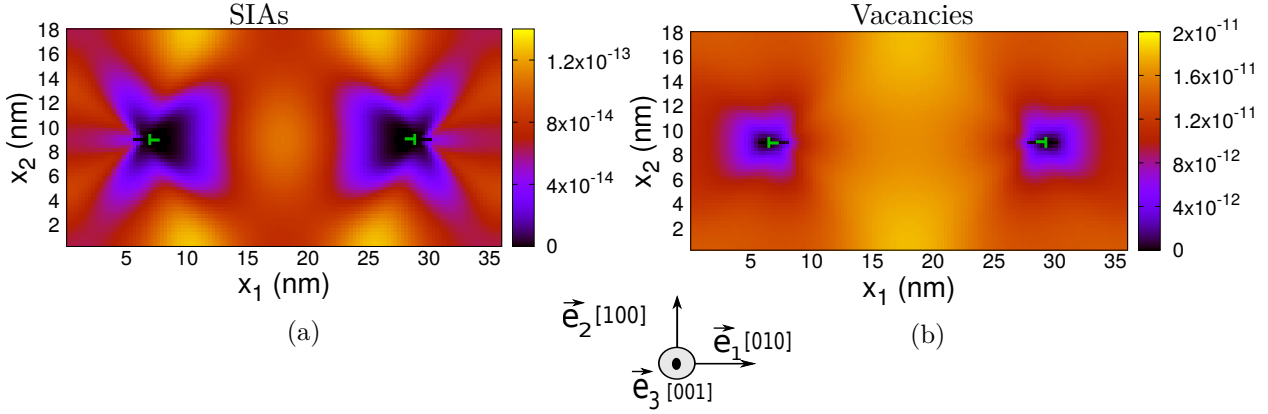


Figure 3.27: Atomic fraction map of a) SIAs and b) vacancies at $t = 596$ s (simulation type 1).

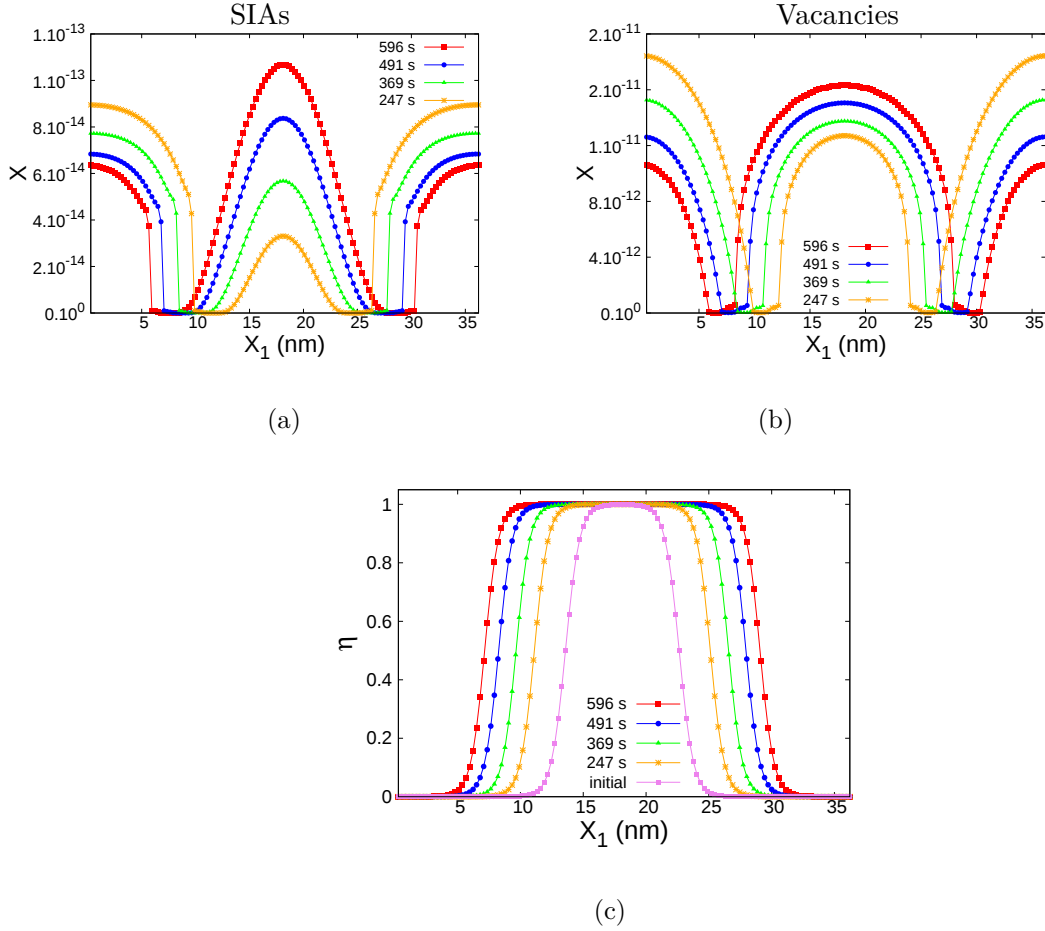


Figure 3.28: Atomic fraction profile of a) SIAs, b) vacancies and c) profile of the field η along the dipole ($x_2 = 9.06$ nm) at different times (simulation type 1).

The spatial PD fraction in the simulation domain is influenced by the sink position: the PD fraction is higher in regions far from the sink than in regions close to it. Thus, the increase of the PD fraction inside the loop is due to the remoteness of the dislocations and the decrease in the bulk to their rapprochement since periodic boundary conditions are used. The PF stationary climb rate obtained is $v_\eta = 1.12 \times 10^{-11} \text{ m.s}^{-1}$ which is in good agreement with the one predicted analytically $1.16 \times 10^{-11} \text{ m.s}^{-1}$. The climb rate evolution as a function of the dislocation density $\rho = 2/N_1 N_2 a_0^2$ is plotted in Fig. 3.29. The analytical solution of the climb rate (see Eq. 3.51) as a function of dislocation density

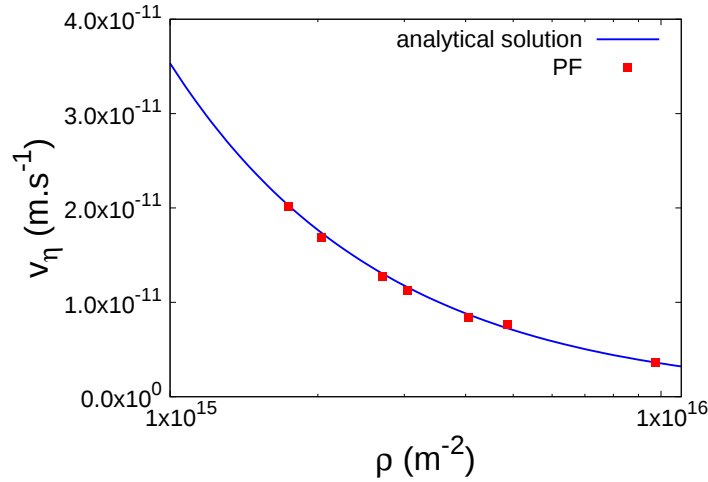


Figure 3.29: Climb rate as a function of the dislocation density in the case of simulation type 1.

is given by (simulation type 1):

$$v_\eta = \frac{1}{a_0 \rho} (K_0^I - K_0^V) \quad (3.68)$$

Fig. 3.29 shows that the climb rate decreases when the dislocation density increases. This result can be explained as follows: for small systems (high dislocation densities), the PD fraction in the bulk (reservoir) is weak at steady-state. The osmotic driving force for dislocation climb is then low which leads to low climb rates. Contrariwise, the greater the reservoir (low dislocation density), the more available PDs in the bulk. Thus, there is a high osmotic driving force and consequently a high climb rate.

3.4.2 Growth of an interstitial loop in a system containing a planar sink (simulation type 2)

A planar sink is introduced in the system as shown in Fig. 3.21 to simulate the growth of an interstitial loop (see Eq. 3.57). PDs are created at an irradiation rate of $K_0 = 10^{-5} \text{ dpa.s}^{-1}$. The physical parameters of tables 3.2 and 3.3 are used and ζ_d^* was fixed to 400 for both PDs as in section 3.4.1. The temperature, loop orientation and elastodiffusion

Table 3.3: Diffusion coefficients and thermal equilibrium fraction of PDs [82].

T (K)	D^I, D^V ($\text{m}^2.\text{s}^{-1}$)	X_{eq}^I, X_{eq}^V
600	$4.42 \times 10^{-9}, 1.07 \times 10^{-11}$	$5.88 \times 10^{-34}, 2.94 \times 10^{-17}$
700	$1.1 \times 10^{-8}, 7.2 \times 10^{-11}$	$3.28 \times 10^{-29}, 1.21 \times 10^{-14}$
800	$2.32 \times 10^{-8}, 3.02 \times 10^{-10}$	$1.2 \times 10^{-25}, 1.11 \times 10^{-12}$
900	$4.03 \times 10^{-8}, 9.2 \times 10^{-10}$	$7.11 \times 10^{-23}, 3.73 \times 10^{-11}$

effects on the climb rate are successively studied.

3.4.2.1 Temperature effect

Simulations were performed for different temperatures for the $\langle 100 \rangle$ -type loop orientation. The PD thermal equilibrium fractions were fixed to zero (typically 10^{-30}) and to their real values given in table 3.3 to investigate their effects on the climb rate. In Fig. 3.30 the climb rate is represented as a function of the temperature and it can be seen that for $X_{eq}^d = 10^{-30}$, the climb rate decreases linearly with the temperature. The analytical solution of Eq. 3.58 is also represented on Fig. 3.30 and shows the same linear variation of the climb rate with temperature. For X_{eq}^d close to zero the analytical solution of Eq.

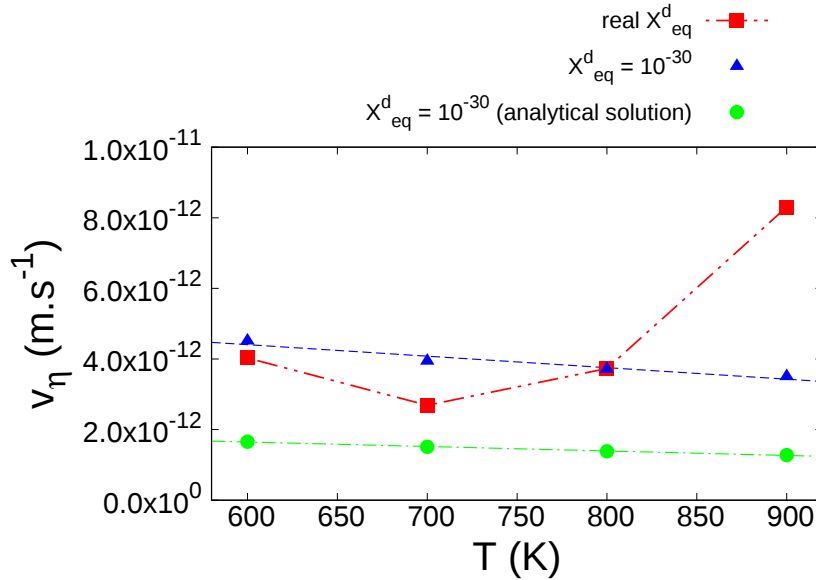


Figure 3.30: Climb rate of a $\langle 100 \rangle$ -type interstitial loop as a function of temperature in the case of simulation type 2, for a dislocation density of $3.048 \times 10^{15} \text{m}^{-2}$ and an interplanar spacing of 18 nm.

3.58 depends only on the sink strength, V and K_0 being fixed. Thus, as the dislocation sink strength decreases with temperature due to the attenuation of elastic interactions, the climb rate decreases also. When the real PD thermal equilibrium fractions are considered, Fig. 3.30 shows a decrease followed by an increase of the climb rate with temperature. This evolution of the climb rate with temperature by considering the real X_{eq}^d can be explained as follows. At low temperatures $T < 800$ K, the average fraction $\bar{X}_d$ at steady state is far from the thermal equilibrium fraction for both PDs as shown in Figs. 3.31 and 3.32. Thus, there is an important osmotic driving force for climb for both PDs due to the large excess of PD fraction available in the bulk. The climb rate evolution with temperature is therefore mainly controlled by the elastic interactions in this range of temperature. Consequently, the climb rate decreases with temperature for $T < 800$ K, like in the case of previous simulations for which $X_{eq}^d = 10^{-30}$. For high temperatures $T > 800$ K, the vacancy fraction at steady state doesn't exceed anymore the thermal equilibrium value, while the opposite behavior is observed for SIAs (see Figs. 3.31 and 3.32), since the SIA thermal equilibrium fraction remains small. The osmotic force due to vacancy tends to zero in this range of temperature ($T > 800$ K), while the one due to SIAs remains significant. Since the osmotic force due to vacancy contributes to the decrease of the climb rate of the interstitial loop, its decrease with the temperature leads therefore to the climb rate increase (see Fig. 3.30). These results show that the PD equilibrium fraction plays a significant role on the loop growth rate estimation, especially at high temperatures.

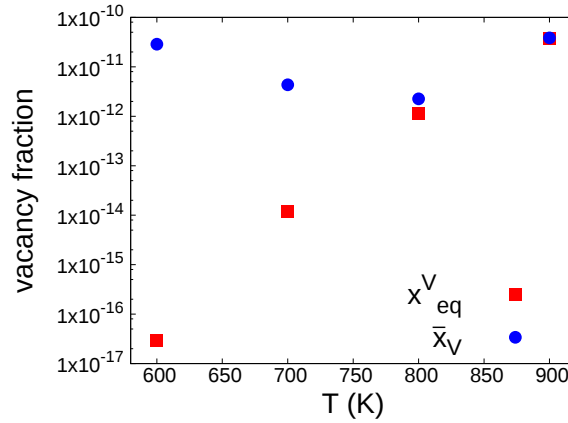


Figure 3.31: Vacancy fraction as a function of the temperature at thermal equilibrium (red square) and at steady state in the PF simulations of type 2 (blue circle), for a dislocation density of $3.048 \times 10^{15} \text{m}^{-2}$ and an interplanar spacing of 18 nm.

The evolution of the climb rate as a function of the dislocation density and temperature is plotted in Fig. 3.33. This figure shows that the climb rate globally increases when the dislocation density decreases which is expected for the reasons given in section 3.4.1.

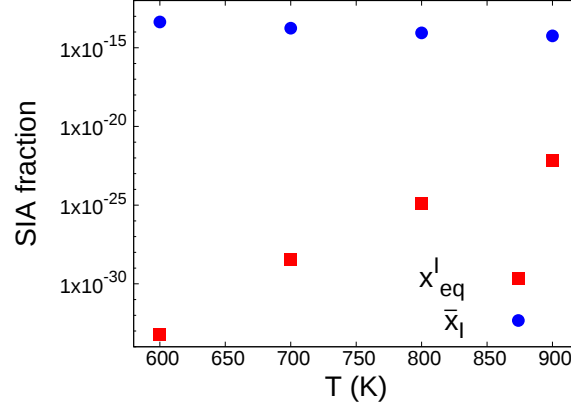


Figure 3.32: SIA fraction as a function of the temperature at thermal equilibrium (red square) and at steady state in the PF simulations of type 2 (blue circle), for a dislocation density of $3.048 \times 10^{15} \text{m}^{-2}$ and an interplanar spacing of 18 nm.

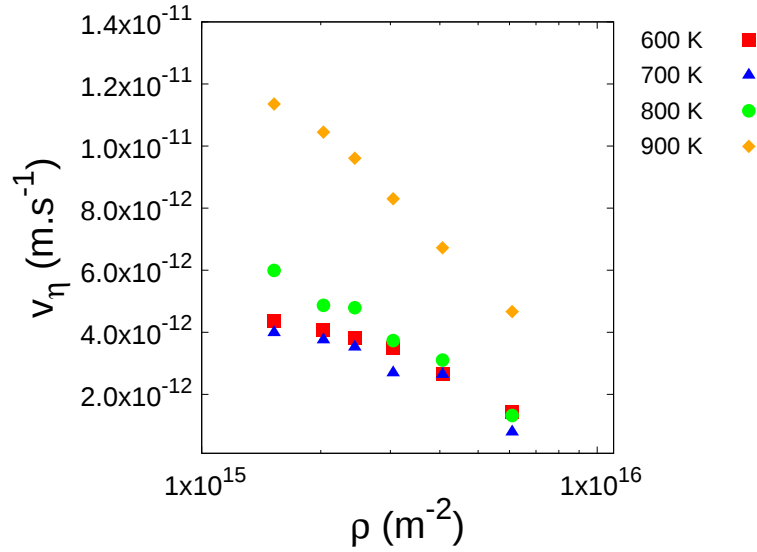


Figure 3.33: Climb rate of a $\langle 100 \rangle$ -type interstitial loop as a function of dislocation density and temperature, for an interplanar spacing of 18 nm (simulation type 2).

3.4.2.2 Loop orientation effect

The loop orientation effect on the climb rate is investigated in this section. The climb rate as a function of temperature has been plotted for the $\langle 100 \rangle$ and $\langle 111 \rangle$ -type loop orientations in Fig. 3.34. It can be seen that the loop growth rate of the $\langle 100 \rangle$ -type is greater than that of the $\langle 111 \rangle$ -type for $T < 900$ K, but smaller at $T = 900$ K. The

differences observed are weak at low temperature ($T < 900$ K) but significant at high temperature ($T = 900$ K).

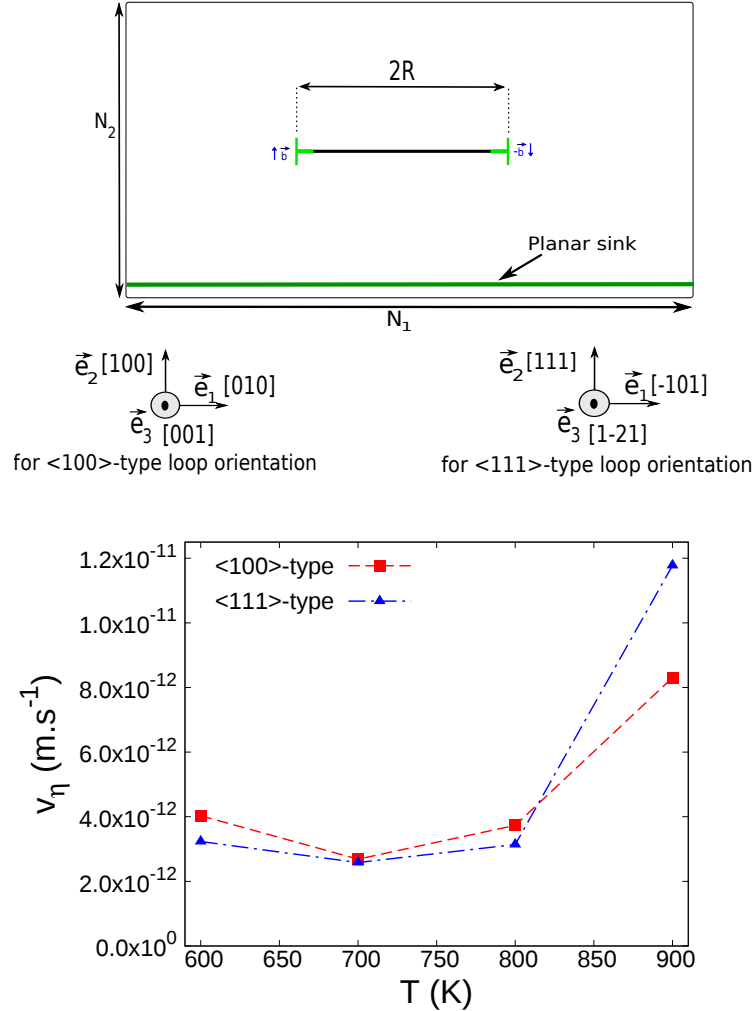


Figure 3.34: Climb rate as a function of temperature and loop orientation, for a dislocation density of $3.048 \times 10^{15} \text{m}^{-2}$ and an interplanar spacing of 18 nm (simulation type 2).

3.4.2.3 Elastodiffusion effect

Simulations were performed without and with elastodiffusion for the $\langle 100 \rangle$ -type loop orientation and the climb rate as a function of temperature is represented in Fig. 3.35. The results show for $T \leq 800$ K that the climb rate of the $\langle 100 \rangle$ -type loop decreases when elastodiffusion effects are taken into account as illustrated in Fig. 3.35 which is consistent with the results of sink strength calculations obtained in section 2.3.3.1. Indeed, the results presented in section 2.3.3.1 showed that the sink bias of edge dislocations in pure Fe decreases when elastodiffusion effects are taken into account compared to the case without, which leads to a decrease of the climb rate. Furthermore, there is a significant

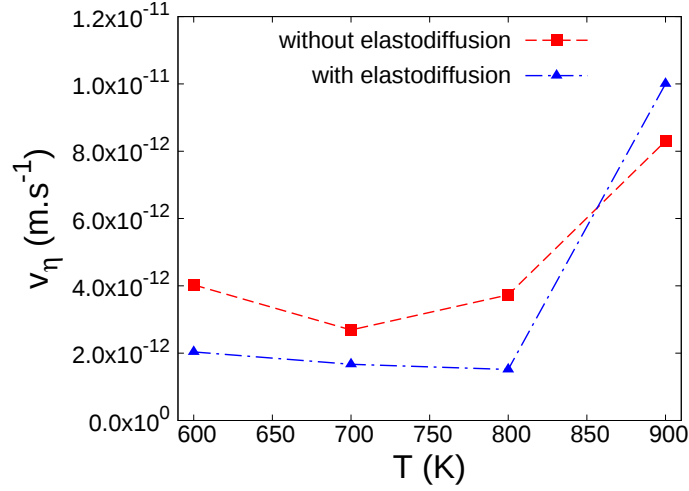


Figure 3.35: Climb rate of a $\langle 100 \rangle$ -type interstitial loop as a function of temperature without and with elastodiffusion effects, for a dislocation density of $3.048 \times 10^{15} \text{m}^{-2}$ and an interplanar spacing of 18 nm (simulation type 2).

decrease of the climb rate with elastodiffusion at 600 K due to the strong effects of elasticity at low temperature. As the sink strength increases with elastodiffusion, at 800 K elasticity keeps playing a predominant role for simulations characterised by a decrease of the climb rate, while the climb rate increases for simulations without elastodiffusion. At 900 K elasticity effects are strongly attenuated for both types of simulations especially without elastodiffusion and as there is no more significant osmotic force for vacancy, the climb rate increases for both cases of simulations and is higher in the case with elastodiffusion compared to the case without.

