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# Physically Justified Models for Crystal Plasticity Developed with Dislocation Dynamics Simulations

This article highlights how dislocation dynamics (DD) simulations provide a unique opportunity for establishing scale transitions in crystal plasticity. Recent progress in this numerical method is briefly reviewed. Based on the standard problem of plasticity in fcc crystals, we show that DD simulation insight provides guidelines for modeling material mechanical properties controlled by the collective behavior of dislocation microstructures. Hence, DD simulation allows more physical input to be incorporated into continuum models for strain hardening, thereby improving their predictive ability.

## Introduction

Due to its importance in many technological problems, including some aerospace industry issues, the development of a plasticity theory based on dislocation mechanics, rather than on an empirical basis, is a long-standing goal in materials science. However, due to its intrinsically multi-scale nature, the problem of reducing dislocation mechanics to a system of partial differential equations compliant with standard continuum computational methods turns out to be a non-trivial problem. In the last decade, important progress has been made with the development of multi-scale modeling strategies bridging models of crystal plasticity from the atomistic to the continuum domains. Within such multi-scale strategies, 3D simulations of dislocation dynamics (DD) that give a physically justified description of the motions and the interactions of large ensembles of dislocations at the mesoscale are strategic [17]. Indeed, DD simulation allows the statistical analysis and integration of the many and complex dislocation properties controlling the plastic deformation of metals and alloys. This is why this simulation technique is essential to improve the constitutive laws used at large scale in continuum mechanics simulations. In addition, DD simulation allows fair and direct comparison with experiments.

The purpose of this paper is to briefly present some of the progress that we have made in the DD simulation method and in the development of physically justified constitutive equations for continuum simulations. We first provide an overview of an important model, the discrete-continuous model, coupling DD simulations and finite-element simulations. Then, we present recent results associated to the key topics of isotropic and kinematic strain hardening modeling. Finally, we present the conclusion and perspective.

## From dislocation dynamics simulation to the discrete-continuous model

### The “microMegas” project

Three-dimensional DD simulations compute plastic strain by integrating the equations of motion for dislocation lines under stress in an elastic continuum. The mutual interactions of dislocations, the formation and destruction of junctions, their line tension and their interactions with other defects are essentially drawn from the elastic theory. Whereas some differences remain among DD simulation codes, there are basic features that all of these have in common. All of the simulation codes discretize dislocations into a finite set of degrees of freedom attached to line segments. The forces on these discrete lines are estimated from the elastic theory of dislocations and the positions of the dislocation segments are updated according to material-dependent equations of motion. Applying periodic boundary conditions to the simulated volume allows a representative volume element of a macroscopic sample to be monitored at the scale of a few tens of microns. A difficult aspect of DD simulation consists in the definition of constitutive or “local” rules that account for dislocation core properties like dislocation cross-slip and nucleation. For this reason, attention must always be paid to these parts of the simulation codes, since they control the peculiarities of the materials. Such validations can be made either from comparison with atomistic simulation results or from dedicated experiments.

The LEM<sup>1</sup> is at the origin and is the main contributor of a free and open source DD simulation code called microMegas<sup>2</sup>(*mM*). *mM* is today one of the most popular lattice-based DD simulation codes and is used by many research groups to investigate different aspects of

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<sup>2</sup> [http://zig.onera.fr/mm\\_home\\_page/index.html](http://zig.onera.fr/mm_home_page/index.html)

crystal plasticity. A full description of this computer code has been presented in numerous studies [7][21] and was recently described in some detail in [8]. Readers interested in DD simulation applications to micro-plasticity problems involving size-effects, such as in sub-micronic objects and nano-structured materials, are referred to this paper.

### The discrete-continuous model

DD simulation codes present some limitations when they have to deal with complex boundary conditions. Indeed, standard simulations compute dislocation-dislocation interactions using classical expressions of the dislocation stress field in infinite media, not taking into account the interactions of dislocations with free surfaces and interfaces. To overcome these limitations, we develop in collaboration with the ONERA Department DMSM the Discrete-Continuum Model (DCM). The DCM is based on a coupling between a DD code and a finite element (FE) code via the Eigenstrain "formalism". In this formalism, a dislocation is introduced in the FE simulation as Volterra loops, regularized in a plate-like inclusion of thickness  $h$  [19][10][25]. In particular, at each time step, the area swept ( $dS$ ) in the DD simulation by each dislocation segment is transmitted to FE and the associated plastic Eigenstrain ( $d\varepsilon^p$ ) is computed using the following expression:

$$d\varepsilon^p = w(r, h) \cdot dS \frac{(b \otimes n + dS \otimes n)}{2} \quad (1)$$

where  $w(r, h)$  is an isotropic distribution function of radius  $r$  with regularization thickness  $h$ ,  $b$  and  $n$  are respectively the dislocation Burgers vector and a unit vector normal to the  $dS$ .

