# DISCRETE-CONTINUUM MODELING OF METAL MATRIX COMPOSITES PLASTICITY

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**Abstract** A computing methodology is reported for modeling the plastic deformation of Metal Matrix Composites. Use is made of a discrete-continuum model based on a coupling between Dislocation Dynamics and Finite Element simulations, which provides a parameter-free quantitative description of the mechanical properties. The model and the first simulation results on MMCs are presented and briefly discussed.

**Keywords:** Metal Matrix Composite, Plastic deformation, Dislocation Dynamics simulation, Finite Element simulation

## 1. INTRODUCTION

The recent interest on materials with increasingly small characteristic length scales has clearly revealed some shortcomings in the modeling of size effects in materials plasticity. These effects, which are explicit in dislocation theory, are usually not reproduced by continuum approaches. For this reason, the prediction of the plastic properties of Metal Matrix Composites (MMCs) is sometimes considered as a bench test for theoretical or numerical models. Indeed, in MMCs the stress-strain behavior is size-dependent for reinforcement sizes and volume fractions in the micrometer range. Further, the matrix stress-strain behavior that needs to be assumed to reproduce experimental results differs from the stress-strain behavior of the unreinforced material [1–3].

As theory and experiment often do not fit very well, some authors [4–6] proposed to validate the predictions of their own theory by comparison with a Dislocation Dynamics (DD) simulation by Cleveringa et al. [7, 8], on a 2D composite material with periodic rectangular reinforcements. Such exercises

were extremely instructive but, nevertheless, care should be exercized when extrapolating two-dimensional models to experiment.

The simulation of dislocation dynamics in 3D MMCs is a challenging problem, which goes much deeper than the usual question of CPU time limitation. One has, in addition, to define precisely the conditions for mechanical equilibrium in such complex hetero-structures (see [9] for detail). Several solutions to this problem are now potentially available [9–14] and a critical comparison of these approaches can be found in ref. [15]. In the present work, use is made of the Discrete-Continuum Model (DCM) [10, 11]. The model and its specific implementation in the case of MMCs are shortly described in part 2. Parts 3 and 4 are dedicated to a presentation of the simulation results and part 5 to concluding remarks.

## 2. THE DISCRETE-CONTINUUM MODEL

In essence, the DCM, is made up of an FE code (ZeBuLon), in which a DD simulation replaces the constitutive formulation for plastic properties. On the one hand, the FE code treats the boundary value problem and cares of the conditions of local equilibrium in a meshed volume element. On the other hand, the DD code cares of the topology and motion of the dislocation lines in the same volume element, hence of the plastic strain, $\underline{\varepsilon}_p$. The coupling is realized with the help of two procedures that control the traffic between the "discrete" and "continuum" codes, a homogenization procedure for the calculation of $\underline{\varepsilon}_p$ and an interpolation procedure for the calculation of the stress tensor $\underline{\sigma}$ at any point of the simulated volume (cf. [11, 15]).

### 2.1 Dislocation Self-Stress Fields

In agreement with Mura's Eigenstrain theory [16], the DCM can theoretically capture all details of the dislocation stress fields in isotropic or anisotropic elasticity. It is then mainly a matter of computation to design a FE mesh for computing the complex stress field of a dislocation line close to its singularity. Unfortunately, for "mass" simulations involving many dislocations, this brute force approach is numerically untractable.

For instance, considering the computational constraints discussed in part 4, the largest regular mesh that can be handled by a good workstation has $(10 \times 16 \times 6)$ quadratic cubic elements of linear length $0.137\mu m$. The mesh length may then be larger than the mean distance between dislocations and the shape function used to interpolate the stress can only reproduce the smooth variations of the dislocation stress fields far from their singularities. Indeed, the Eigenstrains associated to dislocations are homogenized in a small volume surrounding the lines, in order to remove stress singularities. For this rea-