3.4.3 Discussion

The growth of an interstitial loop in pure iron was simulated. The temperature effect on the climb rate was investigated by performing simulations for a system containing an edge dislocation dipole mimicking the interstitial loop and a planar sink. The results showed a decrease of the climb rate followed by an increase when the temperature increases for a given dislocation density of $3.048 \times 10^{15} \text{m}^{-2}$ and interplanar spacing of 18 nm (see Fig. 3.30). The evolution of the climb rate with the dislocation density showed globally an increase of the climb rate with the decrease of dislocation density for all the temperatures (see Fig. 3.33). The temperature dependence of the growth rate of interstitial loop in iron has been measured experimentally on a single thin foil by electron irradiation in [81]. The results of Duparc et al. [81] showed an increase of the growth rate as temperature increases and this increase was following an Arrhenius law as predicted by their analytical solution. The analytical solution of the climb rate given in [81] was obtained using Eqs.

2.1 and 2.2 for $X_d^s \simeq 0$:

$$v = \frac{dR}{dt} = \frac{2V_{at}}{b}(Z_I D_I \bar{X}_I - Z_V D_V \bar{X}_V), \quad Z_d = k_{dislo,d}^2 / \rho \quad (3.69)$$

and under the assumptions that $D_I \gg D_V$, $D_I \bar{X}_I \simeq D_V \bar{X}_V$ at the stationary state, and PD recombination is predominant $D_I \bar{X}_I = \sqrt{K_0 D_V / 4\pi V_{at} r_c}$ which led to:

$$v = \frac{2}{b}(Z_I - Z_V) \sqrt{\frac{K_0 V_{at} D_V}{4\pi r_c}} \quad \text{with} \quad D_V = D_{0V} \exp\left(-\frac{E_V^m}{k_B T}\right) \quad (3.70)$$

Z_d was computed using the solution of Laplace given in table 2.1. Furthermore, a transmission electron microscopy (TEM) study of neutron irradiated iron [11] has revealed a decrease of the dislocation density with the temperature increasing about an order of magnitude for each 50 K (see Fig. 1.4). For example the dislocation density at 623 K was about 10^{14}m^{-2} for irradiation damage of 0.88 dpa and at 773 K about $3 \times 10^{11} \text{m}^{-2}$ for irradiation damage of 0.74 dpa. Fig. 3.33 shows that when the temperature increases and the dislocation density decreases the climb rate increases, which is qualitatively in good agreement with the results of Duparc et al. [81]. Regarding the order of magnitude of the climb rate, the results obtained in [81] showed a variation range of $[10^{-11} - 10^{-9}] \text{m.s}^{-1}$ for a temperature range of $[573 - 873] \text{K}$. The climb rate in our simulations varies as $[10^{-13} - 10^{-11}] \text{m.s}^{-1}$ for a temperature range of $[600 - 900] \text{K}$ and for a dislocation density range of $[10^{15} - 10^{16}] \text{m}^{-2}$ as illustrated on Fig. 3.33. The dislocation density evolution as a function of temperature obtained in [11] is about $[10^{14} - 10^{11}] \text{m}^{-2}$ for temperature increasing from 623 to 773 K. Thus, our range of dislocation density is not representative of what is observed experimentally in [11]. To explore low dislocation densities, large systems are required which is time consuming. However, it can be seen that the order of magnitude of the climb rate obtained in [81] could be obtained by extrapolating the results of Fig. 3.33 to low dislocation densities. Furthermore, the results of Fig. 3.33 were obtained for a fixed interplanar spacing consequently for a fixed sink strength of the surrounding microstructure. As illustrated in figure 3.4 the climb rate depends also on the sink strength of the surrounding microstructure (multi-sink effects). It must be noticed that the climb rate does not necessarily follow an Arrhenius law like in the case of Duparc et al. [81] due to several reasons:

- The assumptions used by Duparc to establish the analytical solution of Eq. 3.70 are not systematically valid and depend on the irradiation conditions. Especially, the kinetic regime was assumed dominated by the PD recombination. In the opposite, the kinetic regime was assumed dominated by sinks in our simulations and therefore PD recombination was neglected.
- The solution used to compute the sink strength of dislocations does not incorporate elastic interactions which depend on the temperature. In addition, the Fig. 3.35 showed that elastodiffusion can affect the climb rate.

3.5 Conclusion

A PF model of dislocation climb under irradiation was developed and presented in this chapter. The model is based on previous ones dealing with dislocation climb via the va-

cancy diffusion [2, 1, 3] suitable for high temperatures. Several tests were carried out in order to validate the new PF model of dislocation climb under irradiation. Especially, a shape function was introduced to ensure the existence of the osmotic force only at the dislocation cores. The model was also adjusted to overcome the modification of the dislocation core structure due to elasticity by applying Eq. 3.64 and by increasing artificially the dislocation core energy. After the model validation, the growth of a prismatic interstitial loop under electron irradiation conditions was investigated. The results showed that the PD equilibrium fraction inside the sink plays a significant role on the loop growth rate calculations especially at high temperatures when the equilibrium vacancy fraction is high as illustrated on Fig. 3.30. The results also showed that the climb rate increases with the combined effects of the decrease of the dislocation density and the increase of the temperature (see Fig. 3.33) for the chosen simulation conditions.

Chapter 4

Radiation induced segregation prediction near prismatic interstitial dislocation loops in Fe-Cr alloys

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A new PF model of dislocation climb under irradiation has been presented and applied to simulate dislocation loop evolution in pure Fe in chapter 3. In this chapter, the phenomenon of radiation induced segregation (RIS) is studied near dislocation cores in Fe-Cr alloys. By means of the new PF model of dislocation climb, climb velocity effects on RIS predictions are investigated.

4.1 Bibliography

Radiation induced segregation (RIS) is a common phenomenon in irradiated materials and plays an important role on the microstructure evolution of these materials. The mobile PDs produced under irradiation migrate towards sinks such as dislocations, dislocation loops and GBs. PD migration is due to atom displacement: the PD fluxes are thus coupled to the atom fluxes. RIS results from this coupling and leads to a **local redistribution** of the alloying elements near sinks [85, 86]. The depletion or enrichment of each element in the vicinity of sinks occurs according to its relative interaction with the PD fluxes. RIS was first predicted by Anthony [87]. Anthony showed in the framework of the **thermodynamics of irreversible process** (TIP) [87, 88, 89, 90] that the segregation tendencies are controlled by the phenomenological coefficients L_{ij} of the **Onsager matrix**. The predictions of Anthony have been first experimentally observed by Okamoto et al. [91] in an austenitic stainless steel Fe-18Cr-8Ni-1Si during electron and ion irradiation. Anthony's model suggested that segregation is due to the coupling between atom fluxes and the flux of excess vacancies, however the observations of Okamoto et al. [91] suggested that undersized atoms Ni and Si which can more accommodate in interstitial sites were diffusing towards sinks, while oversized atoms such as Cr were diffusing away. Thus, in addition to the RIS mechanism through the fluxes of vacancies, Okamoto and Wiedersich [92] proposed a new RIS mechanism involving interstitial atoms. Other experiments [93] allowed to verify this new RIS model.

The Onsager coefficients L_{ij} represent the kinetic response of an alloy subjected to thermodynamic forces and thus allow to obtain the fluxes as described in section 4.2.3. They depend on several parameters such as temperature, PD concentrations, local alloy concentrations and stress field. The L_{ij} -coefficients can be determined from diffusion experiments but for multicomponent and concentrated alloys it is quite difficult to obtain them [86]. Theoretical models have been developed to determine the Onsager matrix. The most popular are the self-consistent mean-field (SCMF) theory based on atomic jump frequencies and the model based on the generalized Einstein relation [94, 95]. In the SCMF theory, L_{ij} are written as a function of the PD migration frequencies which can be computed at the atomic scale (using ab initio calculations, interatomic potentials, broken-bond models) [86]. Tucker et al. [96] for example, computed the atom jump frequencies to access L_{ij} in alloys with a fcc structure (Ni-Cr, Ni-Fe) within the limit of dilute solid solution. In the case of concentrated alloys, the number of jump frequencies becomes large, and approximations are made to compute L_{ij} [97]. The model based on the generalized Einstein relation is particularly suitable to the atomic kinetic Monte Carlo (AKMC) simulations.

RIS has been predicted using SCMF [98] and AKMC [99, 100, 101] simulations. In the AKMC simulations, the PD jumps are described individually and these types of sim-

ulations are time consuming and limited to nanoscale systems [86]. Thus to simulate large systems, it is necessary to rest on continuous descriptions. PF model is particularly adapted to study RIS because diffusion processes are naturally incorporated and elastic interactions can be properly described. This approach has been used by Piochaud et al. [82] to model RIS near a GB assimilated to a planar sink (no elastic interactions) in Fe-Cr alloys. In this study [82], the kinetic equations used in the PF model to simulate RIS are based on the Onsager formalism. The Onsager transport coefficients L_{ij} and the driving force parameters (equilibrium PD concentrations, thermodynamic factors) were computed at the atomic scale using AKMC simulations fitted on DFT calculations. Piochaud et al. compared the prediction obtained by PF method and AKMC simulations, and found a good agreement for all range of compositions and temperatures investigated as illustrated on Fig. 4.1. They also showed that a quantitative PF prediction of RIS requires a precise

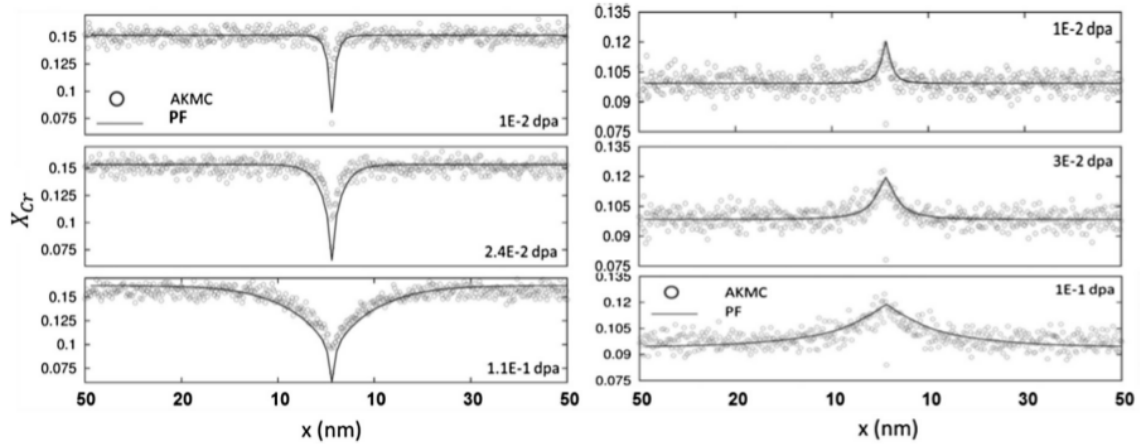


Figure 4.1: RIS profiles obtained using AKMC (symbols) and PF (lines) in Fe-15%Cr at 900 K (left) and in Fe-10%Cr at 700 K (right), as a function of the distance from the grain boundary, x , and for different irradiation doses at $K_0 = 10^{-5} \text{ dpa.s}^{-1}$ [82].

parameterization of the Onsager coefficients, equilibrium PD concentrations and thermodynamic factors. More recently, Thuinet et al. [102] used the kinetic parameterization of [82] to investigate RIS near a dipole of edge dislocations mimicking an interstitial dislocation loop. The results showed that without taking into account elastic interactions between PDs and dislocations, the tendency and the level of segregation near the dislocation cores are comparable to the ones obtained at a planar sink. However, with the elastic interactions, the segregation tendency and level around the cores change strongly. These results illustrate that RIS strongly depends on the elastic interactions between PDs and dislocations. Thus, the criteria established for RIS prediction near neutral sinks based only on kinetic arguments [85] must be reconsidered for biased sinks like dislocations. Z. Li and D. R. Trinkle [103] studied the modification of the Si solute segregation near an edge dislocation due to its strain field via the vacancy diffusion in Ni under irradiation using a mesoscopic approach. They showed that Si atoms segregate in the compression region of the dislocation core despite the fact that Si is an oversized solute in Ni. In these latter studies [102, 103], dislocations act as perfect sinks and are assumed to be static which is also a questionable assumption. This hypothesis would be justified if kinetics

related to PD and atom diffusion was greater than the dislocation climb velocity. It is the case for PDs in most of the cases, but not always verified for atoms.

In this chapter, the RIS prediction using the PF method is investigated near prismatic interstitial dislocation loop in Fe-Cr alloys. Thanks to the PF model of dislocation climb under irradiation presented in chapter 3, the effect of climb rate on RIS prediction is investigated. In section 4.2 we present the PF methodology. Thereafter, we apply the PF model in section 4.3 to simulate RIS near a dipole of edge dislocations mimicking a dislocation loop in 2D.

4.2 PF methodology

In this section, the PF model of section 3.2 is extended to the study of RIS in a binary A-B alloy. We first define the order parameters, the total free energy and the evolution equations are again defined as in section 3.2 by including the chemical species.

4.2.1 Order parameters

The necessary order parameters of the system are the ones described in section 3.2.1 ($X_I, X_V, \eta_I, \eta_V, \eta^l$) to which the atomic fractions X_A and X_B of chemical species A and B respectively are added.

4.2.2 Energy of the system

The total free energy of the system F defined in section 3.2.2 is generalized to a binary system:

$$F(X_\alpha, X_d, \eta^l) = F_{ch}(X_\alpha, X_d) + F_{core}(\eta^l) + F_{el}(X_\alpha, X_d, \eta^l) \quad (4.1)$$

where α stands for the chemical species A and B. The chemical free energy is given by:

$$F_{ch}(X_\alpha, X_d) = \frac{k_B T}{V_{at}} \left(\sum_\alpha \int_V X_\alpha \ln(\gamma_\alpha X_\alpha) dV + \sum_d \int_V X_d \ln\left(\frac{X_d}{X_{eq}^d}\right) dV \right) \quad (4.2)$$

where γ_α is the activity coefficient of the alloying element α . The dislocation core energy $F_{core}(\eta^l)$ is given by Eq. 3.12. To compute the elastic energy $F_{el}(X_\alpha, X_d, \eta^l)$ (see Eq. 3.14), the total eigenstrain (see Eq. 3.15) is written by taking into account the eigenstrain of the alloying elements ϵ^{0, X_α} :

$$\epsilon_{ij}^{0, tot}(\mathbf{r}) = \sum_\alpha \epsilon_{ij}^{0, X_\alpha} X_\alpha(\mathbf{r}) + \sum_d \epsilon_{ij}^{0, X_d} X_d(\mathbf{r}) + \epsilon_{ij}^{0, \eta^l} f(\eta^l(\mathbf{r})) \quad (4.3)$$

4.2.3 Kinetic equations

The evolution equations of the atomic fractions of PDs and chemical species in an A-B binary alloy are given by [86, 82, 102]:

$$\frac{\partial X_d}{\partial t} = -V_{at} \nabla \cdot \mathbf{J}_d(\mathbf{r}, t) \quad (4.4)$$

$$\frac{\partial X_\alpha}{\partial t} = -V_{at} \nabla \cdot \mathbf{J}_\alpha(\mathbf{r}, t) \quad (4.5)$$

where $\mathbf{J}_d$ and $\mathbf{J}_\alpha$ are respectively the fluxes of PDs and chemical species. These fluxes are related to the fluxes of chemical species mediated by PDs $\mathbf{J}_\alpha^d$ through the following equations:

$$\mathbf{J}_d = sg(d) \sum_\alpha \mathbf{J}_\alpha^d \quad (4.6)$$

$$\mathbf{J}_\alpha = \sum_d \mathbf{J}_\alpha^d \quad (4.7)$$

with $sg(d) = 1$ for SIAs and -1 for vacancies. In the framework of the TIP [104], $\mathbf{J}_\alpha^d$ are assumed to be a linear combination of the thermodynamic driving forces $\nabla \mu^\beta$ and $\nabla \mu^d$, and the Onsager kinetic coefficients $L_{\alpha\beta}^d$:

$$\mathbf{J}_\alpha^d = - \sum_\beta L_{\alpha\beta}^d (\nabla \mu^\beta + sg(d) \nabla \mu^d) \quad (4.8)$$

The Onsager matrix of coefficients $L_{\alpha\beta}^d$ is symmetric and positive [105], and depends on the temperature, alloy composition, and internal/external stresses. The evolution equations become, by taking into account the effective PD generation rates, dislocation climb and the presence of other sinks (see sections 3.2.3 and 3.3):

$$\frac{\partial X_d}{\partial t} = \nabla \cdot \left[\sum_\alpha \sum_\beta \frac{l_{\alpha\beta}^d X_d}{k_B T} (sg(d) \nabla \mu^\beta + \nabla \mu^d) \right] - \frac{\partial \eta_d^l}{\partial t} - J_{s,d}^{abs} + K_0^d \quad (4.9)$$

$$\frac{\partial \eta_d^l}{\partial t} = - \frac{V_{at} D^d X_d}{k_B T} \zeta_{\eta^l}^d \left[\frac{1}{X^*} sg(l) sg(d) \mu^{\eta^l} - \lambda(\eta^l) \mu^d \right] \quad (4.10)$$

$$\frac{\partial X_\alpha}{\partial t} = \nabla \cdot \left[\sum_d \sum_\beta \frac{l_{\alpha\beta}^d X_d}{k_B T} (\nabla \mu^\beta + sg(d) \nabla \mu^d) \right] \quad (4.11)$$

where $l_{\alpha\beta}^d$ are the coefficients of the normalised Onsager matrix given by:

$$l_{\alpha\beta}^d = \frac{V_{at} k_B T}{X_d} L_{\alpha\beta}^d \quad (4.12)$$

$J_{s,d}^{abs}$ is given by Eq. 3.34, $\lambda(\eta^l)$ is a shape function associated to the dislocation core defined by Eq. 3.59. The potentials μ^β , μ^d and μ^{η^l} are defined as follows:

$$\mu^\beta = V_{at} \frac{\delta F(X_\alpha, X_d, \eta^l)}{\delta X_\beta}; \quad \mu^d = V_{at} \frac{\delta F(X_\alpha, X_d, \eta^l)}{\delta X_d}; \quad \mu^{\eta^l} = V_{at} \frac{\delta F(X_\alpha, X_d, \eta^l)}{\delta \eta^l} \quad (4.13)$$

The loop evolution is given by:

$$\frac{\partial \eta^l}{\partial t} = \frac{sg(l)}{X^*} \left(\frac{\partial \eta_i^l}{\partial t} - \frac{\partial \eta_v^l}{\partial t} \right) \quad (4.14)$$

The following dimensionless parameters (see Eq. 3.35) are introduced to solve Eqs. 4.9 - 4.11 in their dimensionless form:

$$\begin{cases} F^* = F/H, & \mu^* = \mu/V_{at}H \\ l_{\alpha\beta}^{d,*} = l_{\alpha\beta}^d t_0/a_0^2, & \zeta_{\eta^l}^{d,*} = HV_{at}a_0^2\zeta_{\eta^l}^d/k_B T \\ \nabla^* = a_0 \nabla, & \gamma^* = \gamma/(Ha_0^2) \\ t^{d,*} = t^d/t_0, & t^{\alpha,*} = t^\alpha/t_0 \\ K_0^{d,*} = K_0^d t_0, & J_{s,d}^{abs,*} = t_0 J_{s,d}^{abs} \end{cases} \quad (4.15)$$

t_0 is the reference time and chosen such as $t_0 = \min(t_0^d, t_0^\alpha, t_0^{\eta^l})$ where t_0^d , t_0^α and $t_0^{\eta^l}$ are respectively the characteristic time associated to the PD diffusion, atom diffusion and dislocation motion:

$$t_0^d = \frac{a_0^2}{\max_r(D^d)} \quad (4.16)$$

$$t_0^\alpha = \frac{a_0^2}{\max_r(D^\alpha)} \quad (4.17)$$

$$t_0^{\eta^l} = \frac{a_0}{v_{\eta^l}} \quad (4.18)$$

$\max_r$ refers to the spatial maximum. The diffusion coefficient of atom D^α is given by [86, 82]:

$$D^\alpha = \phi \sum_d \left(\frac{l_{\alpha\alpha}^d}{X_\alpha} - \frac{l_{\alpha\beta}^d}{X_\beta} \right) X_d - \sum_d sg(d) \left(\frac{l_{\alpha\alpha}^d + l_{\alpha\beta}^d}{X_\alpha} \right) X_d \frac{\partial \ln X_{eq}^d}{\partial \ln X_\alpha} \quad (4.19)$$

with ϕ the thermodynamic factor:

$$\phi = 1 + \frac{\partial \ln \gamma_\alpha}{\partial \ln X_\alpha} \quad (4.20)$$

The PD diffusion coefficients D^d are simply written as:

$$D^d = \sum_\alpha \sum_\beta l_{\alpha\beta}^d, \quad D^{d,*} = \sum_\alpha \sum_\beta l_{\alpha\beta}^{d,*} \quad (4.21)$$

v_{η^l} is the climb velocity which is estimated under irradiation condition in section 3.2.5. In practice, t_0 corresponds to $a_0^2/\max_r(D^l)$ due to the fact that SIA diffusion is generally faster than vacancy diffusion, atom diffusion and dislocation motion. The dimensionless evolution equations are:

$$\frac{\partial X_d}{\partial t^{d,*}} = \frac{V_{at}H}{k_B T} \nabla^* \cdot \left[\sum_\alpha \sum_\beta l_{\alpha\beta}^{d,*} X_d \nabla^* (sg(d)\mu^{\beta,*} + \mu^{d,*}) \right] - \frac{\partial \eta_d^l}{\partial t^{d,*}} - J_{s,d}^{abs,*} + K_0^{d,*} \quad (4.22)$$

$$\frac{\partial \eta_d^l}{\partial t^{d,*}} = -\zeta_{\eta^l}^{d,*} D^{d,*} X_d \left[\frac{1}{X^*} sg(l) sg(d) (\mu^{\eta^l,*} - \lambda(\eta^l) \mu^{d,*}) \right] \quad (4.23)$$

$$\frac{\partial X_\alpha}{\partial t^{\alpha,*}} = \frac{V_{at}H}{k_B T} \nabla^* \cdot \left[\sum_d \sum_\beta l_{\alpha\beta}^{d,*} X_d \nabla^* (\mu^{\beta,*} + sg(d)\mu^{d,*}) \right] \quad (4.24)$$

To conserve the shape of the plastic field η^l associated with the loop during climb when elastic interactions are taken into account (see section 3.3), Eq. 3.64 is applied and the dislocation core energy is also artificially increased.