The sum of all of the elementary  $d\varepsilon^p$  gives the total plastic eigenstrain in the FE part. Once the eigenstrain distribution is calculated, the FE code solves the boundary value problem, computing the mechanical equilibrium (stress, strain and displacement field) in the simulated volume. Then, the DD code exploits the FE stress field to compute the dislocation motion.

Unlike with other coupling techniques (e.g., the superposition principle), as stated above, the DCM is able to compute the full mechanical equilibrium in the simulated domain. This is a key property of the method; it thus allows plastic deformation to be naturally simulated in anisotropic media, to simply access periodic boundary conditions and to couple the DCM with other constitutive laws (crystal plasticity).

In order to better illustrate the capability of the DCM, two examples are presented.

The first one in figure 1 highlights the possibility of running micro-mechanic calculations within the framework of anisotropic elasticity. The plastic relaxation onset of SiGe heteroepitaxial nanoislands, due to the lattice mismatch with the Si substrate, has been studied using anisotropic elastic constants. Panel (a) of figure 1 shows the dislocation equilibrium position inside the nano-island, while panel (b) shows the plastic Eigenstrain induced by the dislocation dynamics. Once the equilibrium is computed, it is possible to have access to the stress field (panel c) and to the displacement field (panel d) associated with the plastic deformation inside the nano-object.

