Available online at www.sciencedirect.com
ScienceDirect
C. R. Physique 9 (2008) 427–436
COMPTES RENDUS PHYSIQUE
http://france.elsevier.com/direct/COMREN/

Materials subjected to fast neutron irradiation/Matériaux soumis à irradiation par neutrons rapides

Discrete dislocation dynamics: an important recent break-through in the modelling of dislocation collective behaviour

Marc C. Fivel

SIMaP-GPM2, CNRS, INP Grenoble, BP 46, 38402 Saint-Martin-d'Hères, France

Available online 18 April 2008

Abstract

Recent results obtained by 3D discrete Dislocation Dynamics (DD) simulations are reviewed. Firstly, in the case of fatigued AISI 316L stainless steel, it is shown how DD simulations can both explain the formation of persistent slip bands and give a criterion for crack initiation. The same study is performed in the case of precipitate hardened metals where the precipitate size plays a crucial role. Secondly, we show how molecular dynamics (MD) simulations can feed the DD simulations for two applications. The first concerns the modelling of BCC Fe for which the dislocation mobility is derived from MD simulations. The second considers the modelling of irradiated stainless steels (FCC), where MD is used to define the local rules of interactions between dislocations and Frank loops. ***To cite this article: M.C. Fivel, C. R. Physique 9 (2008).***

Résumé

Dynamique des dislocations discretes : modèlisation du comportement collectif des dislocations. Cet article présente une synthèse des derniers résultats obtenus par simulation de Dynamique des Dislocations. Pour commencer, l'étude du comportement en fatigue de l'acier austénitique 316L montre que les simulations de DD peuvent tout à la fois expliquer la formation des bandes de glissement persistent et prédire un critère physique précisant l'amorçage des premières fissures. Une étude similaire réalisée sur des métaux durcis par précipitation montre le rôle primordiale joué par la taille des particules. Ensuite, il est montré deux applications dans lesquelles des simulations de Dynamique Moléculaire (MD) nourrissent les modèles de DD. La première étude concerne la modélisation du fer BCC pour lequel la mobilité des dislocations est déduite de simulations de MD. La deuxième présente une modélisation de la plasticité d'un acier inoxydable irradié (CFC) pour lequel la MD définit les rêgles locales d'interactions entre dislocations et boucles de Frank. ***Pour citer cet article : M.C. Fivel, C. R. Physique 9 (2008).***

Keywords: Dislocation dynamics; Multiscale modelling; Plasticity

Mots-clés : Dynamique des dislocations ; Plasticité

1. Introduction

The concept of three-dimensional discrete dislocation (DD) simulations has been imagined by L. Kubin, Y. Bréchet and G. Canova in the early 1990s [1,2]. The first code MICROMÉGAS was a simple model for which dislocation lines

E-mail address: Marc.Fivel@inpg.fr.

1631-0705/$ – see front matter
doi:10.1016/j.crhy.2007.11.005

of a f.c.c. single crystal are discretized in sets of edge and screw dislocation segments embedded in a continuum media. For each segment, the velocity is computed from the effective stress resulting from the summation of the applied component with the internal stress field generated by all the other dislocations contained in the simulated box. Typical output of DD simulations are obviously the dislocation microstructure but also many statistical data such as the dislocation densities, the cumulated shear strain, the stored energy, the local stresses. Recently methods have been developed in order to compute the actual shape of any part of the crystal deformed by the dislocations. From some points of view, DD simulations can be seen as an ideal tool to fill the gap between atomic simulations (MD) and continuum modelling. These characteristics explain the large dissemination of this modelling during the past few years. Today, there exist many DD codes over the world [3–7] dedicated to different crystallographic structures but all based on similar ingredients. During the past few years, much progress have been made in terms of computational efficiency and the most recent applications now account for large population of interacting dislocation segments, although the size of the simulation box remains limited to a few tens of microns. This articles presents a review of the most advanced simulations performed at Grenoble using the edge-screw code *Tridis* derived from Canova's initial model [8]. The first application concerns the simulation of the fatigue behaviour of f.c.c. metals both in the case of single phase and precipitate hardened materials. For both cases a detailed analysis of the shape of the persistent slip bands is given and parametric studies of the fatigue life are derived. The second part of the paper is dedicated to ongoing work where MD simulations are used to define local rules used in DD simulations. Example of these multi-scale simulations are given in the case of the modelling of the plasticity of pure Fe for which MD simulations give the dislocation mobility. The second case concerns the simulation of irradiated f.c.c. austenitic steels for which MD simulations give the local rules of interaction of dislocation lines and Frank loops. Finally, perspectives of these studies are presented together with the problems needed to be overcome with a particular focus on problems related to the development of the fusion technology.

2. Simulations of crack initiation in metals

2.1. Case of AISI 316L stainless steel

In powerplants, AISI 316L stainless steel is usually used in the internal parts of the cooling systems. When subjected to thermal fatigue, as in the case of the injection of a cold fluid in the circuit, transgranular fatigue cracks are observed. In order to study the crack formation, the CYTHIA experiment (*CY*clage *TH*ermique par *I*nduction des *A*ciers) has been conceived at the Commissariat à l'énergie atomique (CEA/SRMA). This ideal experiment consists of cyclicly heating a pipe using a high frequency induction coil, where the inner part of the pipe is constantly cooled by flowing water. Transmission Electron Microscopy (TEM) observations of the surface grains located at the outer part of the cylinder show a dense dislocation microstructure organized in bands typical from fatigue behaviour of this kind of material [9–13]. Atomic Force Microscopy (AFM) observations of the grain surface show that with the cycles, the persistent slip bands lead to the development of extrusion and intrusion relief at the surface [14,15] that may induce cracks.