4.2.4 Numerical scheme and multi-time step algorithm

The set of Eqs. 4.22 - 4.24 are spatially discretized using a [staggered grid](#) as in [82] and described in appendix A. The [multi-time step](#) algorithm described in section 3.2.4 is also used to accelerate the convergence towards the steady state. The time steps δt^d , δt^α and δt^{η^l} are chosen such that the following stability criteria are verified:

$$\frac{\delta t^d}{t_0^d} < \frac{1}{2N_{dim}} \quad (4.25)$$

$$\frac{\delta t^\alpha}{t_0^\alpha} < \frac{1}{2N_{dim}} \quad (4.26)$$

$$\frac{\delta t^{\eta^l}}{t_0^{\eta^l}} < 1 \quad (4.27)$$

The dimensionless stability criteria are rewritten according to the reference time $t_0 = a_0^2/\max_r(D_I)$ as follows:

$$\delta t^{I,*} < \frac{1}{2N_{dim}} \quad (4.28)$$

$$\delta t^{V,*} < \frac{1}{2N_{dim}} \frac{\max_r(D^I)}{\max_r(D^V)} \quad (4.29)$$

$$\delta t^{\alpha,*} < \frac{1}{2N_{dim}} \frac{\max_r(D^I)}{\max_r(D^\alpha)} \quad (4.30)$$

$$\delta t^{\eta^l,*} < \frac{1}{2N_{dim}} \frac{\max_r(D^I)}{a_0 v_{\eta^l}} \quad (4.31)$$

As described in section 3.2.4, the PD evolution equations are integrated with $\delta t^{d,*}$ to reach the steady state during the first stage for some given value of η^l and X_α . In the second stage, the evolution equations of X_α and η^l are integrated with the same time step which corresponds to the minimum between $\delta t^{\alpha,*}$ and $\delta t^{\eta^l,*}$. The field $X_d^{t^*+min(\delta t^{\alpha,*}, \delta t^{\eta^l,*})}$ is equal to $X_d^{t^*+n_d \delta t_d^*}$ during this stage, with n_d is the number of iterations needed to reach the steady state. This multi-time step algorithm is illustrated in Fig. 4.2. During the simulations, we chose to set $\delta t^{I,*}$ to 10^{-3} , $\delta t^{V,*} = \delta t^{I,*} \max_r(D^I)/\max_r(D^V)$, $\delta t^{\alpha,*} = \delta t^{I,*} \max_r(D^I)/\max_r(D^\alpha)$, $\delta t^{\eta^l,*} = \delta t^{I,*} \max_r(D^I)/a_0 v_{\eta^l}$ to satisfy the stability criteria.

Now that we have presented the PF methodology describing the evolution of the position-dependent solute and PD atomic fractions coupled to dislocation climb, we apply the model to simulate RIS in Fe-Cr alloys in the vicinity of an interstitial dislocation loop in section 4.3. The elastic interactions and dislocation motion effects on RIS prediction are investigated.

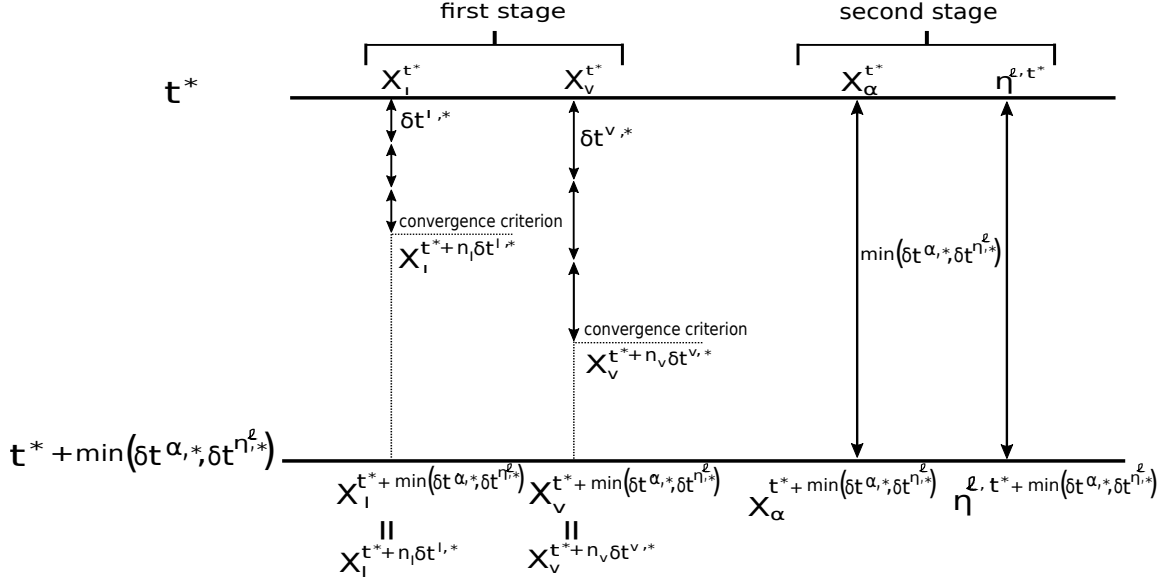


Figure 4.2: Schematic representation of the multi-time step algorithm including PD diffusion, atom diffusion and dislocation motion.

4.3 RIS prediction in Fe-Cr alloys near <100>-type prismatic interstitial dislocation loop

The 2D simulation box mimicking the interstitial dislocation loop is illustrated in Fig. 4.3. The thermodynamic and kinetic parameters (X_d^{eq} , $L_{\alpha\beta}^d$, ϕ) available in [82] were used. The

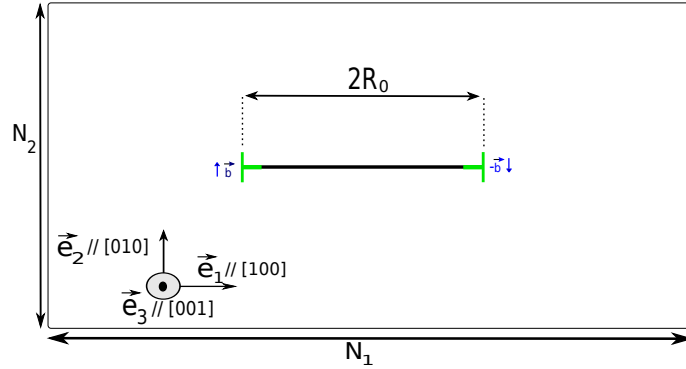


Figure 4.3: 2D simulation mimicking a <100>-type interstitial dislocation loop.

other necessary parameters for the simulations are given in table 4.1. The eigenstrains of the chemical species were set to zero ($\epsilon_{ij}^{0, X_\alpha} = 0$) to compute the elastic interactions due to the negligible difference between the lattice parameters of iron and chromium. $\zeta_{\eta^l}^{d,*}$ was set to 100 for both PDs to reproduce a perfect sink behavior of the dislocations. In section 4.3.1, RIS is predicted assuming that the Cr segregation profiles are not affected by the dislocation motion i.e that atom diffusion is faster than dislocation motion. In section

Table 4.1: Simulation parameters.

b	2.83 Å
dislocation core energy	8 eVÅ ⁻¹
dislocation core width	2.264 nm
domain size	36.2 nm × 18.1 nm
initial loop radius R ₀	4.528 nm
C ₁₁ , C ₁₂ , C ₄₄	243, 145, 116 GPa [59, 60]
Ω _i , Ω _v	1.1V _{at} , -0.05V _{at} [106]
V _{at}	1.13 × 10 ⁻²⁹ m ³

4.3.2, the dislocation motion effects on Cr segregation profile are investigated.

4.3.1 RIS prediction under the assumption of static dislocations

In this part, RIS prediction is simulated without dislocation climb (the loop evolution equation 4.14 is not integrated). We focus first on the Fe-11%Cr alloy at 700 K and Fe-15%Cr alloy at 900 K because these two alloys have been shown to produce opposing effects concerning the Cr segregation near a planar sink [82]: Cr enrichment for Fe-11%Cr and Cr depletion for Fe-15%Cr. PDs are generated at an irradiation rate $K_0 = 10^{-5}$ dpa.s⁻¹ which corresponds to electron irradiation conditions. Simulations were performed without and with elastic interactions. Furthermore, in order to study the effect of the PD equilibrium composition, X_d^{eq} were set close to zero and to their real values.

The Cr atomic fraction maps and profiles without and with elasticity are represented in Figs. 4.4 (Fe-11%Cr at 700 K) and 4.5 (Fe-15%Cr at 900 K). It can be seen that, without elasticity and for $X_d^{eq} = 10^{-30}$, the Cr segregations obtained are qualitatively in good agreement with the results obtained at planar sink [82] for both alloys: in all regions around the dislocation core, Cr enrichment for Fe-11%Cr alloy at 700 K (Fig. 4.4-a) and c)) and Cr depletion for Fe-15%Cr at 900 K (Fig. 4.5-a) and c)). With elastic interactions and for $X_d^{eq} = 10^{-30}$, the Cr segregation tendency is modified: we obtain a Cr enrichment in the traction region of dislocations and Cr depletion in the compression region for both alloys (see Fig. 4.4-d and f)) and 4.5-d) and f)). These results can be explained by the following arguments: vacancies are attracted in the compression zone of dislocation and expelled from the tension zone, while the opposite behavior is observed for SIAs. The fluxes of alloying elements are coupled to the ones of PDs: in the same direction for SIAs and in the opposite direction for vacancies (see Eqs. 4.6 and 4.7). As a consequence, atom enrichment is due to SIAs and depletion due to vacancies. Thus, with elastic interactions, atom enrichment is expected in the tension zone and depletion in the compression zone of the dislocation. Without elasticity, Cr enrichment is obtained in Fe-11%Cr at 700 K (respectively depletion in Fe-15%Cr at 900 K) which means that Cr migrates preferentially through SIAs in Fe-11%Cr at 700 K (respectively through vacancies in Fe-15%Cr at 900 K). Finally, when elastic interactions are taken into account, the Cr segregation is the result of the competition between the kinetic (Onsager coefficients) and the elasticity effects. Thus, in Fe-11%Cr at 700 K there is competition between Cr enrichment-enrichment in

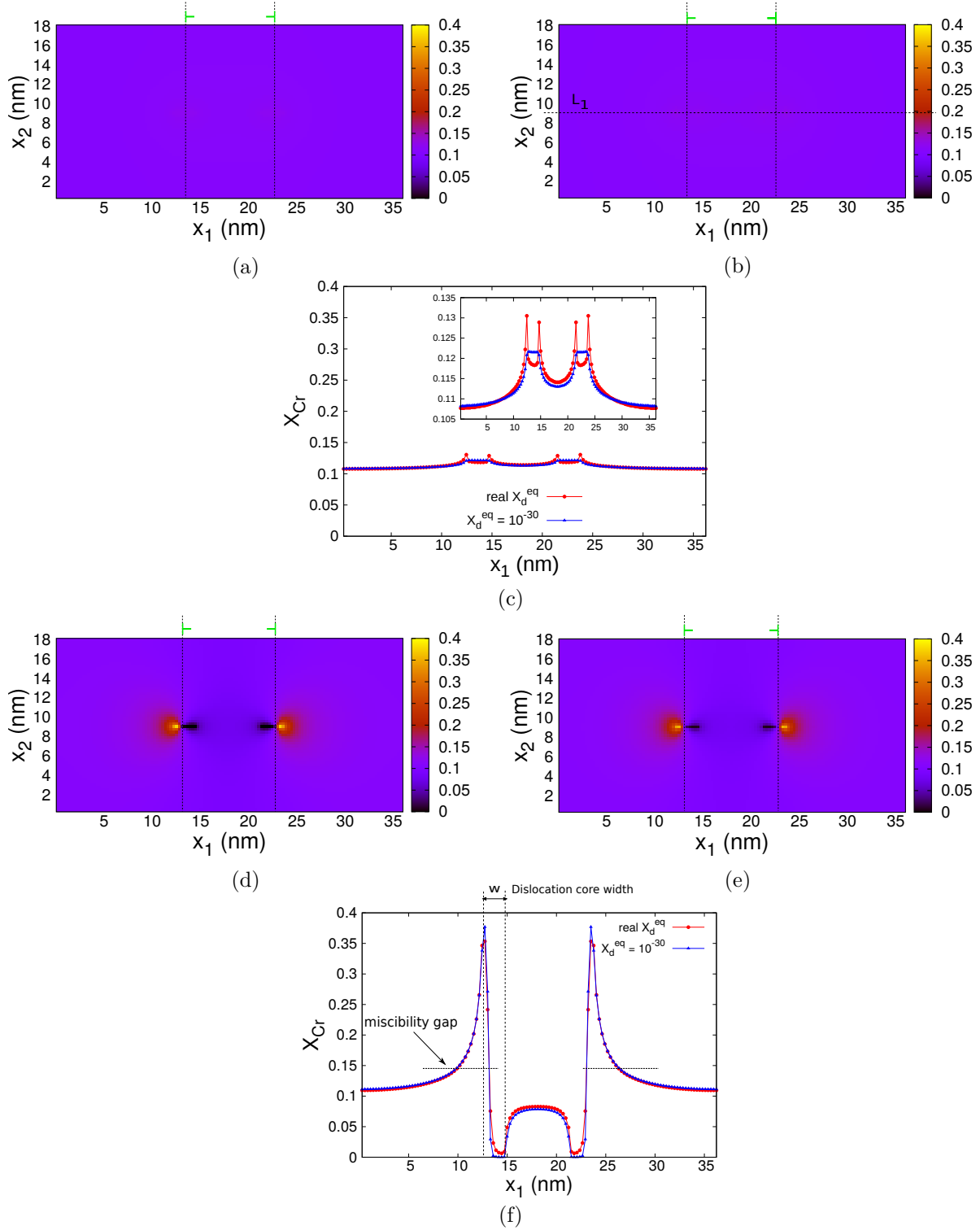


Figure 4.4: Atomic fraction maps of Cr without elasticity a) $X_d^{eq} = 10^{-30}$, b) real X_d^{eq} and with elasticity d) $X_d^{eq} = 10^{-30}$, e) real X_d^{eq} , and the corresponding profiles along the L_1 axis passing through the dislocation cores c) without elasticity and f) with elasticity in Fe-11%Cr alloy at 700 K for a dose of 0.34 dpa, $K_0 = 10^{-5}$ dpa.s $^{-1}$.

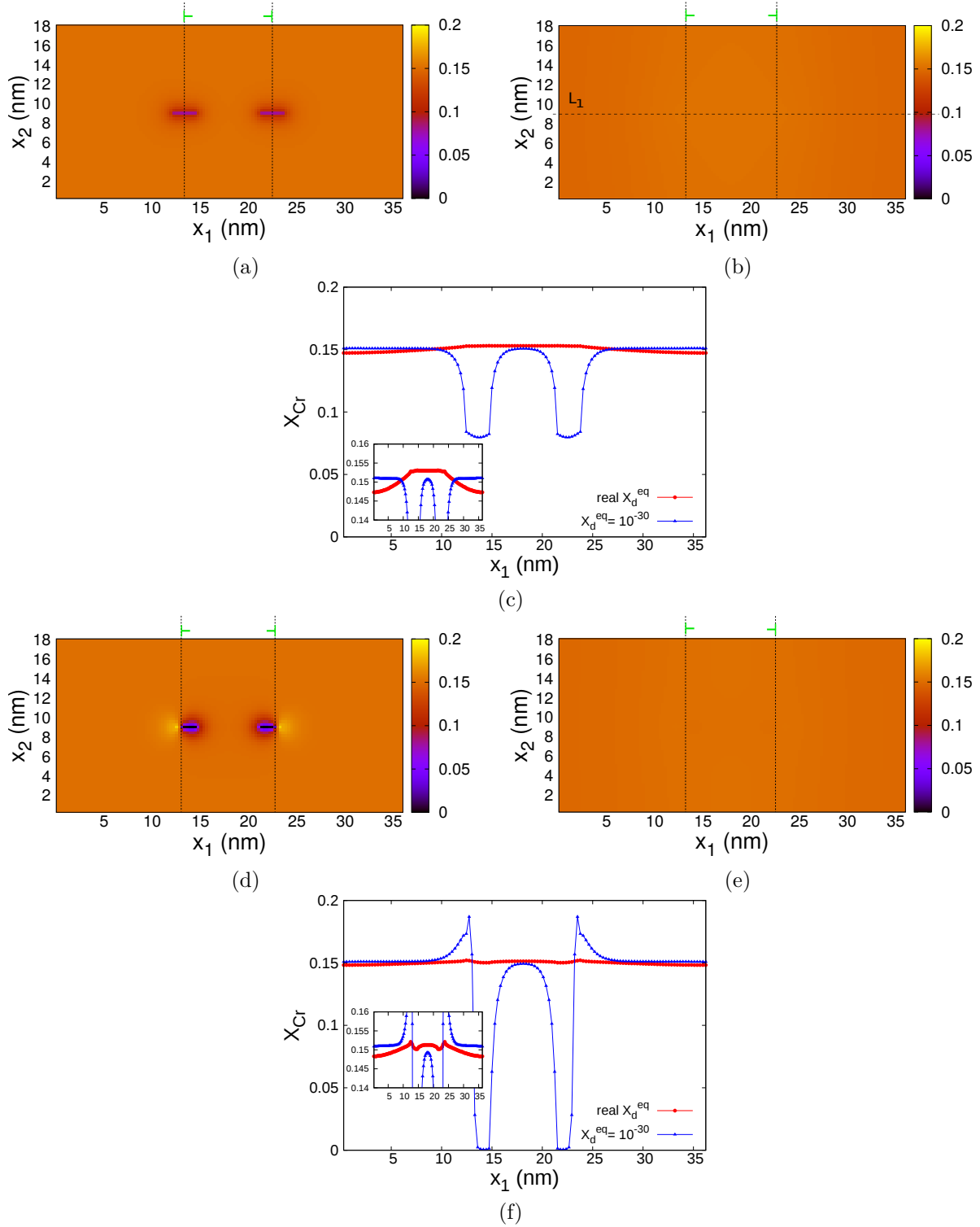


Figure 4.5: Atomic fraction maps of Cr without elasticity a) $X_d^{eq} = 10^{-30}$, b) real X_d^{eq} and with elasticity d) $X_d^{eq} = 10^{-30}$, e) real X_d^{eq} , and the corresponding profiles along the L_1 axis passing through the dislocation cores c) without elasticity and f) with elasticity in Fe-15%Cr alloy at 900K for a dose of 9.5×10^{-3} dpa, $K_0 = 10^{-5}$ dpa.s $^{-1}$.

the tension region and enrichment-depletion in the compression region. This leads finally to Cr enrichment in the tension zone and depletion in the compression zone (see Fig. 4.4-d)). In the same way, there is competition between Cr depletion-enrichment in the tension region and depletion-depletion in the compression region of dislocations in Fe-15%Cr at 900 K which leads to Cr enrichment in the tension region and depletion in the compression region (see Fig. 4.5-d)).

These results show that the Cr segregation is globally controlled by the elasticity effects. Especially, for the Fe-11%Cr alloy, in the tension region where Cr is enriched, the Cr composition locally exceeds the solubility limit (see 4.4-f)) which is not the case without elasticity, and precipitation of the α' phase is expected in this zone. In Fe-15%Cr, the Cr composition in the compression region is close to zero (see 4.5-f)) which can induce locally a sharp decrease in the hardening or corrosion resistance, since Cr improves the hardening of Fe-Cr alloys [107]. Moreover, in the region where kinetic and elasticity effects are antagonists, elasticity plays a predominant role for RIS in the studied alloys. The results presented above are qualitatively the same as those of [102] with the difference that simulations in [102] were performed using Eq. 2.39 for the sink description and the atom fluxes were set to zero inside the core region.

Regarding the effect of X_d^{eq} , simulations have also been performed for the real value of X_d^{eq} . The results show that, in Fe-11%Cr at 700 K, the RIS prediction doesn't change by considering the real X_d^{eq} or zero as illustrated on Figs. 4.4-c) and 4.4-f). On the contrary, in Fe-15%Cr at 900 K, RIS is almost annihilated when the real value of X_d^{eq} is considered (see Figs. 4.5-c) and 4.5-f)), while RIS takes place for $X_d^{eq} = 10^{-30}$. This significant RIS reduction has been obtained in [82] under the conditions X_d^{eq} fixed to zero and X_d^q set to its real value near a planar sink at temperatures above 880 K for $K_0 = 10^{-5}$ dpa.s $^{-1}$. As mentioned by Piochaud et al. [82], at high temperatures, steady-state PD concentrations may no longer exceed the equilibrium concentrations and the PD driving forces tend to zero (consequently the atom driving forces also). It is the case for vacancies in Fe-15%Cr at 900 K for the chosen PD generation rate, but not for SIAs which explains the low Cr segregation observed on Fig. 4.5-c) and f). The vacancy concentration at steady state,

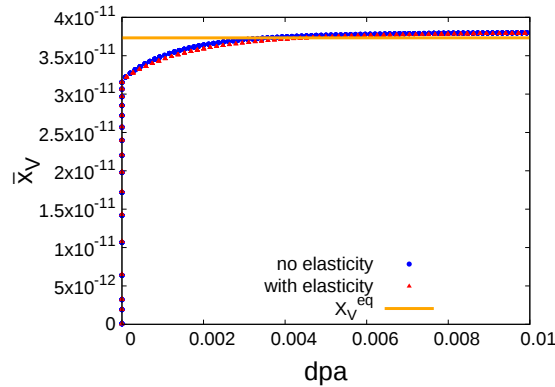


Figure 4.6: Evolution of the average atomic fraction of vacancies as a function of dose in Fe-15%Cr at 900 K for the real value of X_d^{eq} , $K_0 = 10^{-5}$ dpa.s $^{-1}$.

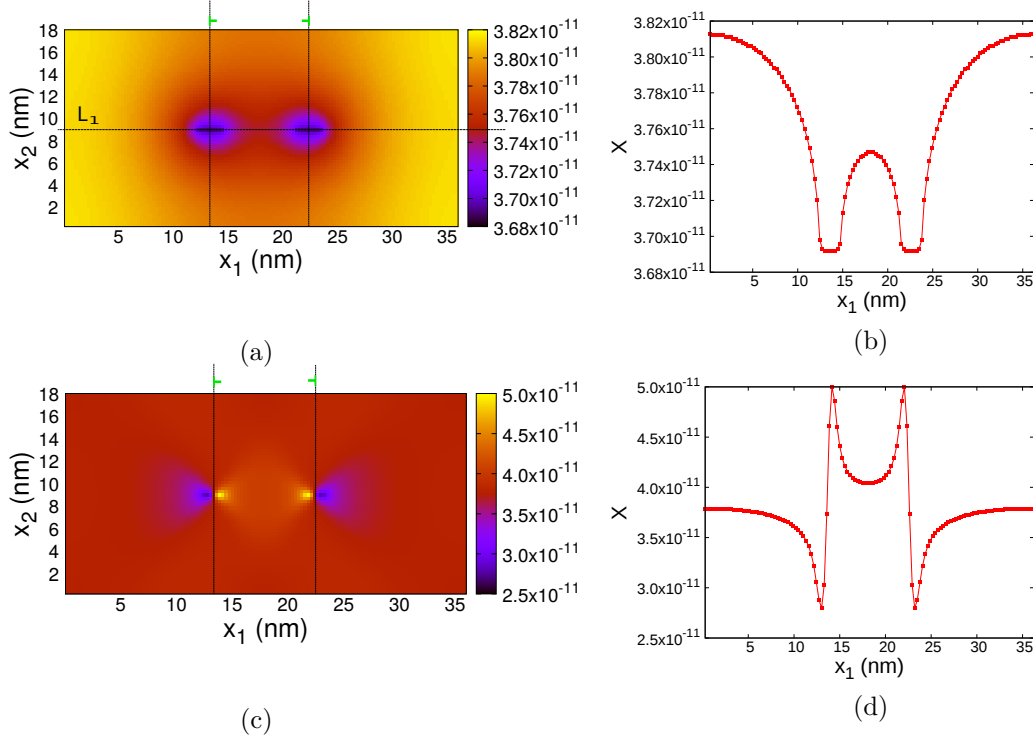


Figure 4.7: Atomic fraction maps of vacancies in Fe-15%Cr at 900 K (real value of X_d^{eq}) a) without elasticity, c) with elasticity, and the corresponding profiles along the dipole b) without elasticity, d) with elasticity, at a dose of 9.5×10^{-3} dpa, $K_0 = 10^{-5}$ dpa.s $^{-1}$.