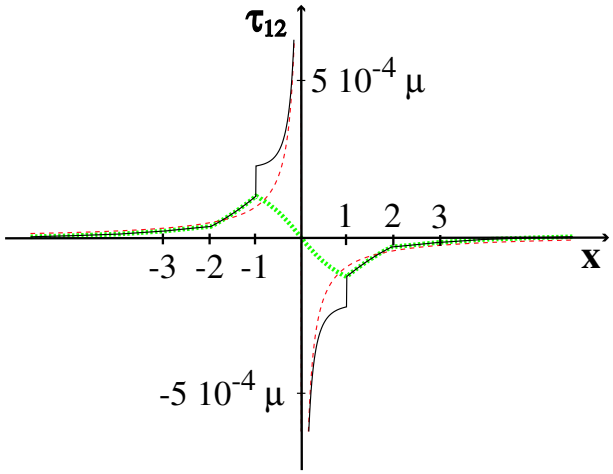


*Figure 1.* Isotropic shear stress field of a rigid screw dislocation calculated along a direction normal to the line. For the sake of comparison, the distances in abscissa are plotted in units of the linear dimension of the quadratic elements used in the present work. Dashed line: theoretical solution. Dotted line: solution yielded by the DCM. Continuous line: DCM solution with a short-distance correction.

son, the previous version of the DCM was restricted to problems of plastic relaxation implying no short-distance reactions between dislocations (see for instance [17]).

A simple solution is proposed to overcome this limitation. In the DD part of the DCM, the analytical (isotropic) self-stress field of a dislocation is superimposed to the stress prediction yielded by the FE code within a small volume surrounding the singularity (see Fig. 1). This volume is limited to the homogenized core region, so that the homogenization volume in the DCM is identical to the volume where the stress correction is performed. Hence, in conformity with dislocation theory, we introduce in the DCM framework the equivalent of an "elastic core surface traction" [18], which does not affect the total mechanical equilibrium (by construction the integral of the additional stress is zero), but improves the local description of dislocation interactions. In other terms, the amount of elastic energy lost in the homogenization procedure is locally restored in the DD code without affecting the consistency of the FE calculations. This correction is an essential one if one wishes to realistically reproduce the strength of dislocation reactions (cf. part 4). It must be noticed that whereas this improvement is easy to implement, it significantly increases the computational burden. This is why the small discontinuity of the stress field generated at the border of the homogenization volume (see Fig. 1) has not been removed so far. This is feasible in technical terms, but does not appears to be critical.

## 2.2 Initial and Boundary Conditions

The need to consider a reference cell as small as possible in order to optimize computations strongly suggests applying periodic boundary conditions (PBCs) in the case of MMCs simulations. Topological problems related to the use of these conditions, when applied with DD simulations, are discussed in [19]. Here, we restrict ourselves to the question of implementing PBCs in a FE code and to some related problems that may affect the simulation results.

As shown in Fig. 2, the simulation cell used for the study of MMCs is a parallelepipedic volume of dimension $(1.368 \times 2.188 \times 0.820)\ \mu m^{-3}$ including four half-fibers of square cross-section at the center of the vertical faces (the edges of the fibers are rounded off in the FE mesh to eliminate local stress concentrations). Modifying the dimensions of the fibers allows obtaining various volume fractions in the simulated cell. By periodic three-dimensional replication of the simulation cell, one obtains a composite material with an hexagonal arrangement of infinitely long fibers. The displacement ($\mathbf{u}$) and strain ($\underline{\varepsilon}$) fields that verify the periodic solution in the reference cell are as follows:

$$\underline{\varepsilon}(\mathbf{u}(\mathbf{r})) = \underline{\bar{\varepsilon}} + \underline{\varepsilon}(\mathbf{u'}(\mathbf{r})) \quad \text{with} \quad \mathbf{u}(\mathbf{r}) = \underline{\varepsilon} \cdot \mathbf{r} + \mathbf{u'}(\mathbf{r}) \tag{1}$$

where $\underline{\bar{\varepsilon}}$ is the mean deformation expected if the material is homogeneous and $\underline{\varepsilon}(\mathbf{u'})$ is a fluctuating quantity that accounts for the presence of the periodic hetherogeneities (in the present case, the fibers). This last term derives from a displacement field $\mathbf{u'}$, *i.e.*, whose values are periodically repeated at the cell boundaries in the directions of the translation vectors. Hence, the mechanical equilibrium in the simulated volume element must satisfy the following equations:

$$\langle \underline{\varepsilon}(\mathbf{u'}(\mathbf{r})) \rangle = \underline{0} \quad \text{and} \quad \langle \underline{\varepsilon} \rangle = \underline{\bar{\varepsilon}} \tag{2}$$

$$div \underline{\sigma}(\mathbf{r}) = \underline{0} \quad \text{and} \quad \underline{\sigma}(\mathbf{r_1}).\mathbf{n} = -\underline{\sigma}(\mathbf{r_2}).\mathbf{n}, \tag{3}$$

where $\mathbf{r_1}$ and $\mathbf{r_2}$ are opposite points at the boundary of the simulation cell and $\mathbf{n}$ is the corresponding boundary translation vector.

The main difficulty encountered when setting up proper initial conditions stems from the fulfillment of the above stress and strain conditions in the presence of a dislocation microstructure. In order for the FE code to account for the elastic fields of dislocations, the latter must imperatively be generated by a Volterra process. This implies that the DCM can only deal with closed dislocation loops. To globally satisfy the equilibrium conditions, the solution that is implemented consists in expanding the initial dipolar loops from random positions in the simulation cell (see Fig. 2-a). All the loops have same diameter, which is taken much larger than the mean distance between dislocations in order to avoid artificial screening effects. The total density is equally distributed

on the twelve slip systems of the fcc structure and the total plastic shear during the Volterra process is set to zero by balancing the signs of the Burgers vectors. In the case of the unreinforced material (cf. part 3), this type of initial microstructure induces a mechanical state very close to equilibrium and only a small relaxation is observed at the beginning of the simulations. The case of the MMCs simulations is more critical and particular attention must be paid to the displacement and strain fields associated to the initial configuration (see Fig. 2-b), particularly with large volume fractions of fibers. Indeed, the fiber-matrix interfaces, which are assumed to be impenetrable barriers to dislocation glide, alter the symmetries of the initial dislocation microstructure. For this reason, it is necessary to check that the randomly generated configuration does not induce high internal stresses that could artificially modify the dynamics. In what follows, we only consider initial microstructures with an initial internal stress sufficiently small not to induce an artificial asymmetry between tension and compression tests. It is worth noting that it could be interesting in some cases to use alternative initial microstructures, for instance for reproducing the residual stresses generated during the processing of MMCs [1].

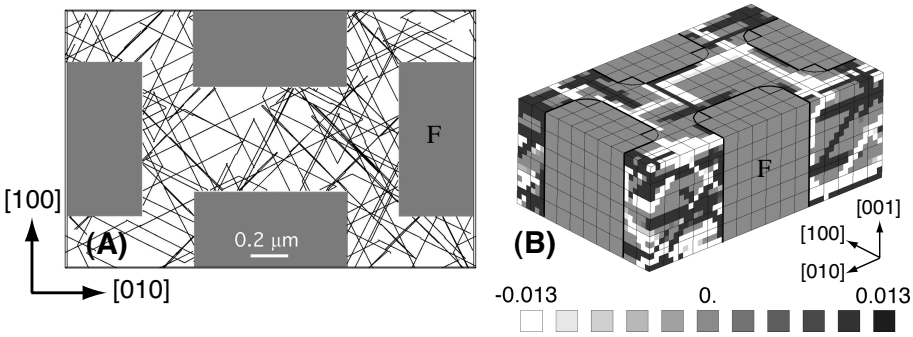


*Figure 2.* Initial conditions for the MMCs problem. A) A random distribution of dipolar dislocation loops generated by Volterra processes in a simulation cell. Whatever the loop positions, the dislocation lines cannot penetrate the fibers (denoted F). B) Surface mapping of the component $\varepsilon_{33}$ of the initial strain field (the mean value is close to zero, as can be seen from the gray scale). Notice that special elements are used at the fiber's edges to avoid local stress concentrations.

Finally, whereas conventional DD simulations with PBCs make use of a cut-off distance for the stress field computations [20], the dislocation dynamics part of the DCM accounts for the totality of the periodic fields. The two types of simulations should then yield slightly different results when long-range elastic effects come into play.