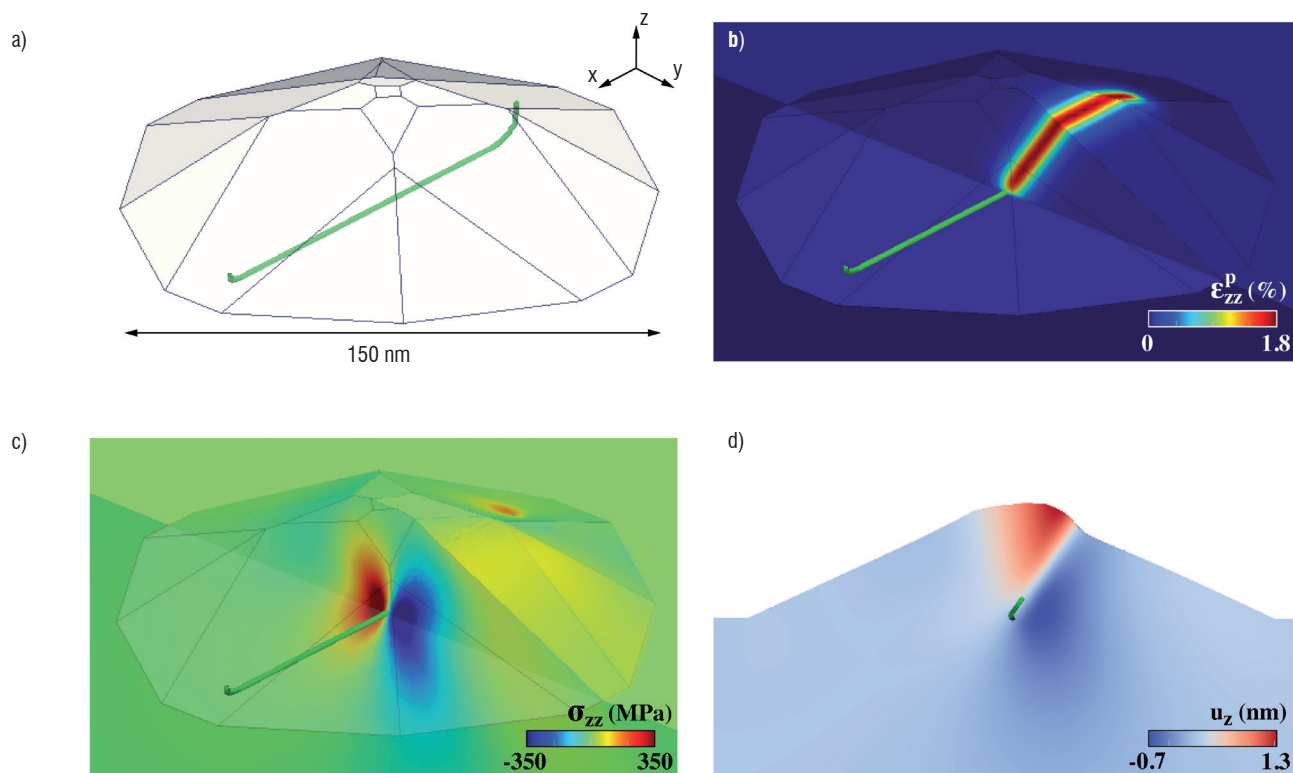


Figure 1 - DCM simulation of a misfit Dislocation line deposited inside a SiGe island  
(a) The dislocation line location and displacements are calculated with the DD code  
(b) The plastic shear associated to dislocation dynamics is locally homogenized and exported to the FE problem  
(c) Dislocation stress field inside the nanoisland at the mechanical equilibrium  
(d) The DCM boundary value problem is solved accounting for crystal rotations and volume shape variations (displacement fields induced by dislocations).

The second example describes the capability of coupling the DCM with other methods, to predict plastic deformation in crystalline materials. In order to model the deformation of a Cu polycrystal in figure 2, a mesh with 16 grains has been created. The central grain exploits the DCM constitutive law, while the surrounding 15 grains are treated with a more phenomenological crystal plasticity model [23][12]. The images of panel (a) and (b) show the Von Mises stress in the polycrystal after 2% of deformation in the  $z$  direction, to highlight the difference between the two different model predictions (DCM vs. crystal plasticity). In panel (a), the dislocation microstructure in the central grain is superposed to the stress field and panel (b) illustrates how, unlike the continuous crystal plasticity model, the DCM is able to capture the stress concentration due to the accumulation of dislocations at the grain boundaries. Hence, it is possible to quantitatively capture the physical process controlling size effects.

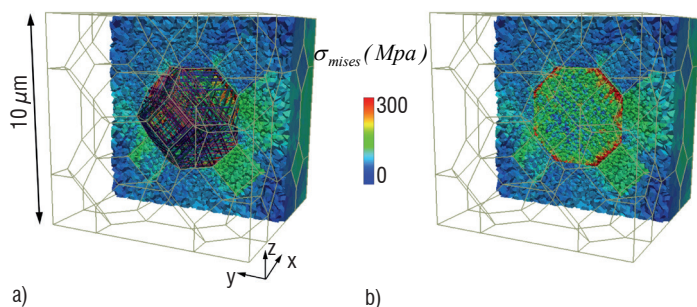


Figure 2 - Example of how the DCM can be coupled with other constitutive law in the FE framework: deformation of a Cu polycrystal. The central grain exploits the DCM constitutive law, while the other 15 Grains in the periodic mesh deform following a phenomenological crystal plasticity law. In panel (a), the dislocation microstructure has been superposed in the central grain to the stress field. Panel (b) highlights how the DCM captures the stress heterogeneities in comparison with the solutions obtain in the other grains.

### Modeling plastic strain hardening

The identification of reliable material constitutive equations for continuum mechanics is an essential ingredient for the development of new materials and structures. Such equations are essential to model the relation between strain and stress inside a material, which is a simple linear relation in the case of elastic analyses (Hooke's law) and a much more complex relation when plastic deformation is involved. Here, we show that the validity of plasticity laws can be considerably improved by making use of information arising from DD simulations. For this purpose, the plasticity of fcc metals is used as a standard problem. It must be noted that the methodology proposed can be extended to other materials, as illustrated by a recent paper dedicated to  $\alpha - Fe$  [22].

Among the many possible choices of constitutive equations for plasticity [2], in this study we consider a well-known dislocation density based model [24] derived from the storage-recovery framework first developed by Kocks and Mecking (see [14] for a review). Nevertheless, the results that we obtained for this model can also be incorporated to alternative continuous models for crystal plasticity. A small strain framework is assumed here, for simplicity reasons.