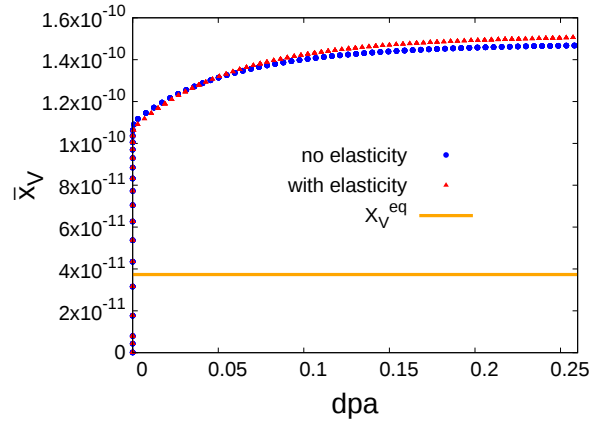


Figure 4.8: Evolution of the average atomic fraction of vacancies as a function of dose in Fe-15%Cr at 900 K for the real value of X_d^{eq} with a PD generation rate of $K_0 = 10^{-3}$ dpa.s $^{-1}$.

in this case, is very close to the thermal equilibrium value (see Fig. 4.6). There is no

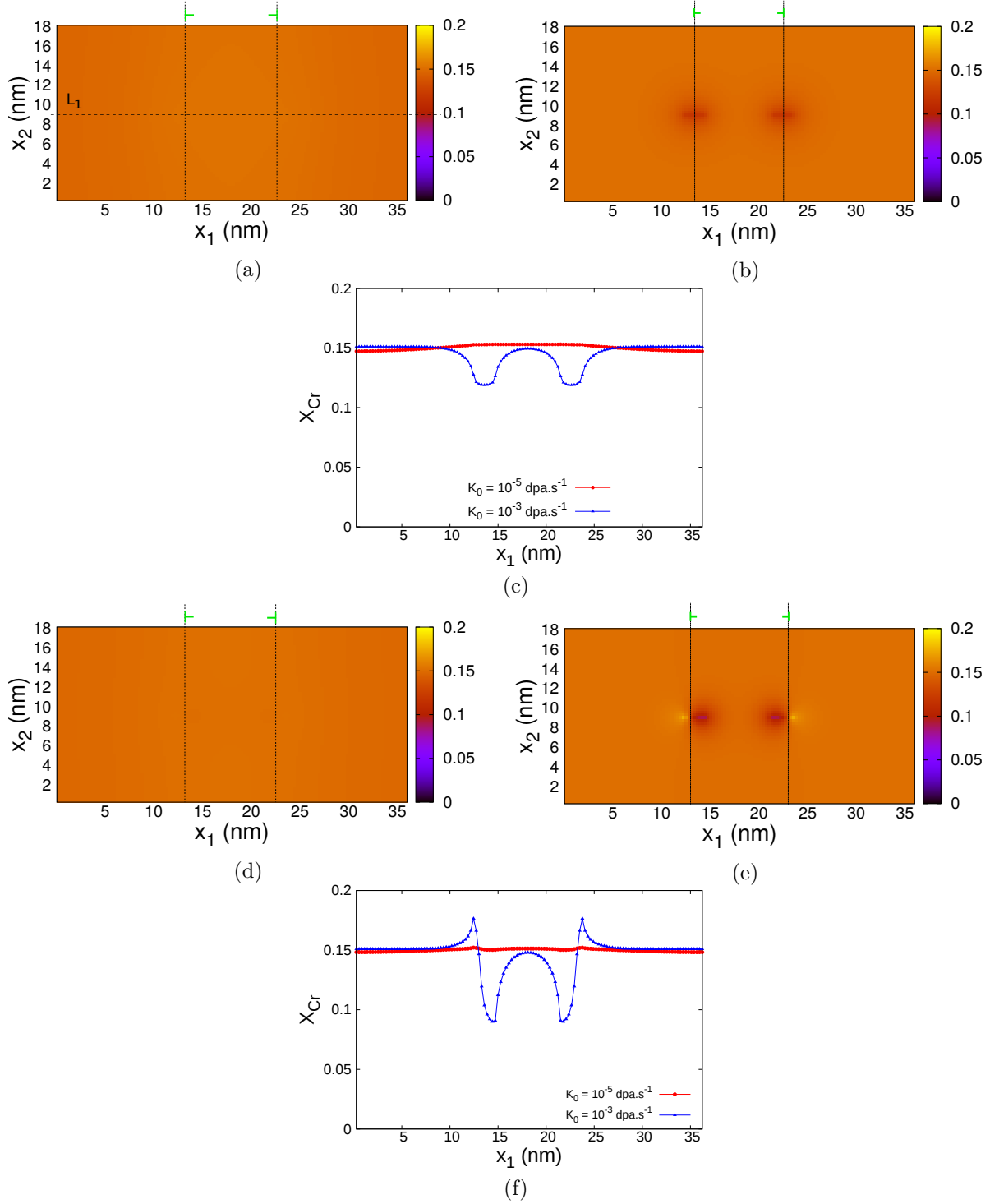


Figure 4.9: Atomic fraction maps of Cr without elasticity a) $K_0 = 10^{-5} \text{ dpa.s}^{-1}$, b) $K_0 = 10^{-3} \text{ dpa.s}^{-1}$ and with elasticity d) $K_0 = 10^{-5} \text{ dpa.s}^{-1}$, e) $K_0 = 10^{-3} \text{ dpa.s}^{-1}$, and the corresponding profiles along L_1 axis passing through the dislocation cores c) without elasticity and f) with elasticity in Fe-15%Cr alloy at 900K for a dose of $9.5 \times 10^{-3} \text{ dpa}$ and for the real value of X_d^{eq} .

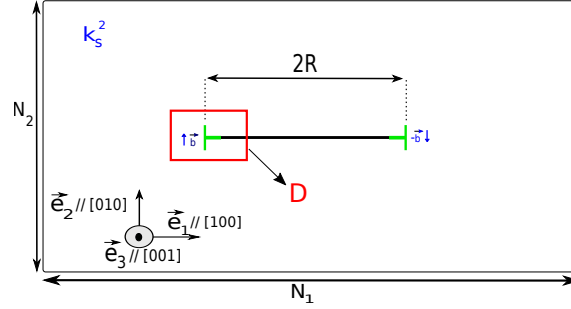


Figure 4.10: 2D simulation box mimicking a $\langle 100 \rangle$ -type interstitial dislocation loop co-existing with other sinks represented by the mean sink strength k_s^2 .

significant concentration gradient of vacancies due to their absorption near the dislocation cores (see Fig. 4.7) which leads to the non significant Cr segregation as shown in Figs. 4.5-c) and 4.5-f). To further explore this issue, the simulations of RIS prediction in Fe-15%Cr at 900 K were performed again but with a PD generation rate of $K_0 = 10^{-3} \text{ dpa.s}^{-1}$. The vacancy concentration at steady state is in this case higher than the thermal value as shown in Fig. 4.8. The Cr maps and profiles along the dipole are plotted in Fig. 4.9 and it can be seen that RIS occurs for the new PD generation rate. Thus, the PD equilibrium concentration plays an important role on RIS prediction especially at high temperatures as shown by the results above.

To conclude this section, RIS was predicted near dislocation cores in a regime where the atom diffusion is faster than the dislocation motion (quasi-static dislocations). The results obtained show that, the prediction changes significantly when elastic interactions are taken into account. It has also been shown that the equilibrium PD fraction at the sink plays an important role. In section 4.3.2, the dislocation motion due to PD absorption is taken into account and we investigate the climb rate effects.

4.3.2 Effects of the dislocation climb rate on RIS prediction

To investigate the effects of dislocation climb on the RIS prediction, simulations described in section 3.2.5 were done: simulation type 1 (system free of any other sink and $K_0^I \neq K_0^V$) and 2 (system including another sink and $K_0^I = K_0^V$). So far, to simulate the presence of another sink, the latter was explicitly introduced in the system (simulation type 2) and the additional term $J_{s,d}^{abs}$ was not used in the PD evolution equations. Another possibility is to use the following expression of $J_{s,d}^{abs}$:

$$J_{s,d}^{abs} = k_s^2 D^d (X_d - X_d^s) \quad (4.32)$$

where k_s^2 is the sink strength of the surrounding microstructure assumed neutral. Thus, the edge dislocation dipole evolves in a system with a mean sink strength k_s^2 associated to the other sinks as illustrated in Fig. 4.10. This configuration will be referred as simulation type 3 in the following. The PD equilibrium composition X_d^{eq} were set to their real values. The subscript l was suppressed in the notation of η for simplicity.

4.3.2.1 Simulation type 1: system containing a dipole of edge dislocations free of any other sink

To obtain a climb velocity at steady state, simulations of type 1 described in section 3.2.5 were first performed (system free of any other sink and $K_0^I \neq K_0^V$). K_0^I and K_0^V were chosen such as $K_0^I > K_0^V$ to obtain an interstitial loop growth. The order of magnitude of K_0^d was chosen such that RIS can occur, according to the results of section 4.3.1. The evolution equations of atom compositions X_α and dislocation loop order parameter η were integrated simultaneously as indicated in the multi-time step algorithm described in section 4.2.4. It clearly appears that two kinetic regimes are possible: the kinetic regime in which the atom diffusion is faster than the dislocation motion $t_0^\alpha < t_0^\eta$, and the other one where the atom diffusion is slower than the dislocation motion $t_0^\alpha > t_0^\eta$. The variations of the ratio t_0^η/t_0^α were estimated at the nominal composition as a function of K_0^I for a fixed value of K_0^V . t_0^η was easily calculated since in simulation of type 1, the climb rate depends only on the PD generation rates and the system volume (see Eq. 3.51). To compute D^α (see Eq. 4.19) and access t_0^α given by Eq. 4.17, the following solution of the PD fraction at steady state for cylindrical sinks (see Fig. 3.1) was used [10]:

$$X_d(\mathbf{r}) = X_d(r_0) + \frac{K_0^d R^2}{2D^d} \left[\ln(r/r_0) - \frac{r^2 - r_0^2}{2R^2} \right] \quad (4.33)$$

The spatial maximum of D^α was considered. Fig. 4.11 shows the variations of the ratio t_0^η/t_0^α in the alloys and thus gives an indication on the choice of K_0^I for K_0^V fixed to observe the two kinetic regimes mentioned above. To distinguish these two regimes, the following

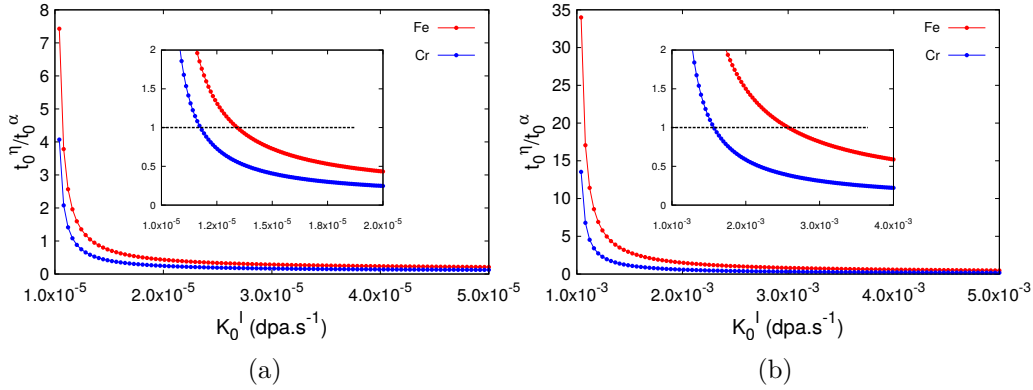


Figure 4.11: Variations of the ratio t_0^η/t_0^α at the nominal composition as a function of K_0^I in a) Fe-11%Cr at 700 K for $K_0^V = 10^{-5}$ dpa.s⁻¹ and b) Fe-15%Cr at 900 K for $K_0^V = 10^{-3}$ dpa.s⁻¹.

values of K_0^I were chosen: $K_0^I = 1.05 \times 10^{-5}$ dpa.s⁻¹ ($t_0^\alpha < t_0^\eta$) and $K_0^I = 2 \times 10^{-5}$ dpa.s⁻¹ ($t_0^\alpha > t_0^\eta$) for Fe-11%Cr at 700 K ($K_0^V = 10^{-5}$ dpa.s⁻¹), $K_0^I = 1.05 \times 10^{-3}$ dpa.s⁻¹ ($t_0^\alpha < t_0^\eta$) and $K_0^I = 2 \times 10^{-3}$ dpa.s⁻¹ ($t_0^\alpha > t_0^\eta$) for Fe-15%Cr at 900 K ($K_0^V = 10^{-3}$ dpa.s⁻¹). These PD generation rates correspond to a climb rate of 5.79×10^{-13} m.s⁻¹ ($t_0^\alpha < t_0^\eta$) and 1.16×10^{-11} m.s⁻¹ ($t_0^\alpha > t_0^\eta$) for Fe-11%Cr at 700 K, 5.79×10^{-11} m.s⁻¹ ($t_0^\alpha < t_0^\eta$) and 1.16×10^{-9} m.s⁻¹ ($t_0^\alpha > t_0^\eta$) for Fe-15%Cr at 900 K.

In the kinetic regime where atoms diffuse faster than the dislocation motion, the size and the shape of the Cr atmosphere around the dislocation cores for both alloys are weakly affected by the dislocation motion as shown by the iso-concentrations of the maps of Figs. 4.12 and 4.13, which is expected. The corresponding Cr profiles for static and moving dislocations given in Fig. 4.12-c) and Fig. 4.13-c) show also that the Cr segregation level is practically unchanged with the dislocation motion. The evolution of the Cr profile as a function of dose in this regime is illustrated in Fig. 4.14 for Fe-11%Cr at 700 K, and shows that the Cr segregation at a given point and dose depends on the dislocation position at this dose. For example, a point located at a given dose in the tension region of the dislocation is Cr enriched but at the passage of the compression region by this point, there is Cr depletion.

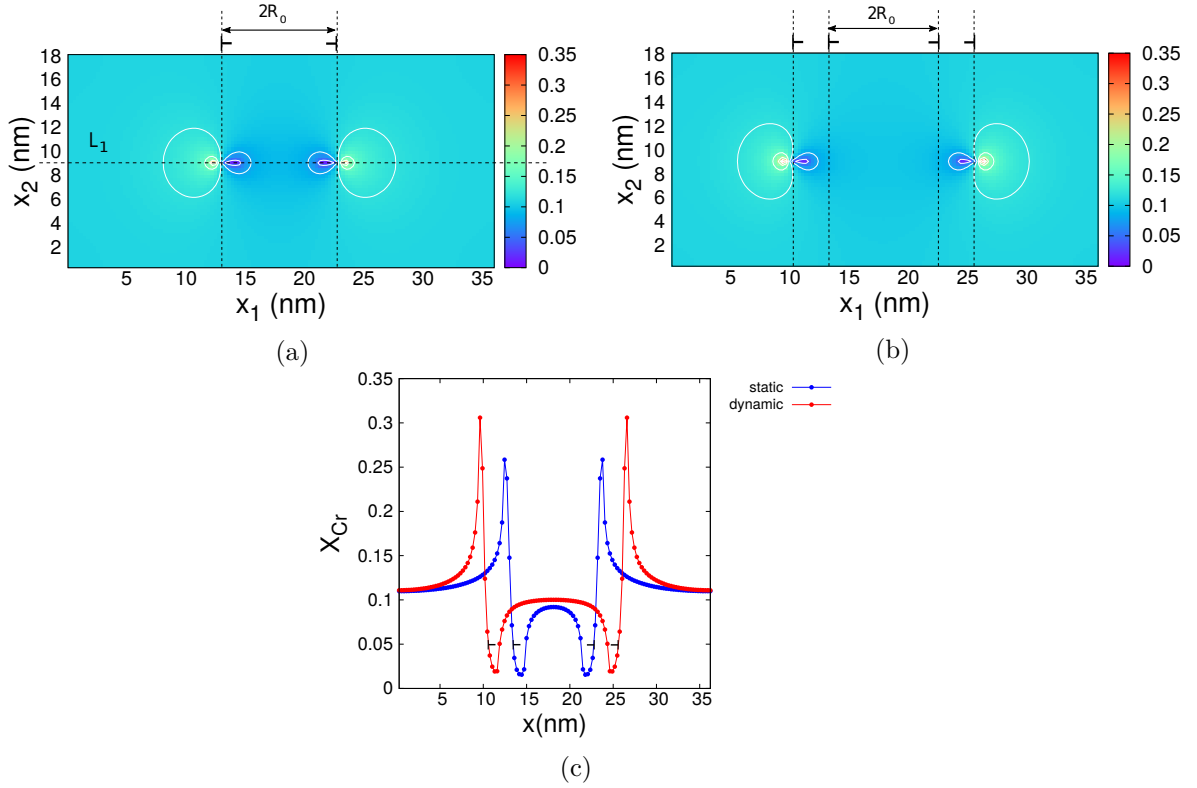


Figure 4.12: Atomic fraction map of Cr for a) static and b) dynamic dislocations, and c) the corresponding profiles along L_1 axis at a dose of 0.058 dpa, in the kinetic regime where the atom diffusion is faster than the dislocation motion ($t_0^\alpha < t_0^\eta$) for Fe-11%Cr at 700 K, $K_0^I = 1.01 \times 10^{-5}$ dpa.s $^{-1}$ and $K_0^V = 10^{-5}$ dpa.s $^{-1}$.

In the kinetic regime where dislocation moves faster than the atom diffusion, there is a significant change in the size and shape of the Cr atmosphere around the dislocation cores for both alloys as illustrated by the iso-concentrations of the Cr maps of Figs 4.15 and 4.16. Indeed, these iso-concentrations are flattened due to the fast motion of dislocation compared to the atom diffusion. The Cr segregation level is also affected by the dislocation motion as shown in Figs. 4.15-c) and 4.16-c). In Fe-15%Cr at 900 K, the Cr segregation

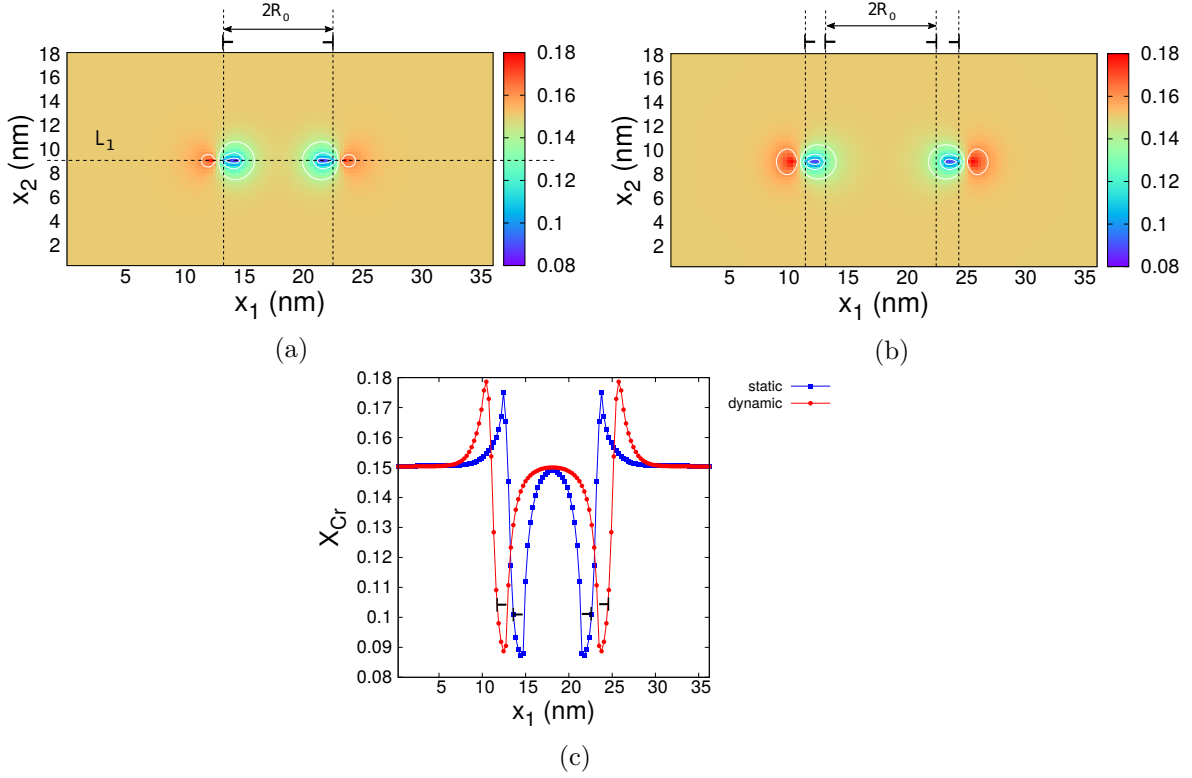


Figure 4.13: Atomic fraction map of Cr for a) static and b) dynamic dislocations, and c) the corresponding profiles along L_1 axis at a dose of 0.01 dpa, in the kinetic regime where the atom diffusion is faster than the dislocation motion ($t_0^\alpha < t_0^\eta$) for Fe-15%Cr at 900 K, $K_0^I = 1.01 \times 10^{-3}$ dpa.s $^{-1}$ and $K_0^V = 10^{-3}$ dpa.s $^{-1}$.