Many DD simulations with various conditions of loading amplitude and grain size were performed with a view to explaining both the formation of the persistent slip bands [16] and the relationship with the surface relief and the nucleation of the first crack [17]. For all the simulations the plastic strain amplitude is imposed and only two glide systems sharing the same Burgers vector are considered. The initial dislocation configuration consists of a single dislocation source whose characteristics are given by the TEM observations performed on CYTHIA samples: the Burgers vector is nearly aligned with the vector normal to the surface. Both pure shear and double glide loading conditions have been tested.

It was found that cross-slip mechanism plays a crucial role in the organisation of the dislocation microstructure [16]. After a few cycles, edge dipoles are formed in the so-called vein structures. When dislocations from the cross-slipped system shear these zones, the dislocation lines recombine and form a complex microstructure containing channels, entangled zones and piled-up dislocations as depicted in Fig. 1.

The dislocations within the channels consist of multipoles made of prismatic loops and helicoidal dislocations. The density of these multipoles increases with the number of cycles, storing more and more energy in the band. Note that the mobility of these dislocations is restricted to a cylinder defined by the loop size and the Burgers vector. Under a homogeneous stress field, the multipoles cannot move. Inversely, when submitted to a stress gradient, they can glide in

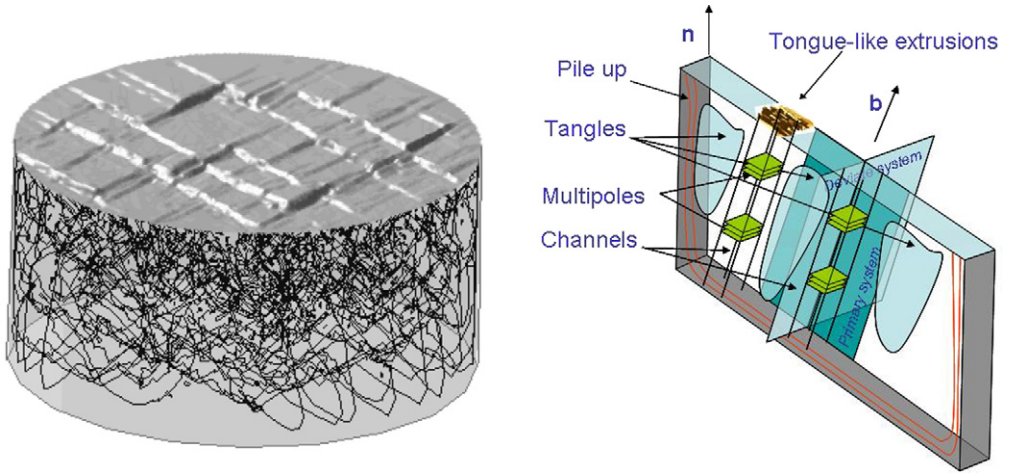

Fig. 1. (a) Typical dislocation microstructure and associated surface relief obtained by DD fatigue simulation of a 316L surface grain (diameter $d = 10$ μm). (b) Schematic description of a persistent slip band as observed in DD simulations.

Fig. 1. (a) Exemple d'une microstructure de dislocations avec le relief de surface associé obtenus par simulation de DD d'un grain de surface d'acier 316L sollicité en fatigue. (b) Description schématique d'une bande de glissement persistent telle qu'observée dans les simulations de DD.

the channel and eventually reach the surface where interstitials loops print tongue-like extrusions, and vacancy loops leave a punch in the surface (intrusion). Detailed analysis of the surface relief obtained by DD when the imposed plastic strain is maximum show that all the plasticity is localised at the interface between the slip band and the matrix. At this place are located highly mobile dislocations which completely accommodate the imposed plasticity. Note that such dislocations are hardly observed in microscopy since observations are usually performed post mortem and only few experiments are done in situ [18]. When these dislocations move, they induced a stress gradient on the multipoles which drive them out of the volume.

The crack nucleation was studied by computing both the energy and the stress state in the bands. As said previously, the multipoles store energy in the band with the cycles. However, DD simulations show that the stress component needed to open a crack is saturating after a few cycles. This means that a crack cannot initiate inside the band, but rather at the surface where the stress is concentrated by the extrusion/intrusion shape of the surface relief. From a simulation campaign performed with different values of the plastic strain amplitude, the mean strain, the grain size, the grain shape and the stress triaxiality, it was possible to derive the effect of these parameters on the fatigue life [17]. It was found that the extrusion growth is a linear function of the strain range and grain size and evolves as a square root function of the number of cycles. When comparing these predictions of the extrusion growth rate with the experimental measures [15,14], one can notice a good agreement for the first few cycles and a discrepancy for the large number of cycles. The difference can be attributed to diffusion of point defects that could change the square-root relationship into a linear form. Despite this limit, the predictions derived from the DD simulations are of great interest since the experiments show that the crack always initiate very early in the cycling process, i.e. where the DD prediction is relevant.

This study was part of C. Déprés's Ph.D. Thesis [19] supported by the Contrat Programme de Recherche SMIRN (*S*imulation des *M*étaux des *I*nstallations et *R*éacteurs *N*ucléaires) which is gratefully acknowledged here.