During plastic deformation, dislocations multiply and their mutual long and short-range interactions hinder their motions. As a consequence, a shear stress increase  $d\tau$  has to be imposed to produce a shear strain increase  $d\gamma$ . By definition, the ratio  $\theta = d\tau / d\gamma$  is the strain hardening rate. In a physically justified approach to crystal plasticity, the density of dislocations in each slip systems ' $i$ ' is a key internal state variable. For this reason, the calculation of the strain hardening can usefully be decomposed in three parts. First, a flow stress relation, has to be identify in order to calculate the critical stress  $\tau_c^i$  for the activation of slip systems. Secondly, the rate at which the critical stress evolves with strain or, equivalently, the rate at which dislocation density evolves under strain in the slip systems ( $d\rho^i / d\gamma^i$ ) (see § " Dislocation storage rate and isotropic strain hardening ") must be defined. Lastly, the plasticity problem is in a closed form by including a flow rule. The latter expression relates, in each slip system, the resolved applied stresses to the critical stress  $\tau^i$  and the strain rate  $\dot{\gamma}^i$ . In fcc materials and for conventional strain rates, a power law expressions is usually considered:

$$\dot{\gamma}^i = \dot{\gamma}_0^i \left\langle \frac{\tau^i - X^i}{\tau_c^i} \right\rangle^m \quad (2)$$

where  $\langle \rangle$  are the Macaulay brackets,  $\dot{\gamma}_0^i$  is a reference strain rate and  $m$  is a material parameter accounting for the strain rate sensitivity. In fcc metals,  $m$  is related to the energetics of jog formation and it does not influence the modeling of plastic strain since at low temperatures its value is large. In eq. (2),  $X^i$  is a long-range back-stress term accounting for the accumulation of polarized dislocation, i.e. the accumulation of geometrically necessary dislocations in regions of the deformed material [1]. For instance, the grain-boundaries (GB) in a polycrystal act as strong barriers to dislocations glide. Then, dislocations are accumulated on both sides of the grain boundaries during plastic deformation. This feature limits the slip system activity and therefore decreases forward deformation of the grains (see § " Modeling kinematic strain hardening ").

### The flow stress relation

Following the work of Franciosi et al. [9], the critical stress for the onset of plastic slip in a system ' $i$ ' interacting with slip systems ' $j$ ' with density  $\rho^j$  can be expressed in a tensor form:

$$\tau_c^i = \mu b \sqrt{\sum_j a_{ij} \rho^j} \quad (3)$$

where  $\mu$  is the elastic shear modulus and  $b$  is the dislocation Burgers vector. In equation (3), coefficients  $a_{ij}$  are the components of a matrix that describes the strength of the interactions between slip systems. In fcc crystals, the number of distinct interaction coefficients between the 12  $\langle 0 1 1 \rangle \{ 1 1 1 \}$  slip systems is reduced to six. Four coefficients are needed to describe slip system interactions involving particular dislocation reactions, that is, the glissile junction, the Hirth and Lomer locks and the collinear annihilation. This last reaction occurs between slip systems that share a common Burgers vector. It does not produce junctions but rather athermal annihilation over an extended range of dislocation line characters [20].

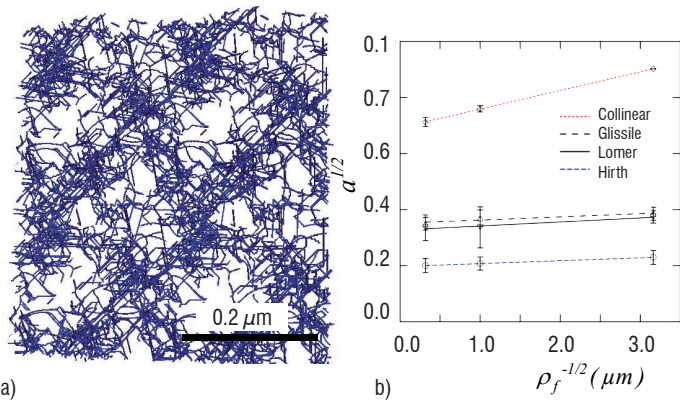


Figure 3 - (a) Example of periodic dislocation microstructure in a (001) foil of thickness  $0.2 \mu\text{m}$  extracted from a simulated volume of Cu deformed under multi-slips conditions. (b) Measurements of slip system interaction strength ( $a^{1/2}$ ) for different forest dislocation densities ( $\rho_f^{-1/2}$ ) including only one type of dislocation reaction, i.e., the collinear annihilation and the glissile, Lomer and Hirth junctions.