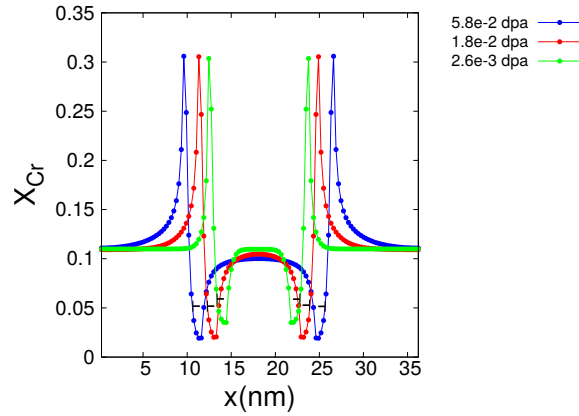


Figure 4.14: Atomic fraction profile of Cr along L_1 axis for dynamic dislocations at different doses, in the kinetic regime where the atom diffusion is faster than the dislocation motion ($t_0^\alpha < t_0^\eta$) for Fe-11%Cr at 700 K, $K_0^I = 1.05 \times 10^{-5}$ dpa.s $^{-1}$ and $K_0^V = 10^{-5}$ dpa.s $^{-1}$.

level along the dipole changes slightly with the dislocation motion (see Fig. 4.16-c)). This may be due to the fact that, for the chosen SIA effective generation rate of 2×10^{-3} dpa.s $^{-1}$,

the ratio t_0^η/t_0^α is not far enough from 1 as shown in Fig. 4.11-b). On the other hand, in Fe-11%Cr at 700 K the ratio t_0^η/t_0^α is further away from 1 (see Fig. 4.11-a)), which allows to explain the remarkable change of the Cr segregation profile as shown in Fig. 4.15-c), especially in the compression region where there is no more Cr depletion compared to the static profile for the dose reached (see Fig. 4.15-c)). The evolution of the Cr profile along

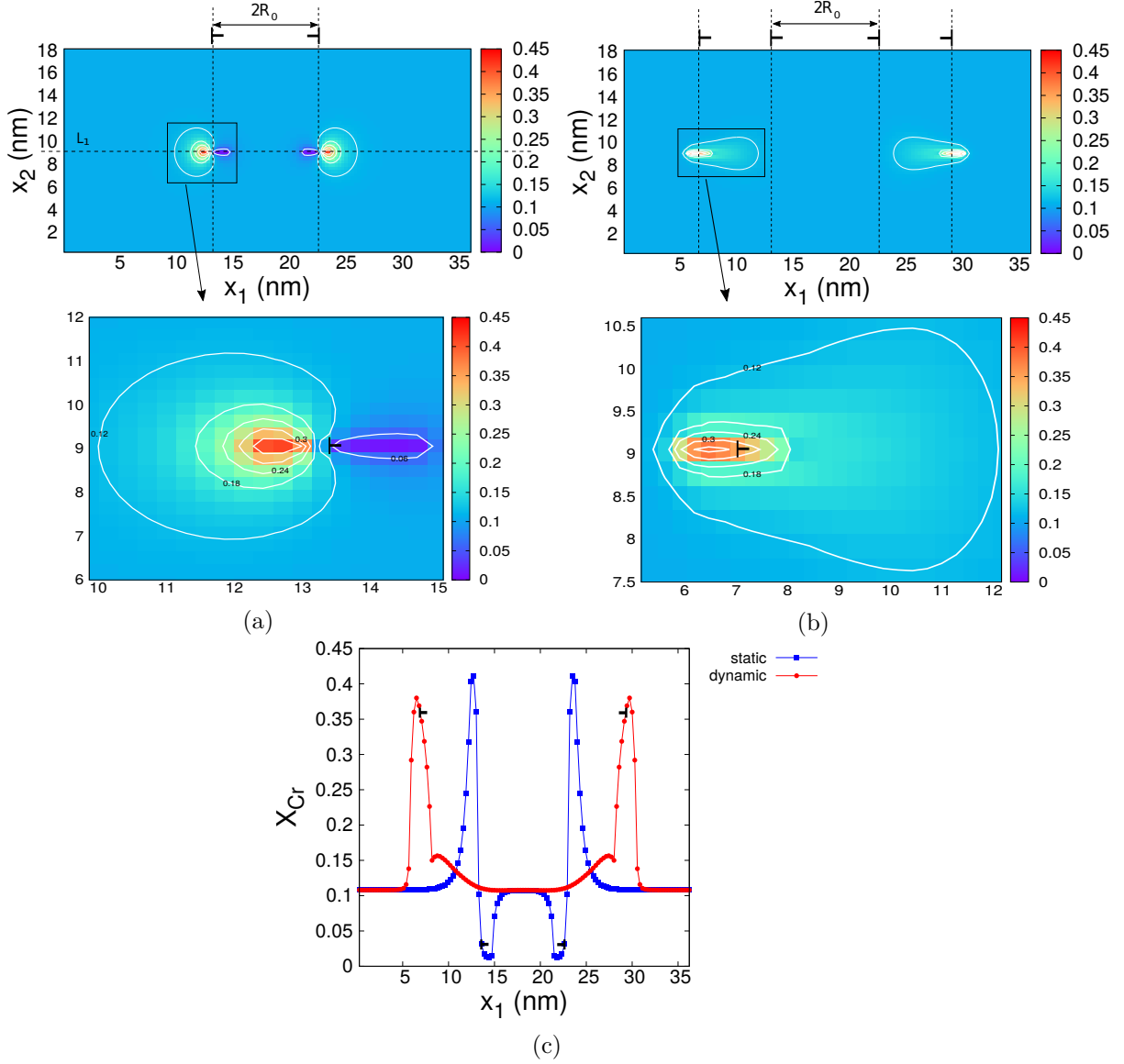


Figure 4.15: Atomic fraction map of Cr for a) static and b) dynamic dislocations, and c) the corresponding profiles along L_1 axis at a dose of 0.012 dpa, in the kinetic regime where the atom diffusion is slower than the dislocation motion ($t_0^\alpha > t_0^\eta$) for Fe-11%Cr at 700 K, $K_0^I = 2 \times 10^{-5}$ dpa.s $^{-1}$ and $K_0^V = 10^{-5}$ dpa.s $^{-1}$.

the dipole as a function of dose during the loop growth is plotted in Figs. 4.17 and 4.18. In Fe-15%Cr at 900 K, the Cr profile hardly changes with dose as shown in Fig. 4.18. In

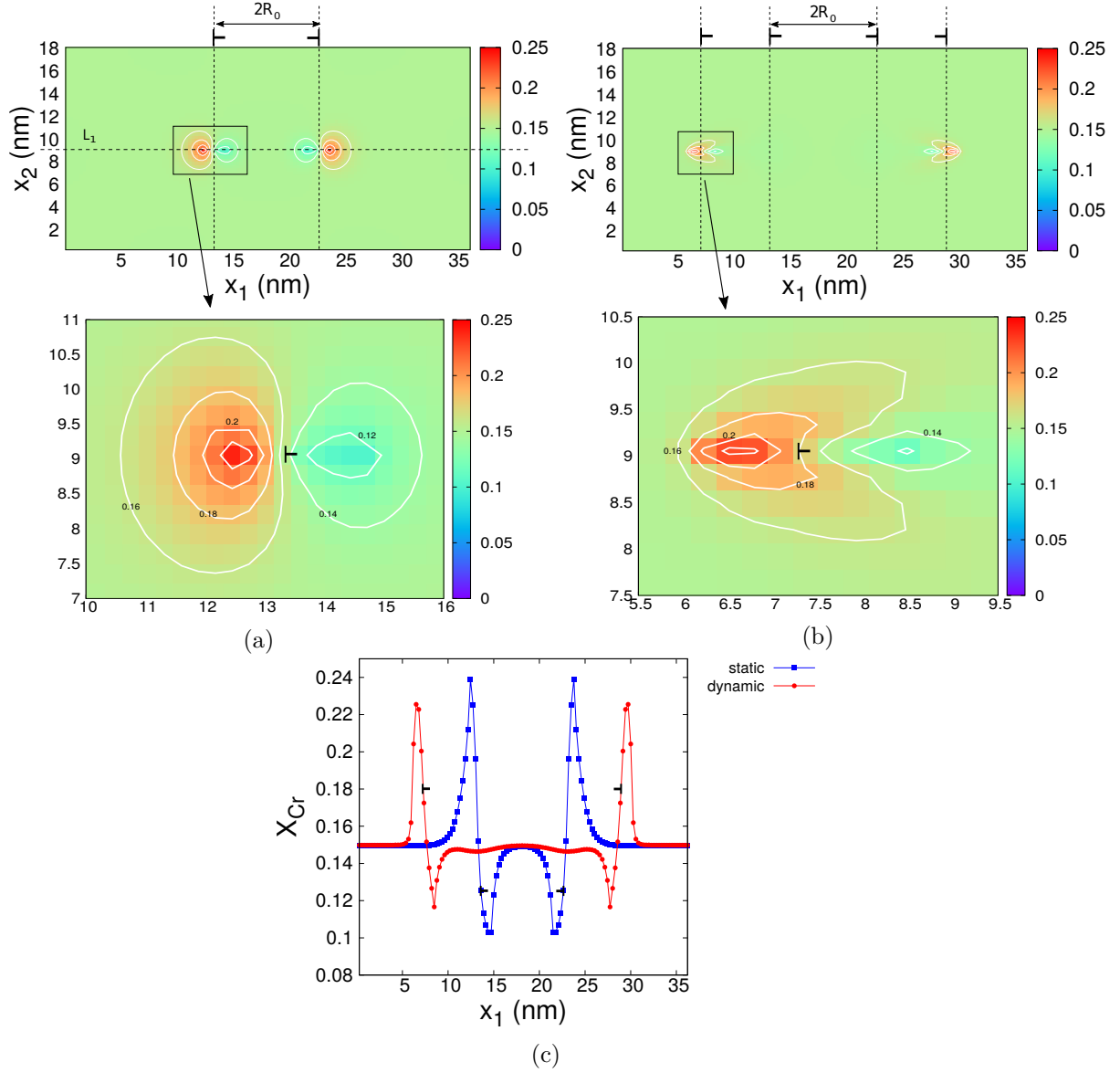


Figure 4.16: Atomic fraction map of Cr for a) static and b) dynamic dislocations, and c) the corresponding profiles along L_1 axis at a dose of 0.011 dpa, in the kinetic regime where the atom diffusion is slower than the dislocation motion ($t_0^\alpha > t_0^\eta$) for Fe-15%Cr at 900 K, $K_0^I = 2 \times 10^{-3}$ dpa.s $^{-1}$ and $K_0^V = 10^{-3}$ dpa.s $^{-1}$.

Fe-11%Cr at 700 K, it can be seen that the static Cr profile tends to be established at the beginning of the loop growth (see Fig. 4.17): Cr enrichment in the tension region and depletion in the compression region of dislocation. During loop growth, the Cr depletion in the compression region is no longer observed and there is only Cr enrichment in all sides of the dislocation. This can be explained by the fact that the compression region moves towards the position where the tension region was previously during loop growth. As the tension region was initially enriched in Cr, this region will become progressively depleted

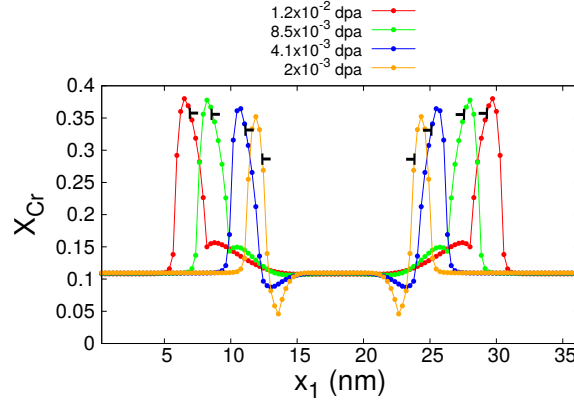


Figure 4.17: Atomic fraction profile of Cr along L_1 axis for dynamic dislocations at different doses, in the kinetic regime where the atom diffusion is slower than the dislocation motion ($t_0^\alpha > t_0^\eta$) for Fe-11%Cr at 700 K, $K_0^I = 2 \times 10^{-5} \text{ dpa.s}^{-1}$ and $K_0^V = 10^{-5} \text{ dpa.s}^{-1}$.

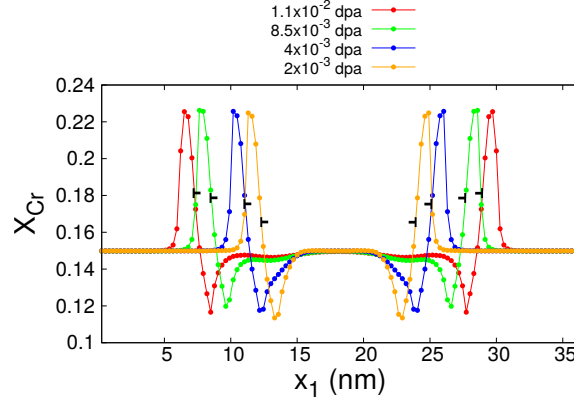


Figure 4.18: Atomic fraction profile of Cr along L_1 axis for dynamic dislocations at different doses, in the kinetic regime where the atom diffusion is slower than the dislocation motion ($t_0^\alpha > t_0^\eta$) for Fe-15%Cr at 900 K, $K_0^I = 2 \times 10^{-3} \text{ dpa.s}^{-1}$ and $K_0^V = 10^{-3} \text{ dpa.s}^{-1}$.

in Cr in order to establish the Cr segregation profile of the compression zone observed in the static case. But due to the faster motion of dislocations, the establishment of this Cr profile in the compression region (depletion) does not have time to fully occur (see Fig. 4.17).

4.3.2.2 Simulation type 2: system containing a dipole of edge dislocations and a planar sink

The system containing the dipole of edge dislocations and the planar sink is illustrated in Fig. 3.21. The effects of the resulting loop growth rate due to biased dislocations (see section 3.2.5) on the RIS prediction were investigated. The PD generation rates were set to $K_0^d = 10^{-5} \text{ dpa.s}^{-1}$ for Fe-11%Cr at 700 K and $K_0^d = 10^{-3} \text{ dpa.s}^{-1}$ for Fe-15%Cr at 900 K. In Figures 4.19 and 4.20 the Cr atomic fraction maps and profiles for both studied alloys in static and dynamic regimes are plotted.

In [82], the case of the static regime (immobile sink), the isolated planar sink (free of any surrounding sink) is enriched in Cr in Fe-11%Cr at 700 K, while depletion is obtained in Fe-15%Cr at 900 K [82] (see Fig. 4.1). Furthermore, the results of section 4.3.1 indicate Cr enrichment in the tension region of dislocation and depletion in the compression zone for both alloys in the system containing only a dislocation dipole. In the case where the

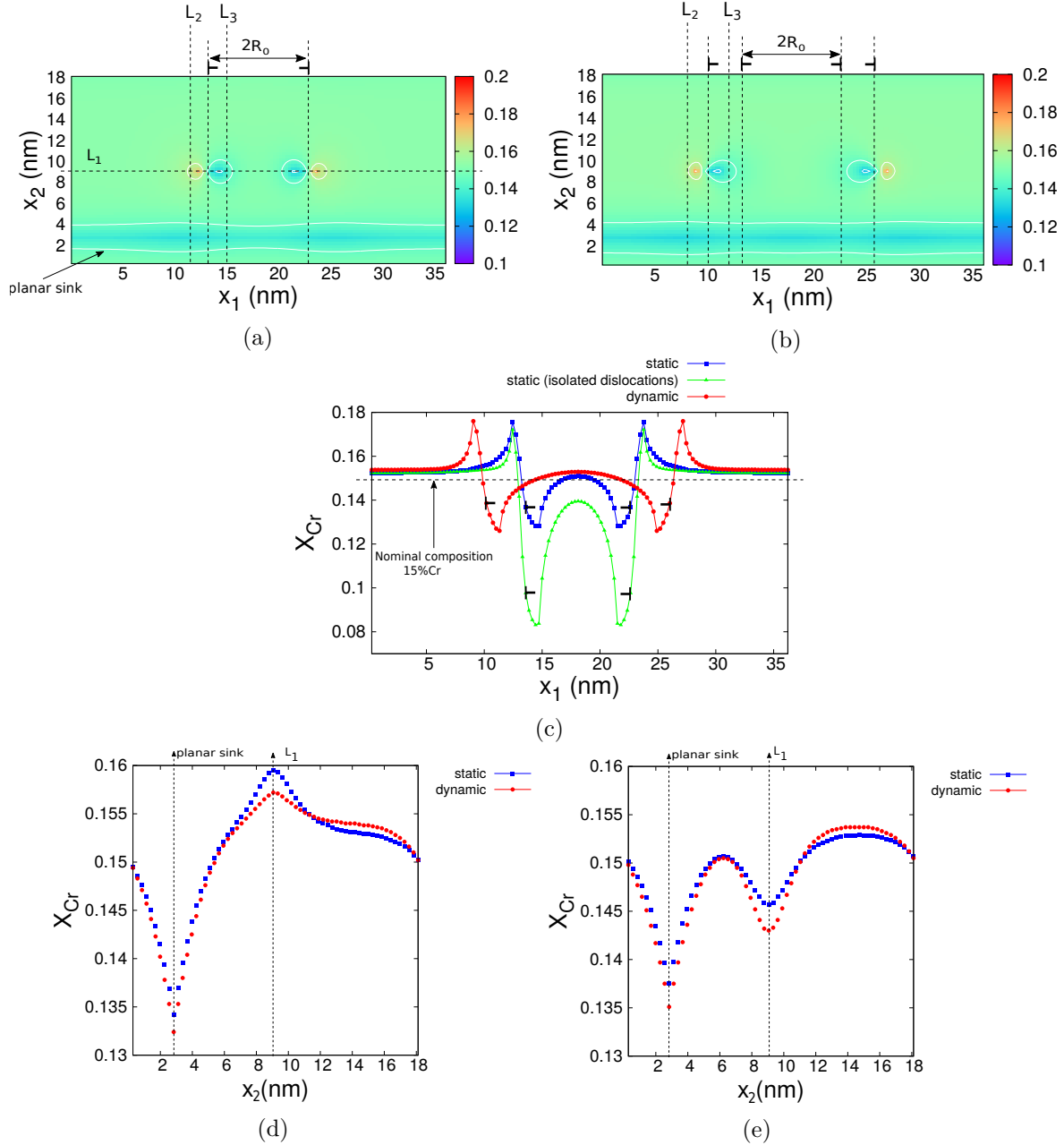


Figure 4.19: Atomic fraction map of Cr for a) static and b) dynamic dislocations, and the corresponding profiles along c) L_1 d) L_2 and e) L_3 axis at a dose of 0.031 dpa for Fe-15%Cr at 900 K, $K_0^d = 10^{-3} \text{ dpa.s}^{-1}$.

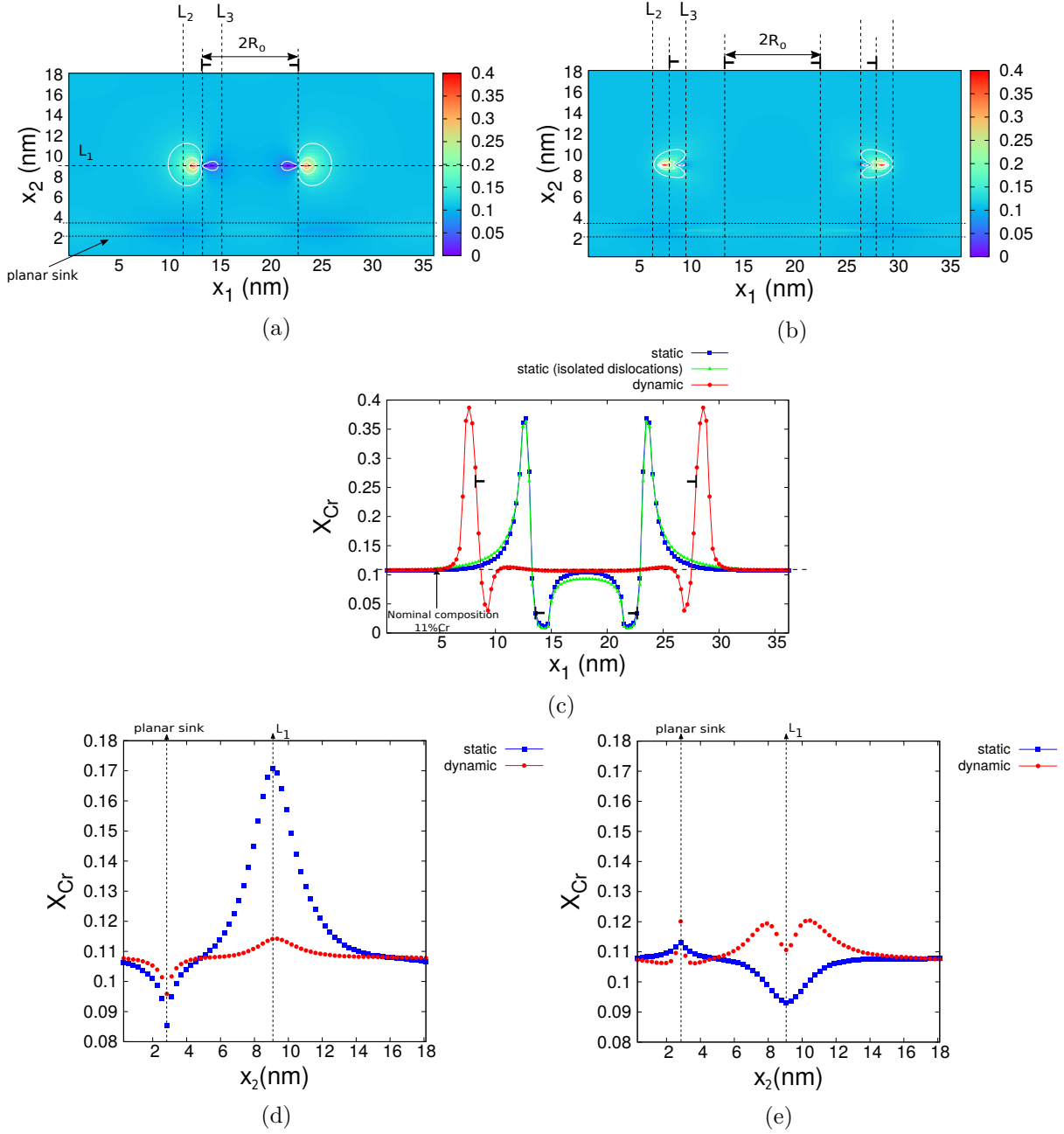


Figure 4.20: Atomic fraction map of Cr for a) static and b) dynamic dislocations, and the corresponding profiles along c) L_1 d) L_2 and e) L_3 axis at a dose of 0.047 dpa for Fe-11%Cr at 700 K, $K_0^d = 10^{-5} \text{ dpa.s}^{-1}$.

system contains both a dislocation dipole and a planar sink, the Cr map (see Fig. 4.19-a)) and profiles (see Figs. 4.19-c), d) and e)) in Fe-15%Cr at 900 K show Cr depletion along the planar sink, Cr enrichment in the tension zone and depletion in the compression zone of dislocations in the static regime, which is qualitatively similar to the tendencies observed when these sinks are not interacting. Furthermore, the Cr segregation level is modified in

the compression region when the planar sink is introduced in the system compared to the case of isolated dislocations (see Fig. 4.19-c)). This is due to the fact that the total Cr flux (see Eq. 4.7) towards the compression region of dislocations is strongly affected by the presence of the planar sink, while the Cr flux in the tension region changes weakly as shown in Fig. 4.21.