2.2. *Case of precipitate hardened metals*

Three-dimensional DD fatigue simulations of precipitate hardened metals is a major challenge in terms of numerical development since they require a code capable of dealing with a large population of dislocations interacting with a large number of precipitates. A preliminary study [20] has nevertheless been conducted using a parallelised version of the DD code [21]. In this new version of TRIDIS, the simulation volume is decomposed into domains and dislocation segments are described through linked-lists. This enables an easy decomposition of the stress fields into short and long-distance stresses and a fast handling of possible dislocation interactions. Load balancing is realised by resizing the size of the different domains so that they all contain a similar number of segments. The efficiency of the parallel

algorithm was tested by comparing the CPU time required to compute 100 steps of a 15 microns large cubic volume submitted to tensile loading. On the IBM p690 architecture with 1.7 GHz POWER4 processors, a speedup factor between 15 and 17 is obtained for 25 CPUs when the number of segments is within the range 40 000 to 80 000. Note that similar efforts have been conducted all other the world to improve the computational efficiency of the different DD codes. As an example, DEMECHA is a parallel version of the UCLA code developed by Ghoniem et al. which demonstrated a speedup factor of 44 with 60 CPUs when dealing with 6000 nodes [22] (a factor 18 is reached for 25 CPUs). The high scalable DD code PARADIS specially developed at Lawrence Livermore National laboratory to run on the BlueGene/L massively parallel computing system consisting in more than 100 000 CPUs reaches a maximum efficiency (about 90%) weakly dependant on the number of degrees of freedom and/or the number of available CPUs [23].

In the case of fatigue simulations, the dislocation segments are mainly localed in confined regions corresponding to the persistent slip bands. Despite the load-balance used in the parallel algorithm of TRIDIS, the dislocation density is highly heterogeneous and the efficiency of the parallel algorithm is reduced.

Theoretically precipitates can be introduced in DD simulation by computing the image forces induced on the dislocations by the difference of elastic moduli. Then, the effective stress field on each dislocation segment is given as the superposition of the internal stresses induced by all the segments contained in the simulation box and the image stresses computed by finite elements. Basic situations of screw and edge dislocations interacting with particles were investigated using such a superposition's technic [24,25]. The numerical model was first validated by comparison with the 2D case of an infinite dislocation interacting with an infinite cylinder. It was found that only 20 node elements give a good approximation of the elastic interactions [25]. In the case of spherical particles [24] the increase in the flow stress due to the difference between the shear moduli is computed by measuring the stress required to force the dislocation line through two particles. The relationship was found to follow a power law with an exponent 0.6. After the first dislocation passage, an Orowan loop is stored around the particles. If new dislocations are emitted in the same glide plane as that of the first dislocation, it is found that the shear stress required to pass the particles linearly depends on the number of loops already stored around the particles. The change in elastic moduli weakly affects the slope coefficient. Finally it was found that when the particle elastic modulus is increased, it favours the cross-slip mechanism so that the particles can be by-passed by double cross-slip. Finally, the effect of the particle shape was studied [25] and it was shown that a cubic particle is more resistant to dislocation climb than a spherical or cylindrical particle.

Fatigue simulations of precipitate hardened metals cannot be simulated using the finite element procedure as depicted above. Indeed, the expected computation time would be much too important and 3D mesh of the entire simulation box including all the particles is very painful. According to the elementary studies summarised above, the image forces induced by the change in elastic modulus can easily be neglected. Thus, for large scale DD simulations, coherent particles can be represented in first approximation by a set of local rules specifying the local strength of each precipitate [20]. In such a modelling, particles are represented by sets of facets with given critical shear stresses defining the minimum effective resolved shear stress a dislocation segment needs to feel to be allowed to shear the precipitate. After each dislocation passage, the facet strength is decreased until a minimum value is reached. This minimum value is introduced to model the dissolution of the particle in the matrix when the surface/volume ratio attains a limit. Using this modelling of the dislocation/precipitate interactions, fatigue simulations are conducted following the same procedure as in the case of AISI 316L austenitic stainless steel detailed in Section 2.1: the simulated volume is a cylindrical surface grain with a 10 microns radius and the imposed plastic strain range is $\Delta\epsilon_p = 10^{-3}$. The simulated alloys contain 14% of particles with three particle distributions: (i) a monomodal distribution of 161 large particles (radius $r_p = 400$ nm) (see Fig. 2(a)), (ii) a monomodal distribution of 2510 small particles ($r_p = 160$ nm) (see Fig. 2(b)) and (iii) a bi-modal distribution containing both particle sizes. For the large particles, the initial facet strength is estimated to 7.5 GPa whereas for the small one it is initialised to 162 MPa. In the case of the monomodal distribution of large particles, it is found that the particles are never sheared and the dislocation microstructure is similar to that of the single phase material.

The shape of the extrusion printed on the surface is more ribbon like with a length comparable to the inter-precipitate distance. In the case of a monomodal distribution of small particles (Fig. 2(b)), the plastic strain is localised in slip bands with characteristics similar to the single phase material but a much larger dislocation density. The mechanical response shows a large value of the initial stress for the first cycle but a severe cyclic softening due to the