Calculation of the  $a_{ij}$  values as a function of the dislocation density is a task that we performed with DD simulations [18][6]. As shown in figure 3-b, for a reference forest density of  $\rho = 10^{12} \text{ m}^{-2}$ , the strength of slip system interaction involving the Lomer junction is found identical to a standard value calculated with the forest model,  $\sqrt{a} \approx \alpha \approx 0.35$ . This result reflects the predominance of the Lomer reaction in the strengthening of fcc single crystals. For the Hirth, glissile and collinear types of interactions, the calculated strengths are approximately  $0.6\alpha$ ,  $\alpha$  and  $2.3\alpha$ , respectively. It is interesting to note that due to the large value of the collinear annihilation coefficient, we explained why, in contradiction with the Schmid law prediction, the simultaneous activity of two slip systems shearing the same Burgers vector can hardly be observed experimentally [15].

The two remaining  $a_{ij}$  coefficients are those associated with the interaction of a slip system with itself and the interaction between coplanar slip systems. DD simulations dedicated to these particular configurations show that the coefficients of the latter are much larger than is often assumed, close to that associated with the Lomer interaction [5].

### Dislocation storage rate and isotropic strain hardening

As illustrated in figure 4, the process of dislocation density storage is, under many deformation conditions, directly related to the dislocation avalanche feature. For this purpose, the concept of dislocation mean free path, which is the distance traveled by a mobile dislocation segment of unit length before it is stored by interaction with the microstructure, is essential. It is intuitive that dislocations mean free path decreases with increasing stored density and depends on the strength of the dislocation obstacles opposing the dislocation motion. A formal modeling of this quantity was performed with DD simulations [3][16]. The full expression of the storage rate derived from DD simulations is too complex to be reported here. Instead, we restrict ourselves to the rather simple form obtained in the absence of dynamics recovery processes and for loading conditions imposing symmetric activity of the slip system. For each mobile slip system and taking into account only forest interactions, we demonstrated that:

$$\frac{d\rho^i}{d\gamma^i} = \frac{\tau_c^i}{\mu b^2 K_{hkl}} \text{ with } K_{hkl} = \left[ \frac{\bar{a}^{-1/2} n (1 + \kappa)^{3/2}}{p_0 k_0 (n - 1 - \kappa)} \right] \quad (4)$$

In eq. 4,  $\tau_c^i$  is the critical stress for the onset of slip systems activity and  $K_{hkl}$  is an orientation-dependent mean free path coefficient. In the  $K_{hkl}$  definition,  $n$  is the number of active slip systems and  $\bar{a}^{-1/2}$  is the average value of the interaction coefficients  $a_{ij}$ . The three coefficients  $p_0 = 0.117$ ,  $k_0 = 1.08$  and  $\kappa = 0.29$  are dimensionless constants. They are related respectively to the probability for forming a stable junction upon crossing a forest dislocation, to the average length of the stored dislocation line segments and to the density of junctions in the microstructure. As illustrated in figure 4, value of these coefficients could be determined from DD simulations [4].

Equations (3) and (4) constitute two essential building blocks for modeling isotropic strain hardening in fcc crystals and in other materials when strain hardening is dominated by dislocation-dislocation interactions. Demonstration was made that their integration on a meshed sample using a crystal plasticity FE code allows for predicting quantitatively the first two hardening stages of FCC single crystals without fitting procedure [16].