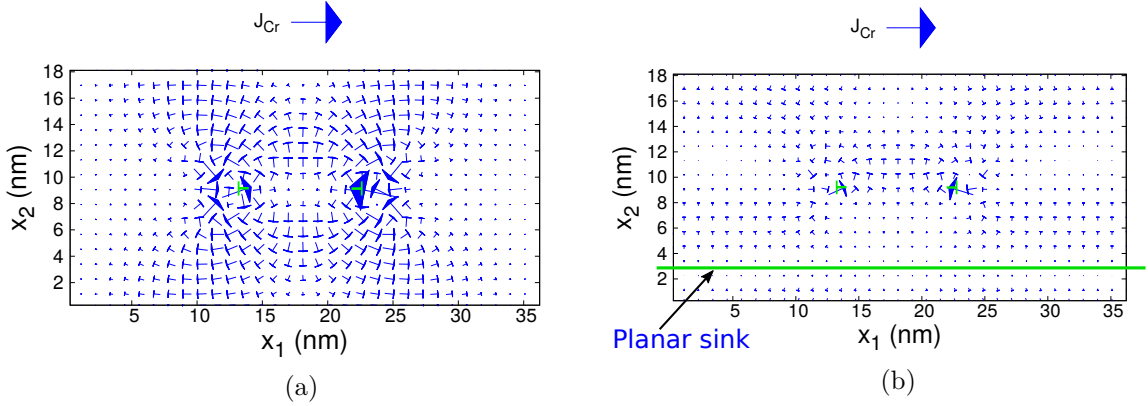


Figure 4.21: Total Cr flux in static regime for a system containing a) an isolated dipole of edge dislocations and b) a dipole of edge dislocations and a planar sink. The length of the vector is proportional to the norm of the flux $\|\mathbf{J}\| = \sqrt{J_1^2 + J_2^2}$.

In Fe-11%Cr at 700 K, there is Cr enrichment and depletion respectively in the tension and compression region of dislocations (see Figs. 4.20-a) and b)) like in the case of isolated dislocations (see Fig. 4.4-d) and f)). However, Cr enrichment is not always obtained along the planar sink (see Figs. 4.20-a), d) and e)) like in the case of a free planar sink. Indeed, the Cr profiles of Figs. 4.20-d) and e) for static dislocations show the Cr depletion in the region of the planar sink located below the tension zone of dislocation, and Cr enrichment in the region of the planar sink located below the compression zone. This can be explained as follows. As SIAs (respectively vacancies) are more attracted towards the tension (respectively compression) region of the dislocation, and as atom fluxes are coupled to PD fluxes (see Eqs. 4.7 and 4.6), the Cr fluxes due to vacancies and SIAs are then affected. Especially, Cr atoms are more drifted towards the tension region due to SIAs (see Fig. 4.22-a) and more expelled from the compression region due to vacancies (see Fig. 4.22-b)). The planar sink being located close to dislocations, the Cr fluxes via SIAs and vacancies along it are consequently affected especially near the part located below the dislocations as shown in Fig. 4.22-a) and b). As the total Cr flow is the sum of the Cr flow due to vacancies and SIAs (see Eq. 4.7), the resulting Cr flow given in Fig. 4.22-c) is also affected along the planar sink which leads to the local dependence of the Cr segregation along it. This result shows that the RIS prediction depends also on the surrounding microstructure.

During the dynamic regime of dislocations, the size and the shape of the Cr atmosphere around dislocations are strongly affected in Fe-11%Cr at 700 K as illustrated on Fig. 4.20-b), but not remarkably in Fe-15%Cr at 900 K as shown on Fig. 4.19-b). Globally, the Cr profiles of Figs. 4.19-c), d), e) and Fig. 4.24 show that the Cr segregation level doesn't change with dislocation motion in Fe-15%Cr alloy. In Fe-11%Cr, the Cr segregation level

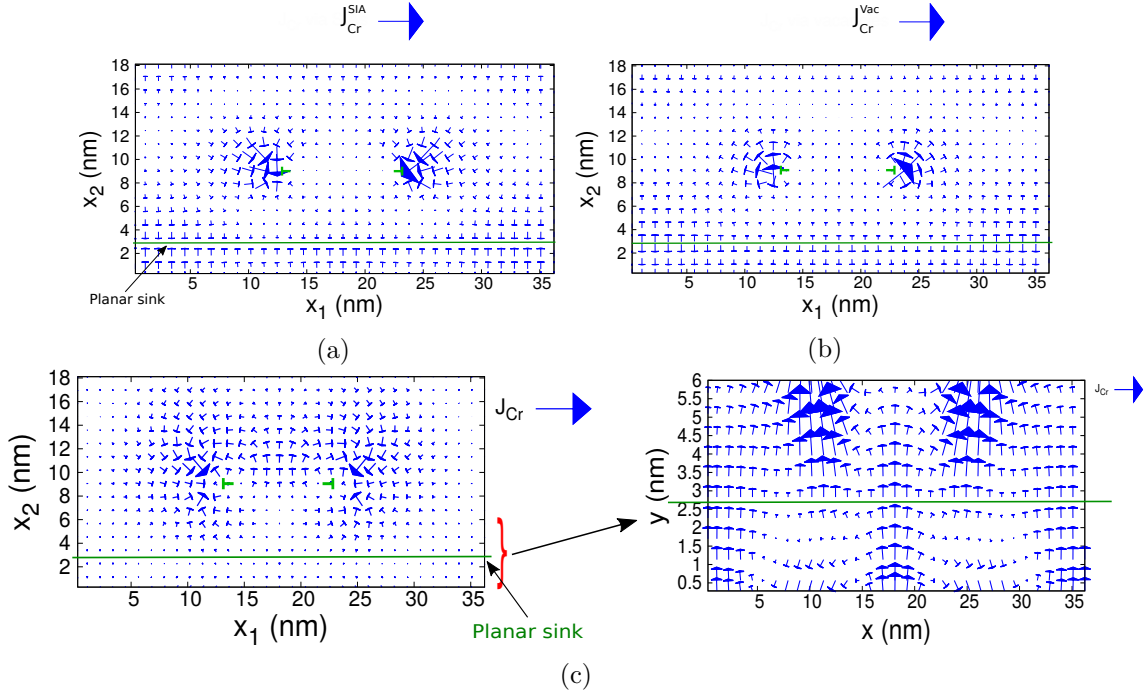


Figure 4.22: Cr flow through a) SIAs, b) vacancies and c) the total Cr flow (see Eq. 4.7) in the static regime of dislocations for Fe-11%Cr at 700 K. The length of the vector is proportional to the norm of the flux $\|J\| = \sqrt{J_1^2 + J_2^2}$, $K_0^d = 10^{-5} \text{dpa.s}^{-1}$.

along the dipole changes weakly as shown by the Cr profiles of Fig. 4.20-c) and Fig. 4.23, however the Cr profiles along the axis passing through the planar sink and the different regions of dislocations (see Fig. 4.20-d) and e)) show a significant change compared to the static profiles.

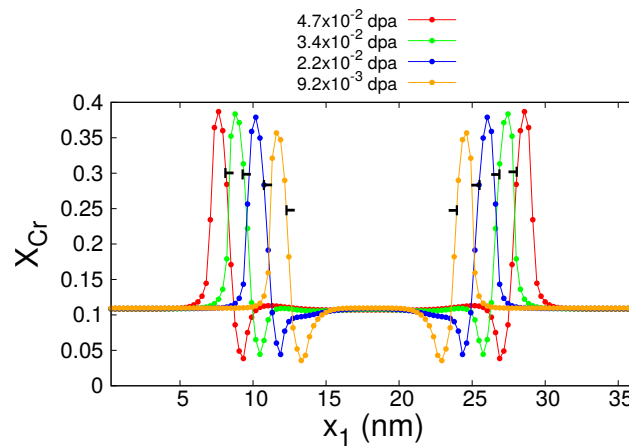


Figure 4.23: Atomic fraction profile of Cr along L_1 axis for dynamic dislocations at different doses for Fe-11%Cr at 700 K, $K_0^d = 10^{-5} \text{dpa.s}^{-1}$.

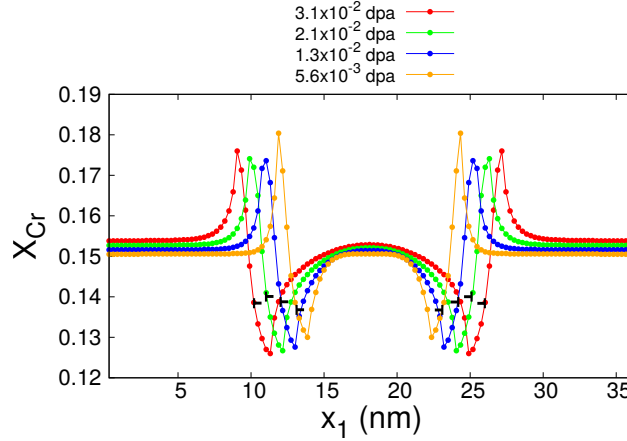


Figure 4.24: Atomic fraction profile of Cr along L_1 axis for dynamic dislocations at different doses for Fe-15%Cr at 900 K, $K_0^d = 10^{-3} \text{ dpa.s}^{-1}$.

4.3.3 Simulation type 3: system containing a dipole of edge dislocations with a mean sink strength k_s^2 associated to the other sinks

Simulations were performed for the Fe-14%Cr and Fe-18%Cr alloys at 800 K ($K_0 = 10^{-3} \text{ dpa.s}^{-1}$) because RIS was recently observed experimentally in these alloys near dislocation lines [108]. The climb rate and the average Cr atomic fraction $\bar{X}_{Cr}^{dislo}$ computed on a given domain D as illustrated in Fig. 4.10 are represented in Fig. 4.25 as a function of k_s^2 . The results of Fig. 4.25 show a good agreement between the climb rate obtained in our simulations and the one predicted analytically. These results show also that globally there is Cr enrichment in Fe-14%Cr and Cr depletion in Fe-18%Cr at dislocations for all the values of k_s^2 , which corresponds to the Cr segregation tendencies observed in [108]. It should be noted that the average Cr atomic fraction computed in our case depends on the choice of the domain D, which is at this stage arbitrary and therefore a more rigorous criterion for the choice of D will be necessary. Furthermore, Fig. 4.25 shows an increase followed by a decrease of the average Cr atomic fraction near dislocations in Fe-14%Cr with the increase of k_s^2 , while only an increase is obtained in Fe-18%Cr. To better understand this evolution of $\bar{X}_{Cr}^{dislo}$ with k_s^2 , the Cr maps and profiles are plotted in Figs. 4.26 and 4.27. These figures show globally that the size, the shape and the level of the Cr segregation around the dislocation core depend strongly on the values of k_s^2 . When we observe the profile of Fig. 4.26-d) the negative segregation zone corresponding to the compression one becomes less intense when k_s^2 increases. The same tendency is observed for Fe-18%Cr but however the average segregation around the dislocation remains negative in this case. On the whole, the segregation is globally positive (respectively negative) in the vicinity of the dislocation for Fe-14%Cr alloys (respectively Fe-18%Cr alloys) at $T = 800$ K. These tendencies are in good agreement with the experimental work of [108], which also reports Cr enrichment around dislocations in Fe-14%Cr at this temperature and Cr depletion in Fe-18%Cr. It must be pointed out that for these two alloys at $T = 800$ K, the study of [108] also reports a negative segregation at the grain boundaries, which is an experimental evidence that the RIS at dislocations and GBs is different. From the simulation results

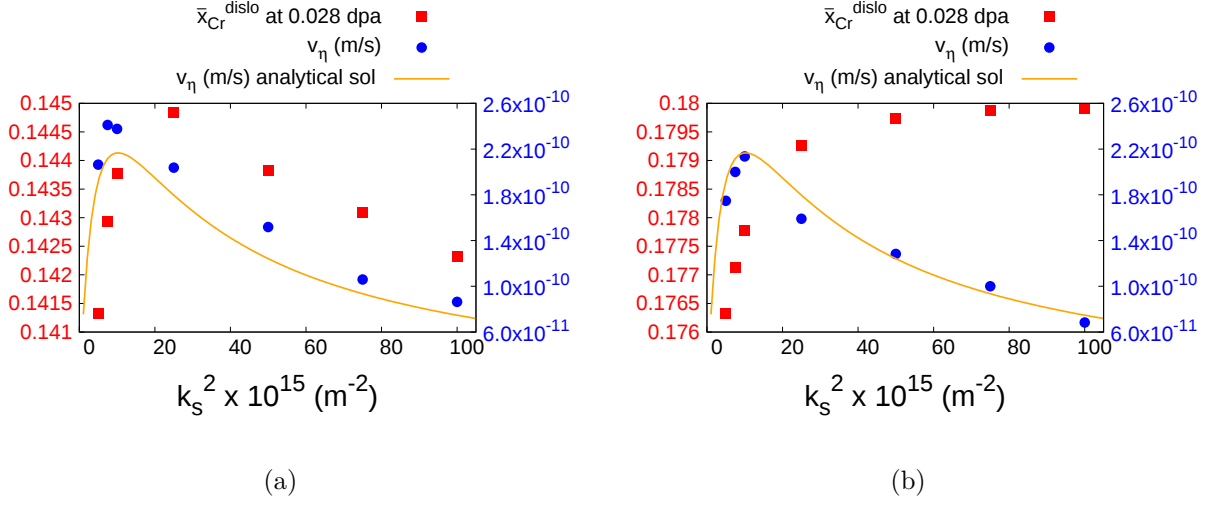


Figure 4.25: Climb rate (blue circle) and average Cr atomic fraction near the dislocation core on the domain D (see Fig. 4.10) (red square) as a function of k_s^2 in a) Fe-14%Cr ($D = 4.528 \times 2.264 \text{ nm}^2$) and in b) Fe-18%Cr at 800 K ($D = 6.792 \times 3.396 \text{ nm}^2$).

obtained, the phase field model incorporates features (dislocation motion, multi-sink effects,...) allowing to predict RIS near dislocations.

In summary of this section, the loop growth rate effects on the RIS prediction were investigated. Simulations of type 1 in which the system contained only a dipole of edge dislocations and $K_0^I \neq K_0^V$ were first performed. We showed by an analytical approach that a suitable choice of K_0^I for a fixed value of K_0^V allowed to observe the kinetic regime where atoms diffuse faster than the dislocation motion, and the opposite one. The results showed that in the kinetic regime where the atom diffusion is slower than the dislocation motion, the size and the shape of the Cr atmosphere around dislocations are strongly modified, as well as the Cr segregation level: the RIS prediction then depends on the [sink mobility](#). Secondly, simulations of type 2 in which the system contained a dipole of edge dislocations and a planar sink and $K_0^I = K_0^V$, were performed. These simulations showed that the local Cr segregation near sink can be changed significantly when another sink is nearby ([multi-sink effects](#)). Finally, a third type of simulations was proposed, in which other sinks present in the microstructure are represented by a mean sink strength k_s^2 . It was applied on Fe-14%Cr and Fe-18%Cr alloys, for which data on RIS at dislocations are available. The simulation results are promising since the obtained segregation tendencies at dislocations are similar to the experimental ones.

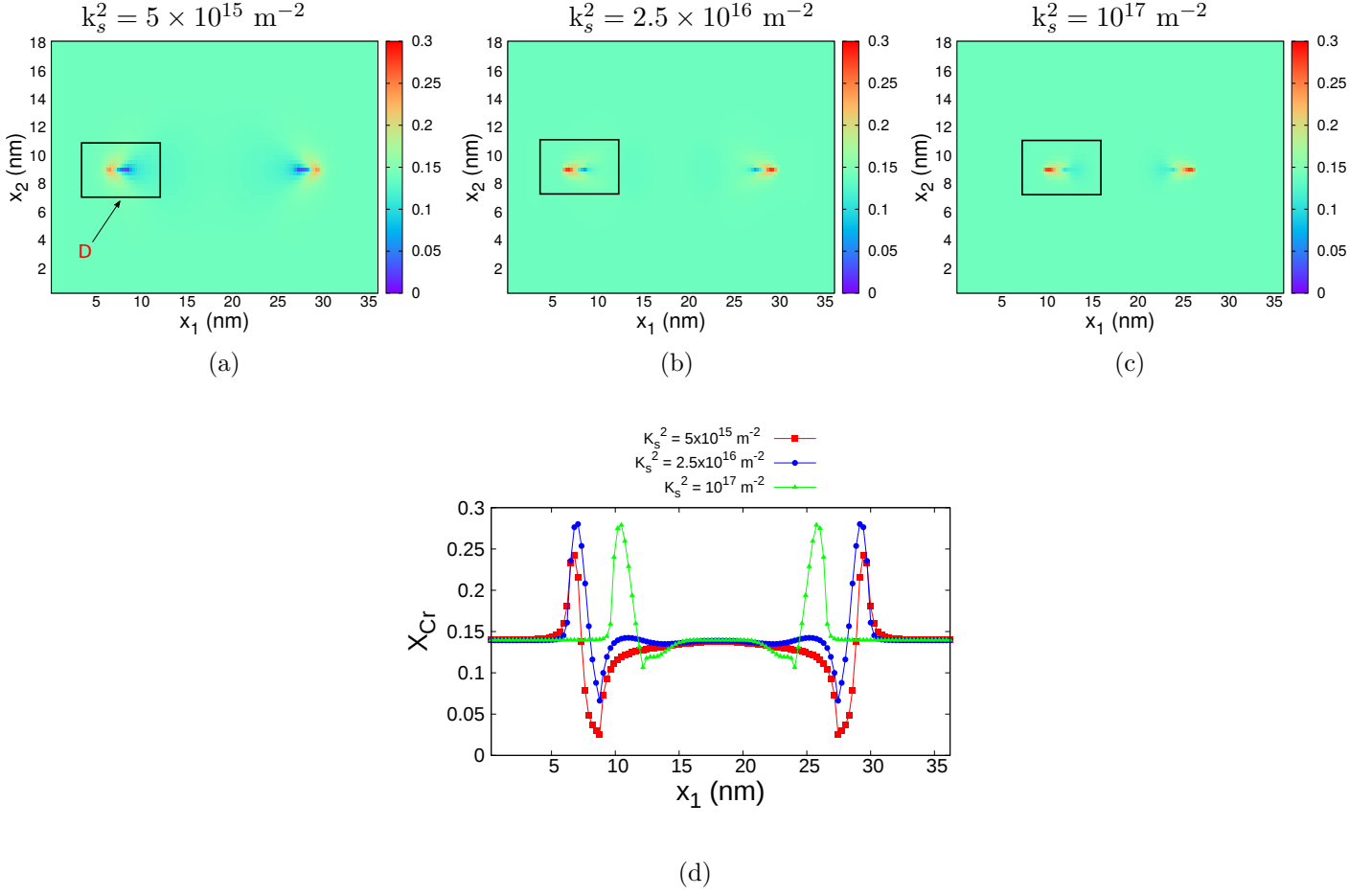


Figure 4.26: Cr atomic fraction in Fe-14%Cr for a) $k_s^2 = 5 \times 10^{15} \text{ m}^{-2}$, b) $k_s^2 = 2.5 \times 10^{16} \text{ m}^{-2}$, c) $k_s^2 = 10^{17} \text{ m}^{-2}$, and d) the corresponding profiles along the dipole.

4.4 Conclusion

A PF method allowing to predict RIS phenomenon near moving dislocations has been presented in this chapter. The model has been applied to simulate RIS in Fe-Cr alloys, and the main conclusions are the following. The RIS prediction can be strongly affected when elastic interactions are taken into account as shown by the results of section 4.3.1. Indeed, Cr enrichment and Cr depletion are predicted near dislocation cores respectively in Fe-11%Cr at 700 K and in Fe-15%Cr at 900 K without elasticity. However with elasticity, there is Cr enrichment in the tension region of dislocations and depletion in the compression region for both alloys which shows that elasticity has a predominant role on RIS prediction. The climb rate effects have been also investigated in section 4.3.2. The results of section 4.3.2.1 showed that, in the kinetic regime where dislocations move faster than atom diffusion, the size and shape of the solute atmosphere, the solute segregation level and tendency around dislocation cores are modified. Furthermore, the results of sections 4.3.2.2 and 4.3.3 also showed that the solute segregation level and tendency at

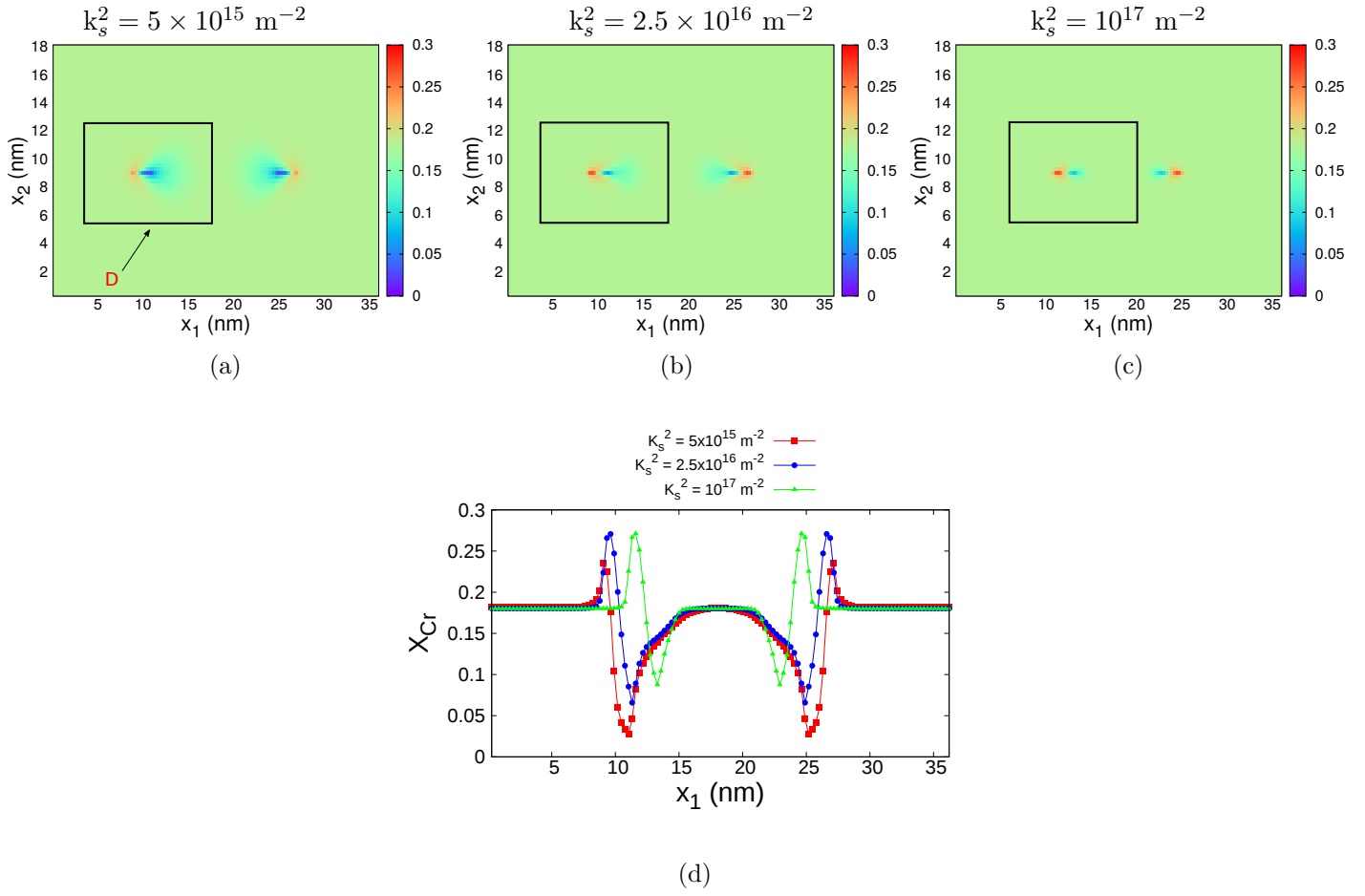


Figure 4.27: Cr atomic fraction in Fe-18%Cr for a) $k_s^2 = 5 \times 10^{15} \text{ m}^{-2}$, b) $k_s^2 = 2.5 \times 10^{16} \text{ m}^{-2}$, c) $k_s^2 = 10^{17} \text{ m}^{-2}$, and d) the corresponding profiles along the dipole.

a given sink can be strongly modified due to the surrounding microstructure ([multi-sink effects](#)).