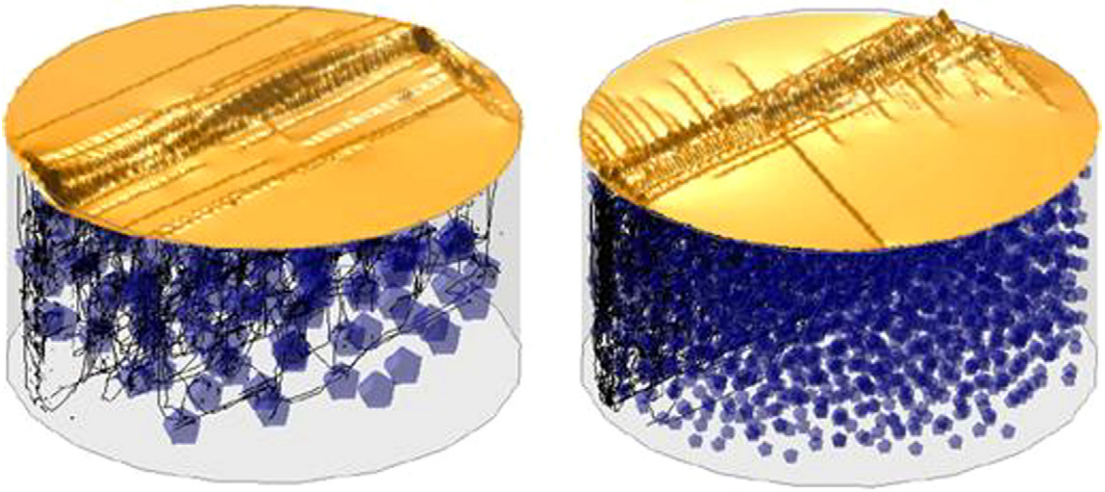

Fig. 2. DD fatigue simulations of precipitate hardened metals. (a) Case of 161 large particles ($r_p = 400$ nm). (b) Case of 2510 small particles ($r_p = 160$ nm).

Fig. 2. Simulations DD de la fatigue de métaux durcis par précipitation pour deux tailles de particules. (a) Cas de 161 grosses particules ($r_p = 400$ nm). (b) Cas de 2510 petites particules ($r_p = 160$ nm).

particle shearing. Finally, the case of bimodal distributions reveals an intermediate mechanical response. Unlike in the case of the monomodal distribution of large particles, some large particles are sheared in the bimodal distribution.

A first conclusion could be derived from this preliminary study. The particle size is an important parameter for fatigue life of precipitate hardened metals. For a given volume fraction of precipitates, large particles increase the stress level with a weak cyclic softening. However, if the particle size if dispersed, the benefit induced by the presence of the large and hardly shearable particles can be lost since some of the large particles are also sheared because of the localisation of the plastic strain induced by the small sheared particles.

These study was part of C.S Shin's Ph.D. [26] supported by program FAMICRO (*Fa*tigue de matériaux métalliques structuraux à partir de mécanismes physique *micro*scopiques) which is gratefully acknowledged here.

3. Scale transition: from molecular dynamics to dislocation dynamics

3.1. Multiscale modelling of dislocation plasticity in body-centred-cubic Fe

In the case of face-centred-cubic (FCC) crystals, DD simulations have demonstrated that they can give insights into the physical mechanisms involved during plasticity and they can explain the formation of dislocation microstructure as observed by microscopy. On the other hand, DD simulations of body-centred-cubic (BCC) metals are still challenging today since there remains large uncertainties regarding the dislocation mobility in these crystals. The main differences with FCC structures concern the sensibility to the temperature and the asymmetry observed in traction/compression. In the thermally activated regime, plasticity of BCC metals is mainly controlled by the slow motion of the $a/2\langle 111\rangle$ screw dislocations via successive double-kinks, whereas the edge dislocations glide at a much higher velocity. This behaviour has been well-known for a long time [27] and is attributed to the core structure of the screw dislocations [28]. First tentative of BCC DD modelling in three dimensions started in 1998 [29,30] mainly motivated by the US Department of Energy and with applications dedicated to tantalum or molybdenum. In these studies, the dislocation mobility was assumed thermally activated with activation energies fitted from experiments. Simultaneously, three-dimensional atomistic studies using the nudged elastic band method were conducted to compute the activation paths followed by a screw dislocation during its motion [31]. This explained the pencil glide and the zigzag patterns of slip [32].

Only very recently, molecular dynamic (MD) simulations were able to reproduce the thermally assisted kinetics of the screw motion in pure BCC Fe [33,34]. Since then, it is theoretically possible to use MD results to define the mobility laws needed for DD codes. The uncertainties now come from the realism of the interatomic potentials

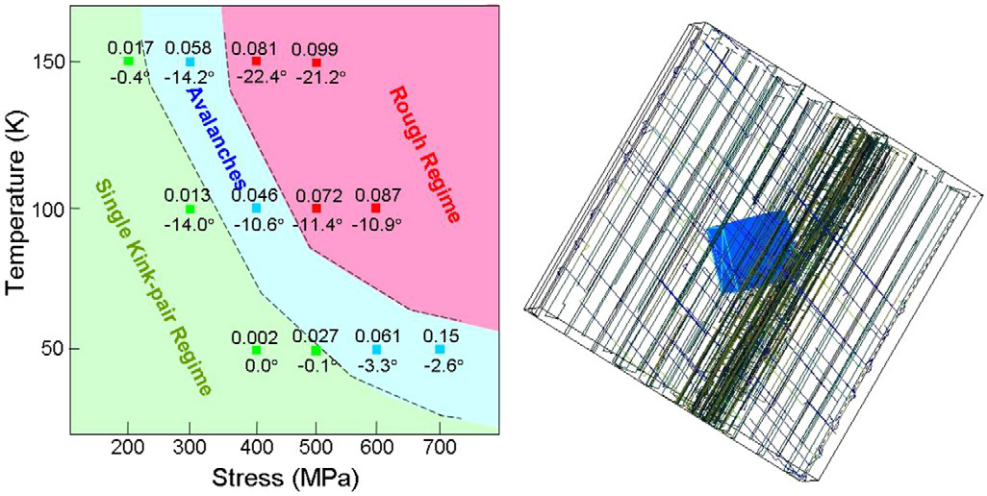

Fig. 3. (a) Behaviour map obtained by MD simulations giving both the plane angle and the dislocation velocity (given in 10^3 ms^{-1}) for different stresses and temperatures [34]. (b) DD simulations of a Fe lath (BCC) submitted to bending (inside cubic volume is defined to compute local concentration of elastic energies).