## 3. VALIDATION TESTS

In order to validate the short-distance stress correction discussed in Sec. 2.1, simulated tensile tests have been carried out on copper crystals. The flow stress of pure fcc metals being controlled by dislocation reactions [20], such tests should be critical ones. An equivalent simulation, not reproduced here, were performed on an aluminum crystal, to determine the plastic properties of unreinforced matrix in $Al_2O_3/Al$ MMCs. The results are very similar in both cases.

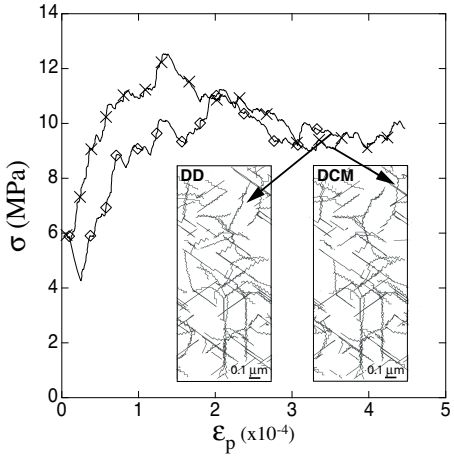


*Figure 3.* Tensile [100] stress-strain curves for a copper crystal, as obtained by DD ($\Diamond$) and DCM ($\times$) simulations with periodic boundary conditions. In both cases, the dimension of the reference cell is about $(10\mu m)^3$, the initial dislocation density is $10^{12}\ m^{-2}$ and the simulated specimen is deformed with a total imposed strain rate of $20\ s^{-1}$. The insets show thin foils extracted from the two simulations. One can check that the dislocation microstructures and the positions of the junctions at the end of the two simulations are nearly identical.

Figure 3 shows the results of DD and DCM simulations on a copper crystal with same loading conditions. In both cases the yield stress is exactly the one experimentally measured for a dislocation density of $10^{12}\ m^{-2}$ [20]. As a result of the small differences between PBCs in the two simulations (cf. Sec. 2.2), the two stress-strain curves slightly differ at low strains. This, actually, results from the truncation of the long-range stresses in the DD simulations. Beyond the yield stress, these differences vanish and the very good agreement between the two computations is interpreted as follows. In fcc crystals, long range interactions do not significantly contribute to the flow stress. The latter is controlled by the dislocation line tension and the numerous dislocation reactions taking place at the intersections between active slip planes.

This well-known result is illustrated in Fig. 3 by two thin foils extracted from the two simulated stress-strain curves at the same strain value. The same junctions are found at the same places in the two simulated microstructures and one has to look closely to find differences in the detail. From this result, we conclude that the local stress correction discussed in Sec. 2-1 is efficient and allows reproducing in the DCM the short-range interactions of dislocations, i.e., essentially the zipping and unzipping of junctions and dipoles. In addition, we verify that the energetic and dynamic aspects of the DCM are now consistent with their equivalents in DD simulations.

# 4. LONGITUDINAL TENSILE TEST IN $Al_2O_3/Al$

## 4.1 Simulation Conditions

In the present study, an $Al$ matrix with infinitely long $Al_2O_3$ fibers is considered as a generic model for MMCs with long reinforcements. The mechanical properties for this composite are well documented in the literature [3], which allows performing direct comparisons with experiment. To be consistent with the dislocation microstructures generated during the processing of such MMCs, the initial dislocation density is set, in all cases, to the rather large value of $\rho_0 \approx 0.7\ 10^{14}\ m^{-2}$. Three different volume fractions of fibers are investigated, $5\%$, $20\%$ and $45\%$, with respective fiber cross-sections of $(0.274 \times 0.274)\ \mu m^2$, $(0.547 \times 0.547)\ \mu m^2$ and $(0.828 \times 0.828)\ \mu m^2$. The distances between the centers of the fibers is constant and equal $1.29\ \mu m$, in order to check the possible occurrence of size effects. As most of the existing analyses of experimental results make use of isotropic elasticity, two isotropic matrices of elastic constants are used in the FE part of the DCM. The Young's moduli and Poisson's ratio for the two phases are, respectively, $E_{Al}$ = 71.3 GPa, $E_{Al_2O_3}$ = 373 GPa, $\nu_{Al} = 0.347$ and $\nu_{Al_2O_3} = 0.235$.