Conclusions and perspectives

This thesis was devoted to the modelling of microstructure evolution under irradiation using a PF approach. As described in chapter 1, during irradiation ageing several phenomena are observed such as dislocation loop growth/shrinkage, RIS, swelling, irradiation creep and are explained by the evolution of microstructural defects (PDs, dislocation loops, cavities, ...). The evolution of these microstructural defects depends on their ability known as sink strength to absorb PDs. Thus, a precise prediction of microstructural evolution requires an accurate computation of sink strengths. Furthermore, the different phenomena can occur at the same time and therefore correlation effects may exist. For example, RIS can occur near a dislocation loop during its growth and the RIS prediction can depend on the loop growth rate. The purpose of this work was first to compute accurately the sink strength for various sinks in pure metals by taking into account the elastic interactions between PDs and sinks (see chapter 2). This type of calculation was already done by Rouchette et al. [4] who took into account elastic effects in the total free energy of the system, however Dederichs and Schroeder [41] showed that the PD diffusion tensor is also modified in a strained system, which is known as elastodiffusion. Our simulations incorporated the elastodiffusion effects and the role of PD anisotropy at saddle state was investigated. Secondly, based on the PF model of dislocation climb of Geslin et al. [1] a new model was developed and generalized to vacancies and SIAs which allows to simulate dislocation loop growth/shrinkage under irradiation (see chapter 3). Finally, this new PF model of dislocation climb under irradiation was coupled to atom diffusion in chapter 4 to predict RIS near a growing interstitial dislocation loop and investigate the climb rate effects on the prediction.

Summary of the results

The sink strength was computed for edge dislocations, low-angle STGBs (array of edge dislocations) and spherical cavities in pure fcc (Al, Ni) and bcc (Fe) metals by including elastodiffusion effects in chapter 2. During the calculations, by solving the PD diffusion equation, we used a staggered grid scheme to compute the strain field and the PD flux

to handle the appearance of artifact oscillations and numerical instabilities which can occur due to sharp variations of the diffusion tensor coefficients in the vicinity of the sink. The results showed globally an increase of the sink strength with full elastodiffusion (real elastic dipole tensor of PD at saddle point) for both PDs in the case of edge dislocations and low-angle STGB compared to the case without elastodiffusion, and an increase for SIAs and a decrease for vacancies in the case of cavities for all the metals investigated. The results showed also a decrease of the sink bias with full elastodiffusion in the case of edge dislocations for all the materials, a decrease for Al and Ni and an increase for Fe in the case of STGB, and an increase in the case of cavities for all the materials. The order of magnitude of the cavity bias obtained for all the materials with full elastodiffusion ($\simeq 10\%$) showed that these defects can be no longer considered as neutral sinks as it is the case in [10]. Otherwise, the results of the STGB sink biases obtained showed also that STGBs with low inter-spacing ($d < 30$ nm) are biased sinks when elastic interactions are considered. These results showed globally that the elastodiffusion plays an important role on the sink strength calculation and its effects depend on the PD elastic dipole properties at saddle point.

In chapter 2 the sink strength was calculated under the assumption of immobile sinks, however the climb of edge dislocations occurs by absorption of PDs for example. Chapter 3 was dedicated to the development of a new PF model of dislocation climb under irradiation inspired from that of Geslin [1], and application of this new model to simulate the growth of an interstitial dislocation loop in pure iron. Several tests were performed to validate the new model and these tests led to the introduction of a shape function to ensure that the climb process occurs due to the existence of the osmotic driving force only at dislocation cores. Furthermore, the dislocation core structure modelled as a diffuse interface is modified during climb when elastic interactions are taken into account and to overcome this change the dislocation core energy had to be artificially increased and Eq. 3.64 applied. The application in pure iron to simulate the growth of an interstitial loop showed that the PD equilibrium fraction inside the sink plays a significant role on the loop growth rate calculations especially at high temperatures when the equilibrium vacancy fraction is high. A direct comparison of our results of the climb rate evolution with the irradiation temperature, with those of the literature [81] was not possible due to the differences in irradiation conditions. Nevertheless, we saw that the order of magnitude of the climb rate obtained experimentally in [81] can be reached by extrapolating our results to low dislocation densities.

The phenomenon of RIS was studied in Fe-Cr alloys near an interstitial dislocation loop in chapter 4. The elasticity effects on RIS prediction were investigated and by means of the new PF climb model developed in chapter 3, the climb rate effects were also studied. The results showed a predominant role of elasticity on RIS prediction compared to the kinetic effects. For example, under the assumption of immobile sinks the precipitation of the α' phase is locally expected in the tension region of dislocation in Fe-11%Cr alloy at 700 K when elasticity is taken into account which was not the case without elasticity. When we take into account motion of the dislocation, we showed that when the atom diffusion is faster than the dislocation motion, the solute atmosphere around the dislocation cores and the level of segregation do not change during the loop growth. In the opposite case, the solute atmosphere and the level of segregation are strongly modified. Preliminary

comparisons between PF and experimental results on Fe-Cr alloys around dislocations are encouraging, and illustrate the relevance of the PF method to investigate RIS in complex microstructures.

Perspectives

In this work, different points were addressed namely the sink strength calculations, dislocation loop evolution and RIS prediction. The results obtained made it possible to provide some answers in the understanding and PF modelling of the microstructure evolution under irradiation and they open new perspectives at the same time.

The sink strength calculations presented in chapter 2 which take into account the elastodiffusion effects could be performed by considering the PD polarizability. Indeed, in the presence of an elastic strain field such as the one generated by a dislocation, the elastic dipole tensor of PD is modified [35, 109, 110]:

$$P_{ij}(\varepsilon_{kl}) = P_{ij}^0 + \alpha_{ijkl}\varepsilon_{kl} \quad (4.34)$$

where P_{ij}^0 is the permanent elastic dipole in an unstrained system and α_{ijkl} the PD dielastic polarizability tensor. As we showed that the elastic dipole tensor anisotropy at saddle state plays an important role on the sink strength calculations, the dependence of the P_{ij} -tensor with the local strain could have significant effects.

The PF model of dislocation climb developed in chapter 3 was applied to simulate the growth of an interstitial loop in 2 dimensions in pure bcc iron. The study could be extended to 3D simulations and the multi-sink effects on the climb rate could be also investigated especially in the presence of 3D defects such as cavities. However, the assumption that dislocations are perfect sinks which means a high jog density was considered in application but for low jog density, this assumption is no longer valid. The PD diffusion towards the dislocation is no longer invariant along the dislocation line due to the PD flux along this line. The climb process is then limited by the mechanism of PD absorption/emission at jogs. As a consequence, the shape of the dislocation loop may change during its evolution. The dislocation loop border could be discretized into different segments, each of which being characterized by a kinetic coefficient L_{η}^d . Furthermore, our model is limited to a single loop and a single slip plane, and its reformulation for multiple dislocations is necessary to get closer to a realistic creep situation.

The RIS simulations presented in chapter 4 showed that local precipitation of a new phase is expected near dislocations due to elasticity. A future work could be to incorporate precipitation in the model. In chapters 2 and 3, we showed that elastodiffusion can have significant effects on the PD fluxes and on the climb rate. Thus, the effects of the Onsager coefficients dependence with the local strain (elastodiffusion) on the RIS prediction and on the loop growth rate could be investigated. For the binary alloys Fe-Cr considered, the difference between the lattice parameters of Fe and Cr is negligible and the atomic size effects on the climb rate and RIS prediction were not studied. To study the effect of atomic size, other chemical species could be considered.

In this work, the PD recombination and the PD emission by the sink were neglected and could be taken into account in future works. Finally, the systems studied were considered free of any external strain/stress and strained systems could also be considered.

Appendix A

Numerical scheme and algorithm to treat the diffusion equation when elastodiffusion is considered

An explicit Euler scheme is used to solve Eq. 2.51:

$$X_d^{t^*+\delta t^*} = X_d^{t^*} + \left(\frac{\partial X_d}{\partial t^*}\right)^{t^*} \delta t^* \quad (\text{A.1})$$

A [finite difference scheme](#) is used for the spatial discretization. The mechanical equilibrium equation 2.34 in dimensionless form and the diffusion equation 2.51 have been solved using the classical derivative operators:

$$\nabla_1^* \phi(r_1^*, r_2^*, r_3^*) = \frac{[\phi(r_1^* + 1, r_2^*, r_3^*) - \phi(r_1^* - 1, r_2^*, r_3^*)]}{2} \quad (\text{A.2})$$

$$\tilde{\nabla}_1^* \tilde{\phi}(q_1^*, q_2^*, q_3^*) = \frac{[\exp(i_c q_1^*) - \exp(-i_c q_1^*)]}{2} \tilde{\phi}(q_1^*, q_2^*, q_3^*) \quad (\text{A.3})$$

$\tilde{\nabla}_i^*$ is the Fourier transform of the gradient operator ∇_i^* . ∇_2^* and ∇_3^* (respectively $\tilde{\nabla}_2^*$ and $\tilde{\nabla}_3^*$) are defined in the same way as ∇_1^* (respectively $\tilde{\nabla}_1^*$). Firstly, the strain field generated by the sink (dipole of edge dislocations for example) has been computed in the case of isotropic system using the input parameters given in table 2.2. Simulations have been performed in a 2 dimension box containing a dipole of edge dislocations as illustrated in Fig. A.1-a). In Fig. A.1-b) the map of the component $\epsilon_{11}(\mathbf{r})$ is illustrated. This map shows artifact oscillations, which are similar to those expected in [111]. To eliminate these oscillations, [shifted derivative operators](#) [111, 112, 113] are introduced and defined as:

$$\nabla_1^{*,+} \phi(r_1^*, r_2^*, r_3^*) = \phi(r_1^* + 1, r_2^*, r_3^*) - \phi(r_1^*, r_2^*, r_3^*) \quad (\text{A.4})$$

$$\nabla_1^{*,-} \phi(r_1^*, r_2^*, r_3^*) = \phi(r_1^*, r_2^*, r_3^*) - \phi(r_1^* - 1, r_2^*, r_3^*) \quad (\text{A.5})$$

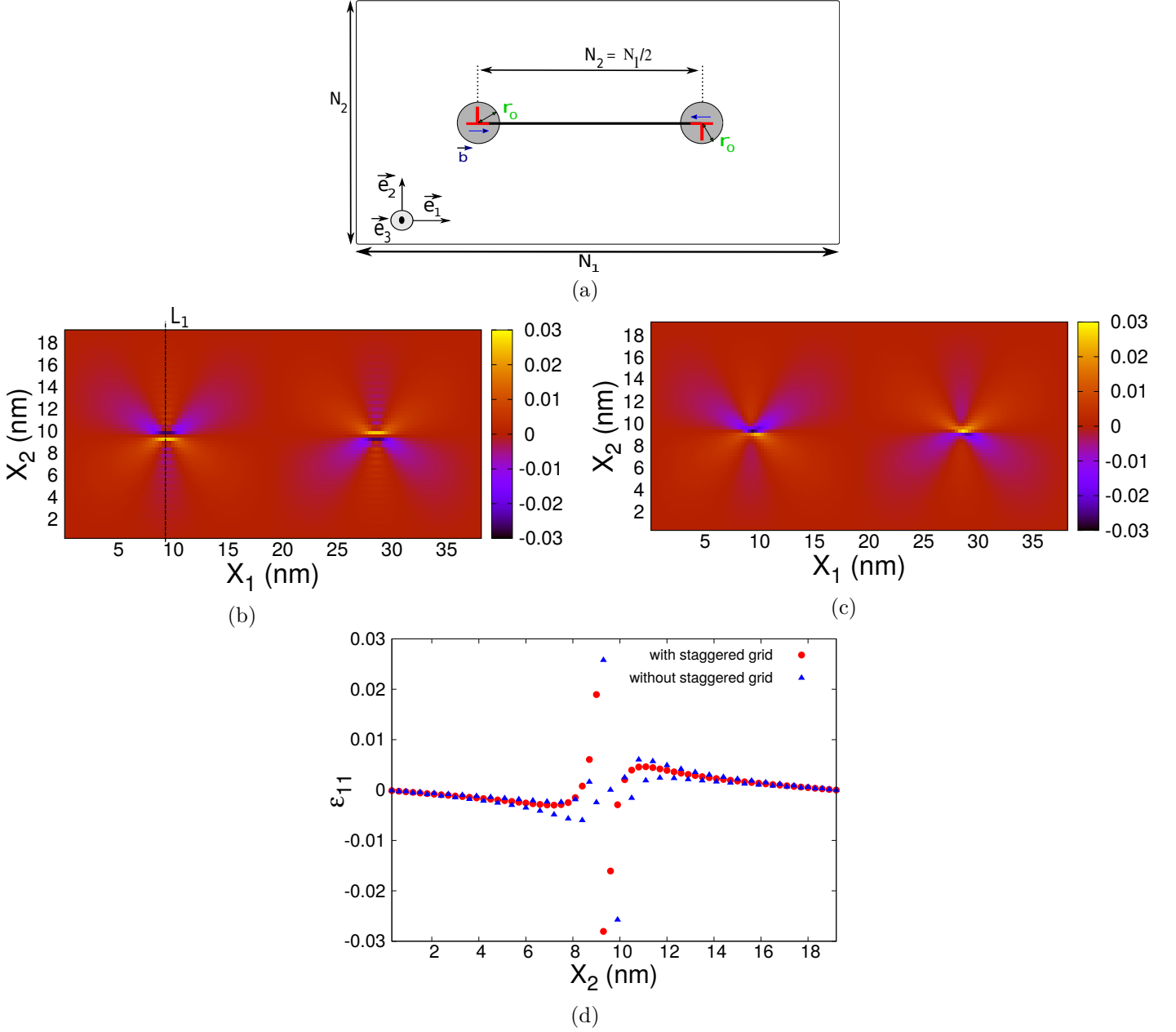


Figure A.1: a) 2D simulation domain containing a dipole of edge dislocations. Map of the strain field component $\varepsilon_{11}(\mathbf{r})$ b) without staggered grid and c) with staggered grid. d) Corresponding profiles along L_1 .

$$\tilde{\nabla}_1^{*,+} \tilde{\phi}(q_1^*, q_2^*, q_3^*) = (\exp(icq_1^*) - 1) \tilde{\phi}(q_1^*, q_2^*, q_3^*) \quad (\text{A.6})$$

$$\tilde{\nabla}_1^{*,-} \tilde{\phi}(q_1^*, q_2^*, q_3^*) = (1 - \exp(-icq_1^*)) \tilde{\phi}(q_1^*, q_2^*, q_3^*) \quad (\text{A.7})$$

The displacement and the strain fields are thus evaluated on **staggered grids** schematized in Fig. A.2. An important fact about using staggered grids is that: one staggered grid (centers of the PF cells) is dedicated to the diagonal components of the strain tensor, and one for each off-diagonal component (see Fig. A.2). The heterogeneous strain $\delta\epsilon_{ij}(\mathbf{q}^*)$

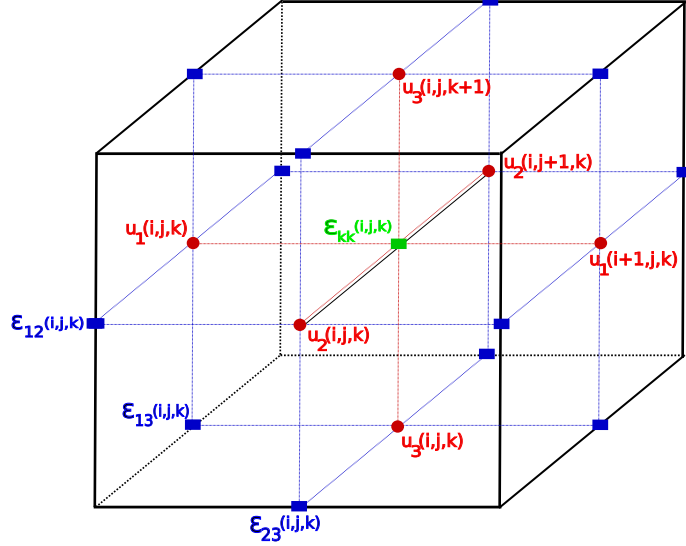


Figure A.2: Staggered finite difference grids [111]. The total volume represent a unit PF cell.

given by Eq. 2.30 is then written in the Fourier space using the shifted derivative operators as follows:

$$\delta\tilde{\epsilon}_{kl}(\mathbf{q}^*) = \frac{1}{2}[\tilde{\nabla}_l^{*,\pm}\tilde{u}_k + \tilde{\nabla}_k^{*,\pm}\tilde{u}_l](\mathbf{q}^*) \quad \text{where} \quad \tilde{\nabla}_{l,k}^{*,\pm} = \begin{cases} \tilde{\nabla}_{l,k}^{*,+} & \text{if } k = l \\ \tilde{\nabla}_{l,k}^{*,\pm} & \text{if } k \neq l \end{cases} \quad (\text{A.8})$$

The mechanical equilibrium (equation 2.31) becomes:

$$\tilde{\nabla}_j^{*,\pm} C_{ijkl}^* (\epsilon_{kl}(\mathbf{q}^*) - \epsilon_{kl}^{0,tot}(\mathbf{q}^*)) = 0 \quad \text{where} \quad \tilde{\nabla}_j^{*,\pm} = \begin{cases} \tilde{\nabla}_j^{*,\pm} & \text{if } i = j \\ \tilde{\nabla}_j^{*,\pm} & \text{if } i \neq j \end{cases} \quad (\text{A.9})$$

Using Eq. A.8 and Eq. 2.24, Eq. A.9 leads to:

$$C_{ijkl}^* \tilde{\nabla}_j^{*,\pm} \tilde{\nabla}_l^{*,\pm} \tilde{u}_k(\mathbf{q}^*) = C_{ijkl}^* [\sum_d \epsilon_{kl}^{0,X_d} \tilde{\nabla}_j^{*,\pm} \tilde{X}_d(\mathbf{q}^*) + \epsilon_{kl}^{0,\eta_s} \tilde{\nabla}_j^{*,\pm} \tilde{\eta}_s(\mathbf{q}^*)] \quad (\text{A.10})$$

with

$$\tilde{\nabla}_j^{*,\pm} = \begin{cases} \tilde{\nabla}_j^{*,\pm} & \text{if } i = j \\ \tilde{\nabla}_j^{*,\pm} & \text{if } i \neq j \end{cases} \quad \text{and} \quad \tilde{\nabla}_l^{*,\pm} = \begin{cases} \tilde{\nabla}_l^{*,+} & \text{if } k = l \\ \tilde{\nabla}_l^{*,\pm} & \text{if } k \neq l \end{cases} \quad (\text{A.11})$$

Eq. A.10 can be written as:

$$[G_{ik}^{*,\pm}(\mathbf{q}^*)]^{-1} \tilde{u}_k(\mathbf{q}^*) = C_{ijkl}^* [\sum_d \epsilon_{kl}^{0,X_d} \tilde{\nabla}_j^{*,\pm} \tilde{X}_d(\mathbf{q}^*) + \epsilon_{kl}^{0,\eta_s} \tilde{\nabla}_j^{*,\pm} \tilde{\eta}_s(\mathbf{q}^*)] \quad (\text{A.12})$$

where

$$[G_{ik}^{*,\pm}(\mathbf{q}^*)]^{-1} = C_{ijkl}^* \tilde{\nabla}_j^{*,\pm} \tilde{\nabla}_l^{*,\pm} = \begin{cases} C_{ijkl}^* \tilde{\nabla}_j^{*,+} \nabla_l^{*,+} & \text{if } i = j \text{ and } k = l \\ C_{ijkl}^* \tilde{\nabla}_j^{*,+} \nabla_l^{*,+} & \text{if } i = j \text{ and } k \neq l \\ C_{ijkl}^* \tilde{\nabla}_j^{*,+} \nabla_l^{*,+} & \text{if } i \neq j \text{ and } k = l \\ C_{ijkl}^* \tilde{\nabla}_j^{*,+} \nabla_l^{*,+} & \text{if } i \neq j \text{ and } k \neq l \end{cases} \quad (\text{A.13})$$

The oscillations are then overcome as illustrated by the map in Fig. A.1-c) obtained using the staggered grids. The suppression of the oscillations does not affect significantly the values of the strain far from the sink as shown by the profiles plotted in Fig. A.1-d).