Fig. 3. (a) Carte de comportement du Fer BCC obtenue par MD donnant à la fois la vitesse des dislocations vis (donnée en 10^3 ms^{-1}) et l'angle du plan de glissement pour différentes valeurs de la contrainte appliquée et de la température. (b) Exemple de simulation DD d'une latte de ferrite (BCC) soumise à une flexion (un volume cubique est dessiné à l'int''erieur de la boîte de simulation pour calculer les concentrations d'énergie élastique).

used in the MD simulations (see paper from D. Rodney in this issue [35]). Such a scale transition from MD to DD has nevertheless been re-allied within the PhD work of J. Chaussidon [34]. In this study, the embedded atom potential developed by Mendelev et al. [36] was selected because it gives a non-degenerate and compact core structure for the screw dislocation which allows the motion along {110} planes as observed experimentally. MD simulations both predicted the traction-compression asymmetry for BCC Fe and the effect of the temperature on the dislocation mobility. Fig. 3 summarises results of all the MD simulations. Depending on the applied stress and the imposed temperature, different regimes for the dislocation motion are observed. In the single kink-pair regime, the double kinks created on the screw dislocation have time to expand along the entire dislocation line before new kinks are nucleated. In the avalanche regime, a new double kink is nucleated while the first one is still printed on the dislocation. For higher stresses, the rough regime is observed when multiple double kinks are nucleated in different planes leaving defects behind the dislocation. The temperature dependence of the non-Schmid behaviour is quantified by the angle between the mean glide plane followed by the screw dislocation and the plane of maximum resolved shear stress. This effect is directly introduced in DD simulations through the cross-slip law.

As shown in Fig. 3, MD simulations also give the magnitude of the dislocation velocity as a function of the temperature and the applied stress level. This information cannot be used in DD simulation since the values found are much too high and only apply to high stress levels. This is an intrinsic limitation of MD simulations. Indeed, the time step being small, one needs to apply a large stress to observe a double-kink event within a reasonable computation time. As detailed in [35], this makes impossible to check thermally assisted processes with activation energies greater than 0.5 eV using direct MD simulations. Thus, in the DD code, the screw velocity is classically written as a thermally activated equation with activation energies measured from experiments. The MD-DD scale transition is finally limited to the selection of the glide planes in the cross-slip probability law with temperature dependence. In collaboration with CEA/SRMA, the BCC version of TRIDIS is now used to study plasticity of ferritic laths of bainitic steels (see Fig. 3(b)), the objective being to quantify the effect of temperature on cleavage initiation. DD results will be compared with experiments conducted in 16MND5 pressure vessel steel [37].

3.2. Multiscale modelling of irradiated austenitic stainless steels

In nuclear environments, irradiation affects the mechanical properties of the structural materials such as the austenitic steels and the pressure vessel steels. The elastic limit is increased whereas the ductility is decreased. At

the atomic level, depending on the material and the irradiation dose, the irradiation is characterised by vacancies or interstitials that cluster respectively into stacking fault tetrahedra (ex: Cu, Ni(low dose)) or Frank loops (316L, Ni(high dose)). The interactions of these defects with the mobile dislocations explain the increase of the elastic limit. The softening is generally associated to the formation of defect free zones (clear channels) where plasticity is localised. Dislocation dynamics modelling has been extensively used to give physical insights of the clear band formation. As an example, Ghoniem et al. and Khraishi et al. have investigated the interactions between mobile dislocations and both stacking fault tetrahedra and self-interstitial atom clusters in the case of irradiated copper [38–40] and paladium [40,41] and also the interactions of dislocations and micro voids in irradiated BCC Fe [42]. In these studies, the irradiated defects are always taken as point obstacles with a given strength imposed by a critical angle for the dislocation unpinning. As pointed out by the authors, such rules could ideally be derived from atomistic computer simulations. Modelling irradiated materials is indeed a good candidate for molecular dynamics simulations. The typical size for the irradiation defect is around 10 nm and the average distance is around 50 nm (leading to a realistic density close to 10^{23} m^{-3}). MD studies generally consists of introducing a single SFT or few Frank loops in the simulation box and modelling the mobility of an edge or screw dislocation that will react with the defects [43]. Then MD results include both the local reactions between the dislocation and the defects and the obstacle strength [44,45].

In the case of austenitic stainless steels, irradiation-induced defaults consist of interstitial Frank loops [46]. Using Ni and Cu as model FCC materials with potentials based on the embedded atom method, MD simulations have evidenced all the possible interactions with screw and edge dislocations [44,45]. It was found that screw dislocations un-fault the Frank loops and the local reaction transforms the dislocation line into an helical dislocation that can now glide in another plane parallel to the initial one. On the other hand, edge dislocations mainly shear the loops and cannot explain the defect removal in the clear channels. These features were introduced in TRIDIS through local rules. Frank loops are randomly spread in the simulation box as a set of prismatic loops. Initially, these loops are arbitrarily immobilised in order to simulate the sessile character of the faulted loops. Then edge or screw dislocations are introduced in the simulations through a Frank–Read multiplication mechanism. When a dislocation segment encounters a Frank loop segment, different reactions are realised depending on the local character of the moving dislocation. If the dislocation segment is close to a screw part, the Frank loop is now considered as a perfect prismatic loop with a Burgers vector equal to that of the moving dislocation. Dislocation and prismatic loops then react leading to an helical turn on the dislocation as observed in MD. If the dislocation segment is closer to an edge part, the segment is pinned at the contact with the Frank loop and will be free to move when a critical angle between the neighbouring segments bowing around the loops is reached. The value of the critical angle has been set to 100 degrees in order to fit with the MD estimations of the obstacle strength. Fig. 4 shows DD simulations of dislocations and Frank loops using these ingredients. For clarity, only the Frank loops transformed into perfect mobile prismatic loops are shown. When the dislocations are emitted from an edge character Frank–Read source (Fig. 4(a)), it is shown that the edge parts of the dislocations have a longer mean free path than the screw component that have more difficulty to propagate. Same effect is observed in the case of a screw character source (Fig. 4(b)). Finally, whatever the dislocation source, the dislocation microstructure mainly consists of long screw dislocations with many helical turns in good agreement with transmission electron microscopy observations [47]. As shown in Fig. 4, prismatic loops and dislocation debris are moved along the Burgers vector and pile up at the border of the simulated box. Such a characteristic has also been observed experimentally [47].