### Modeling kinematic strain hardening

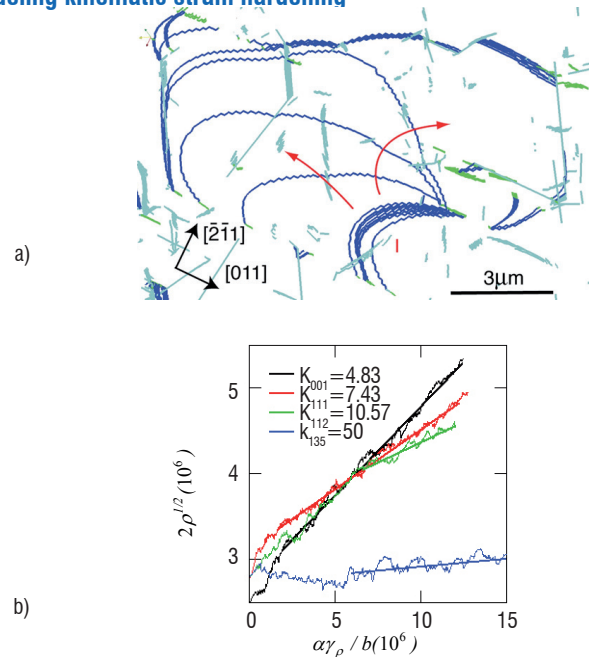


Figure 4 - (a) Dislocation avalanche (or strain burst) observed with DD simulation in a tensile test of a [001] Cu crystal. This dynamic feature controls the relation between plastic strain production and dislocation density storage (b) Determination of the dislocation mean free path coefficients by DD simulations for different single crystal tensile test orientation.

Other obstacles than dislocations can contribute to strain hardening. For instance, in a polycrystal with grain size  $d_g$ , GB distances necessarily limit the mean free path of dislocations. For this reason in a polycrystal, an additional storage term accounting for the accumulation of polarized dislocations (GND) must be added to eq. (4). For simple dimensional reasons, this term take the form:

$$\frac{d\rho_{GND}^i}{d\gamma^i} = \frac{k_{GND}}{b r_{GB}} \quad (5)$$

with  $r_{GB}$  the shortest distance to GBs and  $k_{GND} \approx 0.5$  a storage rate parameter accounting for a specific organization of the GND density