The dimensionless elastic energy (see Eq. 2.36) is also rewritten using the shifted derivative operators:

$$F_{el}^* = \frac{1}{2} \sum_m C_{ijkl}^* \varepsilon_{ij}^{0,\theta_m} \varepsilon_{kl}^{0,\theta_m} \bar{\theta}_m - \frac{1}{2} \sum_m \sum_n C_{ijkl}^* \varepsilon_{ij}^{0,\theta_m} \varepsilon_{kl}^{0,\theta_n} \bar{\theta}_m \bar{\theta}_n - \frac{1}{2} \sum_m \sum_n \int \tilde{\nabla}_j^{*,\pm} \sigma_{ij}^{0,\theta_m*} G_{ik}^{*,\pm}(\mathbf{q}^*) \sigma_{kl}^{0,\theta_n*} \tilde{\nabla}_l^{*,\pm} \tilde{\theta}_m(\mathbf{q}) \tilde{\theta}_n(\mathbf{q}) d^3 q^* \quad (\text{A.14})$$

$$\text{with } \tilde{\nabla}_j^{*,\pm} = \begin{cases} \tilde{\nabla}_j^{*,+} & \text{si } i = j \\ \tilde{\nabla}_j^{*,+} & \text{si } i \neq j \end{cases}, \quad \tilde{\nabla}_l^{*,\pm} = \begin{cases} \tilde{\nabla}_l^{*,+} & \text{si } k = l \\ \tilde{\nabla}_l^{*,+} & \text{si } k \neq l \end{cases}$$

To prevent the appearance of artifact oscillations during the resolution of the diffusion equation, a staggered grid is employed to compute the PD flux as done in [82]. This new scheme allows to handle numerical instabilities which can occur due to sharp variations of the diffusion tensor coefficients when elastodiffusion is taken into account. The PD flux is rewritten using the shifted derivative operators:

$$J_i^{d,*+}(\mathbf{r}^*, t^*) = - \sum_j D_{ij,j}^{d,*+}(\mathbf{r}^*) X_{d,j}^+(\mathbf{r}^*, t^*) \nabla_j^{*,+} (\mu_{chem}^{d,*}(\mathbf{r}^*, t^*) + \mu_{el}^{d,*}(\mathbf{r}^*, t^*)) \quad (\text{A.15})$$

$$J_i^{d,*-}(\mathbf{r}^*, t^*) = - \sum_j D_{ij,j}^{d,*-}(\mathbf{r}^*) X_{d,j}^-(\mathbf{r}^*, t^*) \nabla_j^{*,+} (\mu_{chem}^{d,*}(\mathbf{r}^*, t^*) + \mu_{el}^{d,*}(\mathbf{r}^*, t^*)) \quad (\text{A.16})$$

with

$$\begin{cases} D_{ij,1}^{d,*+}(r_1^*, r_2^*, r_3^*) = \frac{D_{ij}^{d,*}(r_1^*+1, r_2^*, r_3^*) + D_{ij}^*(r_1^*, r_2^*, r_3^*)}{2} \\ D_{ij,2}^{d,*+}(r_1^*, r_2^*, r_3^*) = \frac{D_{ij}^{d,*}(r_1^*, r_2^*+1, r_3^*) + D_{ij}^*(r_1^*, r_2^*, r_3^*)}{2} \\ D_{ij,3}^{d,*+}(r_1^*, r_2^*, r_3^*) = \frac{D_{ij}^{d,*}(r_1^*, r_2^*, r_3^*+1) + D_{ij}^*(r_1^*, r_2^*, r_3^*)}{2} \end{cases} \quad (\text{A.17})$$

$$\begin{cases} D_{ij,1}^{d,*-}(r_1^*, r_2^*, r_3^*) = \frac{D_{ij}^*(r_1^*, r_2^*, r_3^*) + D_{ij}^{d,*}(r_1^*-1, r_2^*, r_3^*)}{2} \\ D_{ij,2}^{d,*-}(r_1^*, r_2^*, r_3^*) = \frac{D_{ij}^*(r_1^*, r_2^*, r_3^*) + D_{ij}^{d,*}(r_1^*, r_2^*-1, r_3^*)}{2} \\ D_{ij,3}^{d,*-}(r_1^*, r_2^*, r_3^*) = \frac{D_{ij}^*(r_1^*, r_2^*, r_3^*) + D_{ij}^{d,*}(r_1^*, r_2^*, r_3^*-1)}{2} \end{cases} \quad (\text{A.18})$$

$$\begin{cases} X_{d,1}^+(r_1^*, r_2^*, r_3^*, t^*) = \frac{X_d(r_1^*+1, r_2^*, r_3^*, t^*) + X_d(r_1^*, r_2^*, r_3^*, t^*)}{2} \\ X_{d,2}^+(r_1^*, r_2^*, r_3^*, t^*) = \frac{X_d(r_1^*, r_2^*+1, r_3^*, t^*) + X_d(r_1^*, r_2^*, r_3^*, t^*)}{2} \\ X_{d,3}^+(r_1^*, r_2^*, r_3^*, t^*) = \frac{X_d(r_1^*, r_2^*, r_3^*+1, t^*) + X_d(r_1^*, r_2^*, r_3^*, t^*)}{2} \end{cases} \quad (\text{A.19})$$

$$\begin{cases} X_{d,1}^-(r_1^*, r_2^*, r_3^*, t^*) = \frac{X_d(r_1^*, r_2^*, r_3^*, t^*) + X_d(r_1^*-1, r_2^*, r_3^*, t^*)}{2} \\ X_{d,2}^-(r_1^*, r_2^*, r_3^*, t^*) = \frac{X_d(r_1^*, r_2^*, r_3^*, t^*) + X_d(r_1^*, r_2^*-1, r_3^*, t^*)}{2} \\ X_{d,3}^-(r_1^*, r_2^*, r_3^*, t^*) = \frac{X_d(r_1^*, r_2^*, r_3^*, t^*) + X_d(r_1^*, r_2^*, r_3^*-1, t^*)}{2} \end{cases} \quad (\text{A.20})$$

where $J_i^{d,*+}$ and $J_i^{d,*-}$ are respectively the i^{th} component of the PD flux shifted to the right and to the left. In other words, the PD flux is evaluated at the middle of the PF cell boundaries as illustrated in Fig. A.3. Diffusion equation 2.51 becomes:

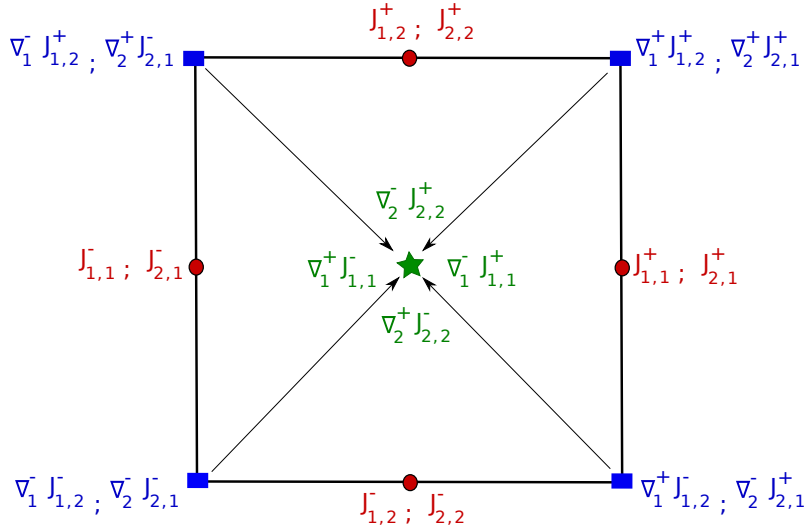


Figure A.3: 2D representation of the staggered grid used to compute the PD flux and its divergence.

$$\frac{\partial X_d}{\partial t^*}(\mathbf{r}^*, t^*) = - \sum_i \sum_j \nabla_i^{*,\mp} J_{i,j}^{d,*\pm}(\mathbf{r}^*, t^*) + K_0^* - J_{s,d}^{abs,*}(\mathbf{r}^*, t^*) \quad (\text{A.21})$$

with

$$J_{i,j}^{d,*\pm}(\mathbf{r}^*, t^*) = D_{ij,j}^{d,*\pm}(\mathbf{r}^*) X_{d,j}^{\pm}(\mathbf{r}^*, t^*) \nabla_j^{*,\pm} \mu^{d,*}(\mathbf{r}^*, t^*) \quad (\text{A.22})$$

where

$$\nabla_i^{*,\mp} J_{i,j}^{d,*\pm} = \begin{cases} -\nabla_i^{*, -} J_{i,i}^{d,*+} & \text{or equivalently} \\ -\nabla_i^{*, +} J_{i,i}^{d,*-} & \text{if } i = j \end{cases} \quad (\text{A.23})$$

and

$$\nabla_i^{*,\mp} J_{i,j}^{d,*\pm} = -\frac{1}{4}[\nabla_i^{*,+} J_{i,j}^{d,*+} + \nabla_i^{*,+} J_{i,j}^{d,*-} + \nabla_i^{*,+} J_{i,j}^{d,*-} + \nabla_i^{*,+} J_{i,j}^{d,*+}]$$

if $i \neq j$ (A.24)

For the diagonal terms of the diffusion tensor, the divergence of the PD flux given by $\nabla_i^{*,\mp} J_{i,j}^{d,*\pm}$ is evaluated at the center of the PF cells. On the other hand for off-diagonal terms, $\nabla_i^{*,\mp} J_{i,j}^{d,*\pm}$ is calculated at the corner of the PF cell boundaries as shown in Fig. A.3. To have the divergence of the PD flux at the center of the PF cells, an average value of all the terms $\nabla_i^{*,\mp} J_{i,j}^{d,*\pm}$ given at each corner is done. In practice, the discretization scheme is more stable when it is only the chemical flux $J_{chem}^{d,*}$ which is evaluated on shifted grids. This may due to the fact that the elastic potential $\mu_{el}^{d,*}$ is computed using the shifted derivative operators, and the diffusion coefficients $D_{ij}^{d,*}$ are also computed using the shifted derivative operators via the strain field.

Appendix B

Dislocation climb: derivation of the evolution equations

The total differential of $F(\phi_I, \phi_V, \eta_I^l, \eta_V^l)$ is given by:

$$dF(\phi_I, \phi_V, \eta_I^l, \eta_V^l) = \frac{\delta F}{\delta \phi_I} d\phi_I + \frac{\delta F}{\delta \phi_V} d\phi_V + \frac{\delta F}{\delta \eta_I^l} d\eta_I^l + \frac{\delta F}{\delta \eta_V^l} d\eta_V^l \quad (\text{B.1})$$

Using the relations $d\phi_I = dX_I + d\eta_I^l$ and $d\phi_V = dX_V + d\eta_V^l$, Eq. B.1 becomes:

$$dF(\phi_I, \phi_V, \eta_I^l, \eta_V^l) = \frac{\delta F}{\delta \phi_I} dX_I + \frac{\delta F}{\delta \phi_V} dX_V + \left(\frac{\delta F}{\delta \phi_I} + \frac{\delta F}{\delta \eta_I^l} \right) d\eta_I^l + \left(\frac{\delta F}{\delta \phi_V} + \frac{\delta F}{\delta \eta_V^l} \right) d\eta_V^l \quad (\text{B.2})$$

Moreover, $dF(X_I, X_V, \eta_I^l, \eta_V^l)$ is given by:

$$dF(X_I, X_V, \eta_I^l, \eta_V^l) = \frac{\delta F}{\delta X_I} dX_I + \frac{\delta F}{\delta X_V} dX_V + \frac{\delta F}{\delta \eta_I^l} d\eta_I^l + \frac{\delta F}{\delta \eta_V^l} d\eta_V^l \quad (\text{B.3})$$

knowing that $dF(\phi_I, \phi_V, \eta_I^l, \eta_V^l) = dF(X_I, X_V, \eta_I^l, \eta_V^l)$, equations B.2 and B.3 are equivalent and the following relations emerge:

$$\left\{ \begin{array}{l} \frac{\delta F(X_I, X_V, \eta_I^l, \eta_V^l)}{\delta X_I} = \frac{\delta F(\phi_I, \phi_V, \eta_I^l, \eta_V^l)}{\delta \phi_I} \\ \frac{\delta F(X_I, X_V, \eta_I^l, \eta_V^l)}{\delta X_V} = \frac{\delta F(\phi_I, \phi_V, \eta_I^l, \eta_V^l)}{\delta \phi_V} \\ \frac{\delta F(X_I, X_V, \eta_I^l, \eta_V^l)}{\delta \eta_I^l} = \frac{\delta F(\phi_I, \phi_V, \eta_I^l, \eta_V^l)}{\delta \phi_I} + \frac{\delta F(\phi_I, \phi_V, \eta_I^l, \eta_V^l)}{\delta \eta_I^l} \\ \frac{\delta F(X_I, X_V, \eta_I^l, \eta_V^l)}{\delta \eta_V^l} = \frac{\delta F(\phi_I, \phi_V, \eta_I^l, \eta_V^l)}{\delta \phi_V} + \frac{\delta F(\phi_I, \phi_V, \eta_I^l, \eta_V^l)}{\delta \eta_V^l} \end{array} \right. \quad (\text{B.4})$$

The evolution equations 3.18 - 3.21 become by using relations B.4 and $\frac{\partial \phi_d}{\partial t} = \frac{\partial X_d}{\partial t} + \frac{\partial \eta_d^l}{\partial t}$:

$$\frac{\partial X_I}{\partial t} = \nabla \cdot [M^I \nabla \frac{\delta F(X_I, X_V, \eta_I^l, \eta_V^l)}{\delta X_I}] - \frac{\partial \eta_I^l}{\partial t} \quad (B.5)$$

$$\frac{\partial X_V}{\partial t} = \nabla \cdot [M^V \nabla \frac{\delta F(X_I, X_V, \eta_I^l, \eta_V^l)}{\delta X_V}] - \frac{\partial \eta_V^l}{\partial t} \quad (B.6)$$

$$\frac{\partial \eta_I^l}{\partial t} = -L_{\eta^l}^I [\frac{\delta F(X_I, X_V, \eta_I^l, \eta_V^l)}{\delta \eta_I^l} - \frac{\delta F(X_I, X_V, \eta_I^l, \eta_V^l)}{\delta X_I}] \quad (B.7)$$

$$\frac{\partial \eta_V^l}{\partial t} = -L_{\eta^l}^V [\frac{\delta F(X_I, X_V, \eta_I^l, \eta_V^l)}{\delta \eta_V^l} - \frac{\delta F(X_I, X_V, \eta_I^l, \eta_V^l)}{\delta X_V}] \quad (B.8)$$

The loop evolution is given by the plastic field η^l (see Eq. 3.9) and η_d^l can be seen as an intermediate parameter which allows to give the loop evolution through the PD d . Since the free energy of the system is given as a function of η^l and not η_d , it is more convenient to write the evolution of η^l . The following relations are verified using Eq. 3.9:

$$\begin{cases} \frac{\delta F(X_I, X_V, \eta_I^l, \eta_V^l)}{\delta \eta_I^l} = \frac{sg(l)}{X^*} \frac{\delta F(X_I, X_V, \eta^l)}{\delta \eta^l} \\ \frac{\delta F(X_I, X_V, \eta_I^l, \eta_V^l)}{\delta \eta_V^l} = -\frac{sg(l)}{X^*} \frac{\delta F(X_I, X_V, \eta^l)}{\delta \eta^l} \end{cases} \quad (B.9)$$

Finally, the evolution equations are as follows:

$$\frac{\partial X_I}{\partial t} = \nabla \cdot [M^I \nabla \frac{\delta F(X_I, X_V, \eta^l)}{\delta X_I}] - \frac{\partial \eta_I^l}{\partial t} \quad (B.10)$$

$$\frac{\partial X_V}{\partial t} = \nabla \cdot [M^V \nabla \frac{\delta F(X_I, X_V, \eta^l)}{\delta X_V}] - \frac{\partial \eta_V^l}{\partial t} \quad (B.11)$$

$$\frac{\partial \eta_I^l}{\partial t} = -L_{\eta^l}^I [\frac{sg(l)}{X^*} \frac{\delta F(X_I, X_V, \eta^l)}{\delta \eta^l} - \frac{\delta F(X_I, X_V, \eta^l)}{\delta X_I}] \quad (B.12)$$

$$\frac{\partial \eta_V^l}{\partial t} = -L_{\eta^l}^V [-\frac{sg(l)}{X^*} \frac{\delta F(X_I, X_V, \eta^l)}{\delta \eta^l} - \frac{\delta F(X_I, X_V, \eta^l)}{\delta X_V}] \quad (B.13)$$

The loop evolution is simply given by $\frac{\partial \eta^l}{\partial t} = \frac{sg(l)}{X^*} (\frac{\partial \eta_I^l}{\partial t} - \frac{\partial \eta_V^l}{\partial t})$. Substituting the total energy into Eqs. B.10 - B.13 and taking the first variational derivatives with respect to X_d and η^l , we obtain the following contracted evolution equations:

$$\frac{\partial X_d}{\partial t} = \nabla \cdot [M^d \nabla (\mu_{chem}^d + \mu_{el}^d)] - \frac{\partial \eta_d^l}{\partial t} \quad (B.14)$$

$$\frac{\partial \eta_d^l}{\partial t} = -L_{\eta^l}^d [\frac{1}{X^*} sg(l) sg(d) (\mu_{core}^{\eta^l} + \mu_{el}^{\eta^l}) - (\mu_{chem}^d + \mu_{el}^d)] \quad (B.15)$$

where $sg(d) = 1$ for SIAs and -1 for vacancies and:

$$\mu_{chem}^d = V_{at} \frac{\delta F_{chem}}{\delta X_d} = E_f^d + k_B T \ln X_d = k_B T \ln (\frac{X_d}{X_{eq}^d}) \quad (B.16)$$

APPENDIX B. DERIVATION OF THE EVOLUTION EQUATIONS

with X_{eq}^d the thermal equilibrium value of PD d, related to its formation energy by the relation:

$$X_{eq}^d = \exp\left(-\frac{E_f^d}{k_B T}\right) \quad (\text{B.17})$$

$$\mu_{el}^d = V_{at} \frac{\delta F_{el}}{\delta X_d}, \quad \mu_{el}^{\eta^l} = V_{at} \frac{\delta F_{el}}{\delta \eta^l} \quad (\text{B.18})$$

μ_{el}^d and $\mu_{el}^{\eta^l}$ are calculated in the Fourier space in which they have the following simple form:

$$\tilde{\mu}_{el}^I(\mathbf{q}) = B_{II}(\mathbf{q})\tilde{X}_I(\mathbf{q}) + B_{IV}(\mathbf{q})\tilde{X}_V(\mathbf{q}) + B_{I\eta^l}(\mathbf{q})\tilde{f}(\tilde{\eta}^l)(\mathbf{q}) \quad (\text{B.19})$$

$$\tilde{\mu}_{el}^V(\mathbf{q}) = B_{VV}(\mathbf{q})\tilde{X}_V(\mathbf{q}) + B_{VI}(\mathbf{q})\tilde{X}_I(\mathbf{q}) + B_{V\eta^l}(\mathbf{q})\tilde{f}(\tilde{\eta}^l)(\mathbf{q}) \quad (\text{B.20})$$

$$\tilde{\mu}_{el}^{\eta^l}(\mathbf{q}) = \tilde{f}'(\tilde{\eta}^l)[B_{\eta^l I}(\mathbf{q})\tilde{X}_I(\mathbf{q}) + B_{\eta^l V}(\mathbf{q})\tilde{X}_V(\mathbf{q}) + B_{\eta^l \eta^l}(\mathbf{q})\tilde{f}(\tilde{\eta}^l)(\mathbf{q})] \quad (\text{B.21})$$

with

$$\left\{ \begin{array}{l} B_{II}(\mathbf{q}) = \sigma_{ij}^{0,X_I} \epsilon_{ij}^{0,X_I} - q_i \sigma_{ij}^{0,X_I} G_{jm}(\mathbf{q}) \sigma_{mn}^{0,X_I} q_n \\ B_{VV}(\mathbf{q}) = \sigma_{ij}^{0,X_V} \epsilon_{ij}^{0,X_V} - q_i \sigma_{ij}^{0,X_V} G_{jm}(\mathbf{q}) \sigma_{mn}^{0,X_V} q_n \\ B_{IV}(\mathbf{q}) = \sigma_{ij}^{0,X_I} \epsilon_{ij}^{0,X_V} - q_i \sigma_{ij}^{0,X_I} G_{jm}(\mathbf{q}) \sigma_{mn}^{0,X_V} q_n \\ B_{VI}(\mathbf{q}) = \sigma_{ij}^{0,X_V} \epsilon_{ij}^{0,X_I} - q_i \sigma_{ij}^{0,X_V} G_{jm}(\mathbf{q}) \sigma_{mn}^{0,X_I} q_n \\ B_{I\eta^l}(\mathbf{q}) = \sigma_{ij}^{0,X_I} \epsilon_{ij}^{0,\eta^l} - q_i \sigma_{ij}^{0,X_I} G_{jm}(\mathbf{q}) \sigma_{mn}^{0,\eta^l} q_n \\ B_{V\eta^l}(\mathbf{q}) = \sigma_{ij}^{0,X_V} \epsilon_{ij}^{0,\eta^l} - q_i \sigma_{ij}^{0,X_V} G_{jm}(\mathbf{q}) \sigma_{mn}^{0,\eta^l} q_n \\ B_{\eta^l I}(\mathbf{q}) = \sigma_{ij}^{0,\eta^l} \epsilon_{ij}^{0,X_I} - q_i \sigma_{ij}^{0,\eta^l} G_{jm}(\mathbf{q}) \sigma_{mn}^{0,X_I} q_n \\ B_{\eta^l V}(\mathbf{q}) = \sigma_{ij}^{0,\eta^l} \epsilon_{ij}^{0,X_V} - q_i \sigma_{ij}^{0,\eta^l} G_{jm}(\mathbf{q}) \sigma_{mn}^{0,X_V} q_n \\ B_{\eta^l \eta^l}(\mathbf{q}) = \sigma_{ij}^{0,\eta^l} \epsilon_{ij}^{0,\eta^l} - q_i \sigma_{ij}^{0,\eta^l} G_{jm}(\mathbf{q}) \sigma_{mn}^{0,\eta^l} q_n \end{array} \right. \quad (\text{B.22})$$

where $\sigma_{ij}^{0,X_d} = C_{ijkl} \epsilon_{kl}^{0,X_d}$ and $\sigma_{ij}^{0,\eta^l} = C_{ijkl} \epsilon_{kl}^{0,\eta^l}$. $\tilde{\mu}$ is the Fourier transform of μ and $\mathbf{q}$ the wave vector as defined in section 2.2.

$$\mu_{core}^{\eta^l} = V_{at} \frac{\delta F_{core}}{\delta \eta^l} = V_{at} \left(\frac{\delta F_{cry}}{\delta \eta^l} + \frac{\delta F_{grad}}{\delta \eta^l} \right) \quad (\text{B.23})$$

with

$$\frac{\delta F_{cry}}{\delta \eta^l} = 2H\eta^l(1-\eta^l)(1-2\eta^l), \quad \frac{\delta F_{grad}}{\delta \eta^l} = \frac{\gamma}{2} \frac{\delta(|\mathbf{n} \wedge \nabla \eta^l|^2)}{\delta \eta^l} \quad (\text{B.24})$$

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