According to these characteristics, when the plastic strain rate is imposed, the dislocation will propagate through the obstacles and helical turns will be printed on the screw components. Then some parts of the dislocation will be emitted in parallel planes and will encounter new loops that will pin the dislocations after few reactions. The stress will then increase and new dislocations will be emitted from the Frank–Read source in the initial glide plane which now contains fewer sessile defects marking the beginning of band clearing. The stress level needed to propagate the plasticity will then decrease so that the first dislocations pinned on the parallel planes will not be pushed further into the crystal. In forthcoming studies, this could simulate both the softening observed experimentally and explain why the thickness of the clear channel is finite.

In conclusion to this ongoing work on irradiated stainless steel, the MD-DD scale transition is performed via local rules depicting the interactions between dislocation segments and Frank loops. The challenge here comes from the DD part of the modelling which was scaled down to the atomic scale (a typical box size was $600 \times 600 \times 120$ nm). Theoretically, the elastic theory is not valid when distances are of the order of the Burgers magnitude. The study reveals that elasticity is robust down to the atomistic level where the elastic limits found by DD for different density

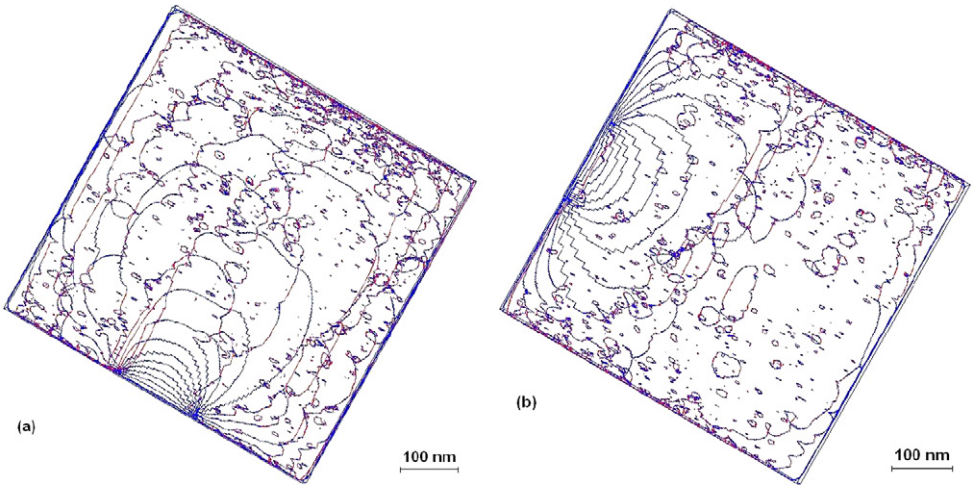

Fig. 4. DD simulations of dislocations interacting with Frank loops. (a) Case of an edge character source. (b) Case of a screw character source.

Fig. 4. Simulations DD de dislocations en interaction avec des boucles de Frank. (a) Cas d'une source de caractère coin. (b) Cas d'une source de caractère vis.

of defects are comparable with the experiments. This work is part of T. Nogaret's Ph.D. funded by European FP-6 project PERFECT (No. FI60-CT-2003-508840).

4. Concluding remarks and perspectives for applications to fusion technology

Recently dislocation dynamics modelling has proven it cannot only reproduce local mechanisms implying dislocations and few defects but also be used in an engineer manner to predict mechanical properties. DD was able to explain the dislocation microstructure in fatigued 316L stainless steel and an estimation of the fatigue life was given. In the case of the simple edge-screw code TRIDIS, a break-through in DD modelling was realised by developing a parallel code that can significantly decrease the CPU time down to a factor 15 when using 25 CPUs. Applications to the modelling of precipitate hardened materials showed the importance of the precipitate size in fatigue life.

DD simulations, being based on elastic theory, need local rules to describe any mechanism not relevant from this theory. This information can come from a smaller scale, for example from MD simulations. Such a scale transition has been done in the case of BCC Fe for which the mobility law for the screw dislocation in the thermally activated regime is obtained by MD simulations. Following the same idea, a scale transition has been setup in order to define the local reactions of dislocations and irradiation defects in a view to an understanding of the formation of clear channels in 316L austenic stainless steels. This study shows that elastic theory is still valid at very small scales. However, in forthcoming DD simulations, a key point needs to be solved concerning the cross-slip law. Indeed, in the actual version of DD codes, cross-slip is taken into account via a thermally activated law which implies activation energies, activation volumes and effective stresses derived from experiments realised on single crystals. Such a law is completely phenomenologic and not adapted to small scale modelling where the stress magnitude is much higher than the effective stress measured at the beginning of stage III of a tensile test. Thus this cross-slip law needs to be improved in order to use DD to simulate plasticity at the submicron scale.

Similarly, the climbing process is a second recovery mechanism that needs to be implemented in the next generation of DD codes to fully account for high temperature plasticity. This implies the introduction in DD codes of the physics of diffusion of point defects. Ideally, DD simulations should be coupled with a diffusion model so that the defect concentration is locally updated in function of the dislocation mobility and vice-versa. The challenge here is to correctly compute the possibility for a dislocation to glide or climb, i.e. two mechanisms for which the kinetics is very different.