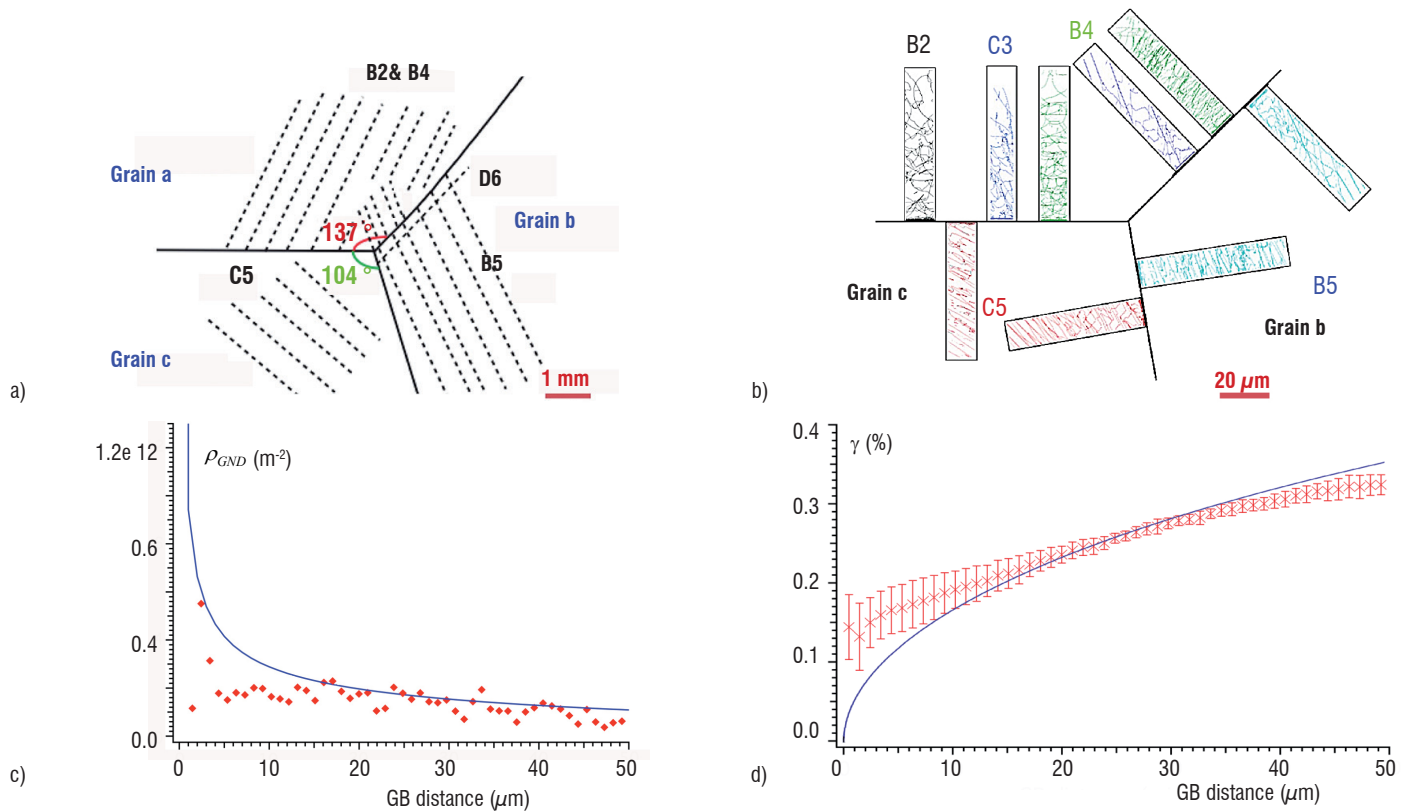


Figure 5 - (a) Schematic of the slip systems activity observed at yield in a Cu tri-crystal compression test (Schmid&Boas slip system notation is used). (b) Illustration of the slip system-GB configurations investigated with DD simulations and reproduced from a Cu tri-crystal deformation test. Dimensions of the simulated volume are  $75 \times 13 \times 10 \mu\text{m}$ . (c) and (d) are respectively, the average profiles of GND density and plastic shear calculated with the DD simulations illustrated in (b). Continuous blue lines are solutions of the classical equation of a one-dimensional pile-up profile and the equations (5) holding from the average dislocation density in the simulated volume.

close to a GB. Integration of eq. 5 reproduces the formation of heterogeneous densities of GND known as a dislocation pile-up distribution. Such configurations are essential since they are the basis for the notion of back stress and the foundation of many size effects like the Hall-Petch mechanism [11]. Again, calculation of the parameters monitoring the formation of 3D pile-up configurations against GBs has been made with DD simulations. As illustrated in figure 5, we systematically studied the dislocation microstructures formed against a GB with different slip system geometries (i.e. different misorientation between slip planes and GB planes). Such simulated configurations were identified from a real Cu tri-crystal deformation test (figure 5-a) and the analysis of active slip system traces at yield.

Unsurprisingly, simulated 3D dislocation microstructures are different from the ideal pile-up configurations discussed in textbooks. The back-stress fields we found are complex construction of the long-range stress fields associated to dislocations sharing the same glide plane, but also from many dislocations positioned on neighboring, parallel or tilted glide planes. Nevertheless, averaging the plastic strain and the GND density, as function of the GB normal distance, shows that simulated 3D dislocation configurations can still be interpreted with a generalized concept of pile-up stress. Hence, a new expression for the back-stress associated to 3D GND microstructures accumulated against a GB was proposed as function of  $r_{GB}$ :

$$X^i(r_{GB}) = \beta \cos(\theta^i) \mu b \sqrt{\rho_{GND}(r_{GB})} \sqrt{r_{GB}} \quad (6)$$

In eq. 6,  $\theta^i$  is the angle between the GB and the slip system, and  $\beta$  is a geometrical parameter accounting for the organization of dislocations in 3D configurations. The latter value was numerically estimated to 37 from many DD simulation results.

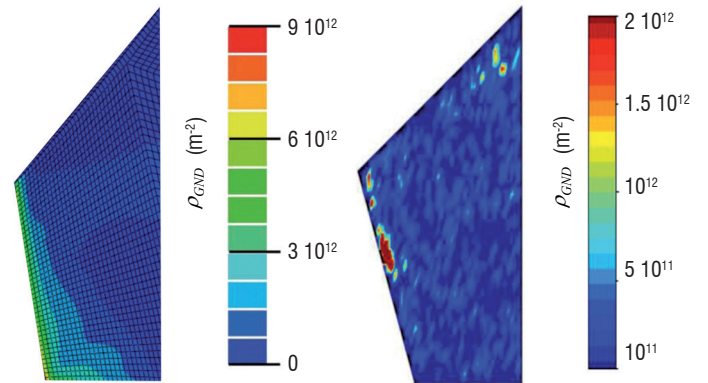


Figure 6 - Comparison between simulated and measured GND density distribution at 0.2% compression strain in a grain part of a tri-crystal (see figure 5-a for the total geometry).