In the case of materials research for fusion technology, multiscale modelling is needed to understand the mechanical behaviour of highly irradiated materials. In this aspect, DD simulations will help to scale up the information from the atomistic modelling realised through MD simulations to continuum mechanics. As an example, the effect of He

bubbles on the mechanical response of structural ferritic/martensitic steels can be simulated using the same procedure as the one used for dislocation-precipitate interactions. Simple situations of a limited number of dislocations and few bubbles could be precisely studied using the BCC version of TRIDIS coupled to a finite element modelling. By comparing the response with MD simulations, it will be possible to measure respectively the part due to elasticity and that induced by the core effect. Then a set of local rules similar to that used in 3.2 to describe the reaction with a Frank loop could be introduced in a DD simulation of BCC Fe in order to perform large scale simulations involving a significant volume fraction of bubbles. DD simulations will then feed continuum modelling through constitutive equations that will account for the physics pointed out at the micron scale.

All the links required in the multiscale modelling will soon be available for a complete scale transition from ab-initio to continuum mechanics. With time, results will always improve stimulated by the development of always more realistic inter-atomic potentials at the lowest scale enforced by always more powerful computers.

References

[1] L.P. Kubin, G.R. Canova, The modelling of dislocation patterns, Scripta Metall. 27 (1992) 957–962.
[2] B. Devincre, V. Pontikis, Y. Brechet, G. Canova, M. Condat, L. Kubin, Three-dimensional simulations of plastic flow in crystals, in: M. Marechal, B.L. Holian (Eds.), Microscopic Simulations of Complex Hydrodynamic Phenomena, Plenum Press, New York, 1992, [413].
[3] H.M. Zbib, M. Rhee, J.H. Hirth, On plastic deformation and the dynamics of 3D dislocations, Int. J. Mech. Sci. 40 (1999) 113–127.
[4] K. Schwarz, Simulation of dislocations on the mesoscopic scale. I. Methods and examples, J. Appl. Phys. 85 (1999) 108–119.
[5] N.M. Ghoniem, S.-H. Tong, L.Z. Sun, Parametric dislocation dynamics: A thermodynamics-based approach to investigations of mesoscopic plastic deformation, Phys. Rev. B 61 (1) (2000) 913–927.
[6] D. Weygand, L.H. Friedman, E. Van der Giessen, A. Needleman, Aspects of boundary-value problem solutions with three-dimensional dislocation dynamics, Modelling Simul. Mater. Sci. Eng. 10 (3) (2002) 437–468.
[7] V.V. Bulatov, W. Cai, Computer Simulations of Dislocations, Oxford University Press, 2006, p. 352.
[8] M. Verdier, M.C. Fivel, I. Groma, Mesoscopic scale simulation of dislocation dynamic in fcc metals: Principle and applications, Modelling Simul. Mater. Sci. Eng. 6 (6) (1998) 755–770.
[9] H. Mughrabi, Introduction to the viewpoint set on: surface effects in cyclic deformation and fatigue, Scripta Metall. Mater. 26 (1992) 1499–1504.
[10] A.F. Armas, I. Alvarez-Armas, C. Petersen, Thermal fatigue behavior and dislocation substructures of 316L-type austenitic stainless steels, J. Nucl. Mater. 191–194 (1992) 672–675.
[11] Y. Li, C. Laird, Cyclic response and dislocation structures of AISI 316L stainless steel. Part 1: single crystals fatigued at intermediate strain amplitude, Mater. Sci. Eng. A 186 (1994) 65–86.
[12] K. Obrtlík, T. Kruml, J. Polák, Dislocation structure in 316L stainless steel cycled with plastic strain amplitudes over a wide interval, Mater. Sci. Eng. A 187 (1994) 1–9.
[13] P. Hahner, B. Tippelt, C. Holste, On the dislocation dynamics of persistent slip bands in cyclically deformed f.c.c. metals, Acta Mater. 46 (1998) 5073–5084.
[14] J. Man, K. Obrtlík, C. Blochwitz, J. Polák, Atomic force microscopy of surface relief in individual grains of fatigued 316L austenitic stainless steel, Acta Mater. 50 (2002) 3767–3780.
[15] J. Man, K. Obrtlík, J. Polák, Study of surface relief evolution in fatigued 316L austenitic stainless steel by afm, Mater. Sci. Eng. A 351 (2003) 123–132.
[16] C. Déprés, C. Robertson, M.C. Fivel, Low-strain fatigue in AISI 316L steel surface grains: a three-dimensional discrete dislocation dynamics modelling of the early cycles i. dislocation microstructures and mechanical behaviour, Philos. Mag. 84 (22) (2004) 2257–2275.
[17] C. Déprés, C. Robertson, M.C. Fivel, Low-strain fatigue in 316L steel surface grains: a three dimension discrete dislocation dynamics modelling of the early cycles. part 2: Persistent slip markings and micro-crack nucleation, Philos. Mag. 86 (1) (2006) 79–97.
[18] J. Lepinoux, L.P. Kubin, In situ TEM observations of the cyclic dislocation behaviour in persistent slip bands of copper single crystals, Philos. Mag. A 51 (5) (1985) 675–696.
[19] C. Déprés, Modélisation physique des stades précurseurs de l'endommagement en fatigue dans l'acier inoxydable austénitique 316L. PhD thesis, INP Grenoble, Laboratories GPM2 – CEA Saclay/DEN/SRMA, 2004.
[20] C.S. Shin, C.F. Robertson, M.C. Fivel, Fatigue in precipitation hardened materials: a three-dimensional discrete dislocation dynamics modelling of the early cycles, Philos. Mag. 87 (24) (2007) 3657–3669.
[21] C.S. Shin, M.C. Fivel, M. Verdier, S.C. Kwon, Numerical methods to improve the computing efficiency of discrete dislocation dynamics simulations, J. Comput. Phys. 215 (2006) 417–429.
[22] Z. Wang, N.M. Ghoniem, S. Swaminarayan, R. LeSar, A parallel algorithm for 3D dislocation dynamics, J. Comput. Phys. (2006) 608–621.
[23] V. Bulatov, W. Cai, J. Fier, M. Hiratani, G. Hommes, T. Pierce, M. Tang, M. Rhee, K. Yates, T. Arsenlis, Scalable line dynamics in paradis, in: Proceedings of the 2004 ACM/IEE Conference on Supercomputing, 2004.
[24] C.S. Shin, M.C. Fivel, M. Verdier, K.H. Oh, Dislocation–impenetrable precipitate interaction: a three-dimensional discrete dislocation dynamics analysis, Philos. Mag. 83 (31–34) (2003) 3691–3704.
[25] C.S. Shin, M.C. Fivel, W.W. Kim, Three-dimensional computation of the interaction between a straight dislocation line and a particle, Modelling Simul. Mater. Sci. Eng. 13 (2005) 1163–1173.

[26] C.S. Shin, 3D discrete dislocation dynamics applied to dislocation–precipitate interactions, PhD thesis, INP Grenoble, Laboratories GPM2 – Seoul National University, 2004.
[27] J. Lothe, J.P. Hirth, Dislocation dynamics at low temperature, Phys. Rev. 115 (3) (1959) 543–550.
[28] M. Duesberry, The influence of core structure on dislocation mobility, Philos. Mag. 19 (1969) 501–526.
[29] M. Tang, L.P. Kubin, G.R. Canova, Dislocation mobility and the mechanical response of bcc (Ta) single crystals: a mesoscopic approach, Acta Metall. Mater. 46 (9) (1998) 3221–3235.
[30] M. Rhee, H.M. Zbib, J.P. Hirth, H. Huang, T. de la Rubia, Models for long-/short-range interactions and cross slip in 3D dislocation simulation of bcc single crystals, Modelling Simul. Mater. Sci. Eng. 6 (1998) 467–492.
[31] M. Wen, A.H.W. Ngan, Atomistic simulation of kink-pairs of screw dislocations in body-centred cubic iron, Acta Mater. 48 (2000) 4255–4265.
[32] M. Wen, A.H.W. Ngan, Dislocation kink-pair energetics and pencil glide in body-centered-cubic crystals, Phys. Rev. Lett. 87 (7) (2001) 075505.
[33] C. Domain, G. Monnet, Simulation of screw dislocation motion in iron by molecular dynamics simulations, Phys. Rev. Lett. 95 (2005) 215506.
[34] J. Chaussidon, M. Fivel, D. Rodney, The glide of screw dislocations in bcc Fe: atomistic static and dynamic simulations, Acta Mater. 54 (2006) 3407–3416.
[35] D. Rodney, Atomic modeling of irradiation-induced hardening, C. R. Physique 9 (3–4) (2008) 418–426.
[36] M. Mendelev, S. Han, D. Srolovitz, G. Ackland, Development of new interatomic potentials appropriate for crystalline and liquid iron, Philos. Mag. 83 (2003) 3977–3994.
[37] K. Obrtlik, C.F. Robertson, B. Marini, Dislocation structures in 16mnd5 pressure vessel steel strained in uniaxial tension, J. Nucl. Mater. 342 (2005) 35–41.
[38] N.M. Ghoniem, B.N. Singh, L.Z. Sun, T. Diaz de la Rubia, Interaction and accumulation of glissile defect clusters near dislocations, J. Nucl. Mater. 276 (2000) 166–177.
[39] N.M. Ghoniem, S.-H. Tong, B.N. Singh, L.Z. Sun, On dislocation interaction with radiation-induce defect clusters and plastic flow localization in fcc metals, Philos. Mag. 81 (11) (2001) 2743–2764.
[40] T. Diaz de la Rubia, H.M. Zbib, T.A. Khraishi, B.D. Wirth, M. Victoria, M.J. Caturla, Multiscale modelling of plastic flow localization in irradiated materials, Nature 406 (2000) 871–874.
[41] T.A. Khraishi, H.M. Zbib, T. Diaz de la Rubia, M. Victoria, Modelling of irradiation-induced hardening in metals using dislocation dynamics, Philos. Mag. Lett. 81 (9) (2001) 583–593.
[42] N.M. Ghoniem, S.H. Tong, J. Huang, B.N. Singh, M. Wen, Mechanisms of dislocation–defect interactions in irradiated metals investigated by computer simulations, J. Nucl. Mater. 307–311 (2002) 843–851.
[43] D. Rodney, G. Martin, Dislocation pinning by small interstitial loops: a molecular dynamics study, Phys. Rev. Lett. 82 (1999) 3272–3275.
[44] D. Rodney, Molecular dynamics simulation of screw dislocations interacting with interstitial frank loop in a model fcc crystal, Acta Mater. 52 (2004) 607–614.
[45] T. Nogaret, C. Robertson, D. Rodney, Atomic-scale plasticity in the presence of frank loops, Philos. Mag. 87 (6) (2007) 945–966.
[46] P. Maziasz, Overview of microstructural evolution in neutron-irradiated austenitic stainless steels, J. Nucl. Mater. 205 (1993) 118.
[47] J.V. Sharp, Deformation of neutron-irradiated copper single crystals, Philos. Mag. 16 (1967) 77–96.