The predictive ability of eq. (5) and (6) in addition with the equations previously defined for isotropic strain hardening was tested with a crystal plasticity code in the case of a Cu tri-crystal compression test. As shown in figure 6, the GND density distribution at 0.2% strain was calculated in a meshed tri-crystal and compared with measurements made with the  $\mu$ Laue-XRD technique in the real sample [13]. In the

early stage of plastic deformation observed experimentally, excellent agreement is found for the slip systems activity between simulation and experience. In addition, good agreement (within the limits of the experimental errors) is found for the GND density amplitude and distribution (i.e. rotation fields) in the grains.

## Conclusion and perspectives

In this paper we have first presented the progress we made in the development and numerical implementation of DD simulations. More specifically, we emphasized the breakthrough made in the last two years in a coupling of DD and FE simulations to solve complex boundary problems. The numerical strategy developed, called the discrete-continuous model (DCM), is now mature and offer many advantages. Then, we have shown that the internal state variables and the mathematical forms used in crystal plasticity calculations can be physically justified and identified with DD simulations. An important effort was first devoted to the modeling of isotropic strain hardening in pure fcc metals. Recently, we started to investigate more complex phenomena at the origin of kinematic strain hardening.

Modeling complex loading with large strain in a multi-phased polycrystalline materials is still a long-term goal, but important progresses have been made that extend the domain of validity of the existing crystal plasticity models. Simulations of the Bauschinger effect and cyclic deformation conditions are the next steps. The constitutive equations used for these problems involve back-stress formulations opening the door to many different interpretations at the dislocation scale. A study with the DCM simulation of the collective and dynamic properties involved here should give useful information for design methods against fatigue of structural materials [13].

Another important problem in which the capability of the DCM simulation will be exploited is the study of plastic relaxation at crack-tip in ductile materials. Here, two main phenomena take place: a dislocation microstructure is locally developed to decrease stress concentration

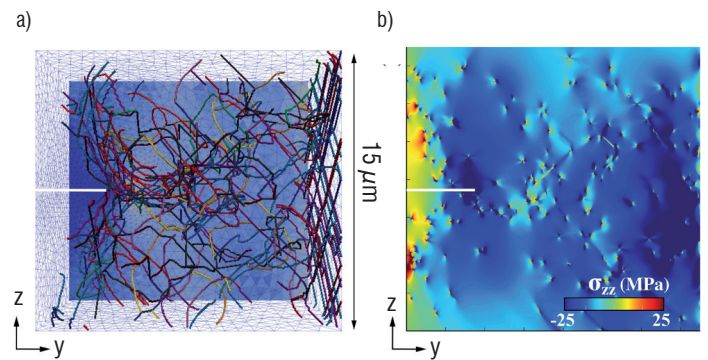


Figure 7 - (a) Example of a dislocation microstructure formed at a crack tip in a Cu sample loaded in Model. The crack location is the thin white segment and the dislocation lines are plotted with colors according to their slip systems. (b) The elastic shielding effect caused by the dislocation microstructure is illustrated in a plane normal to the crack tip. The plotted quantity  $\sigma_{zz}$  is the sum of the dislocation stress fields in the sample and is clearly opposed to the crack opening (Courtesy of L. Korzeczek, PhD work).

ahead of the crack (shielding effect) and the crack tip changes its shape due to the emission/absorption of dislocations (blunting effect). The DCM is suitable to simulate these two phenomena, on the one hand the proper boundary conditions can be imposed to compute the mechanical equilibrium in a material including a crack and on the other hand the evolution of the dislocation microstructure can be precisely investigated. Figure 7 shows one of the first results obtained using the DCM. Here a Cu single crystal is deformed in the  $z$  direction to open a crack in mode I. The crack plane is normal to the (100) direction with a crack tip parallel to the [010] direction. Panel (a) shows how the dislocation pre-existing in the sample reacts to the stress field ahead of the crack tip and rapidly build a plastic zone. The elastic shielding of the dislocation microstructure that works to reduce crack opening is shown in panel (b). Ongoing work is dedicated to this problem for cyclic deformation conditions and in a polycrystalline material to better understand grain size effects ■

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