## 4.2 Results

In a first step, the simulation results are compared with the simple rule of mixtures, which assimilates the material to a composition in series of two elastic phases stressed in uniaxial tension. Hence, along the tensile axis:

$$\sigma = E\varepsilon \quad \text{and} \quad E = E_{Al_2O_3}V + E_{Al}(1-V) \tag{4}$$

where $V$ is the volume fraction of fibers.

The composite behavior, as reproduced by the simulation, is in very good agreement with experiment on the same material [1, 3]. As shown in Fig. 4,

the composite material deformed in the longitudinal direction and with a large volume fraction of fibers deforms quasi-elastically. The rule of mixtures then provides a reasonable prediction of the stress-strain dependency. A smooth deviation from the purely elastic prediction is nevertheless recorded, even at very small strains. Such behavior, viz. the absence of an initial elastic stage, is commonly observed experimentally in $Al_2O_3/Al$ composites. In the present case, the Al matrix is soft, as it has the mechanical properties of a pure single crystal; thus, it starts plastically deforming at rather low applied stresses. As expected, this phenomenon manifests itself all the more as the volume fraction of fibers decreases.

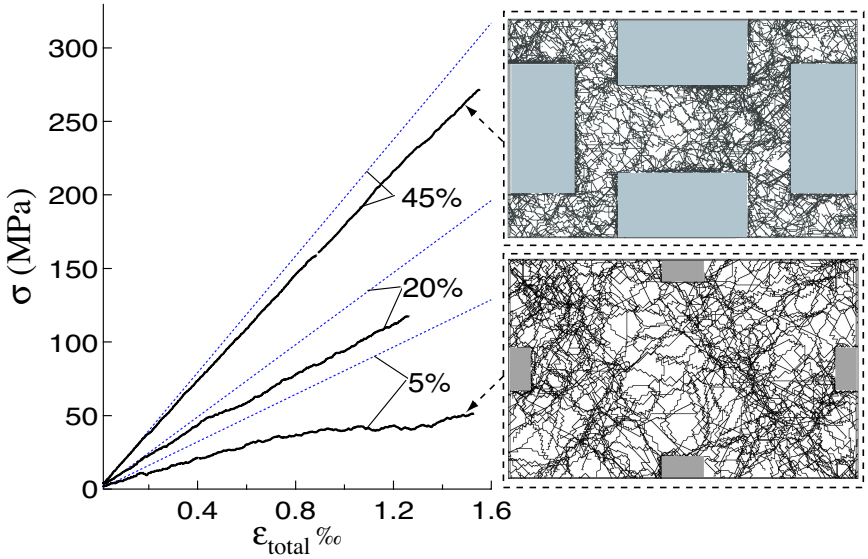


*Figure 4.* Longitudinal tensile stress-strain curves for $Al_2O_3/Al$ MMCs with different fiber dimensions in a simulation cell of constant size. The volume fraction of fibers is V = 5%, 20% and 45%. The dotted lines refer to elastic predictions from the rule of mixtures. The two simulated microstructures show [001] views of the composites parallel to the fiber axis at a strain $\varepsilon = 0.15\%$. The dislocation density is about $1.35\ 10^{14}\ m^{-2}$ for $V = 5\%$ and $1.7\ 10^{14}\ m^{-2}$ for $V = 45\%$. Notice the early departure from elastic behavior for the smallest volume fraction.

When plastic deformation proceeds in the matrix, the dislocation density rapidly increases and a microstructure is formed, which contains many junctions (Fig. 4). The observed persistence of junctions at all the investigated strains is an indirect proof that the stresses developed in the matrix are still compatible with a mechanism of forest hardening. This result is again in agreement with experimental observation [1]. Nevertheless, as illustrated by Fig. 4, the differences in microstructure arrangement and dislocation density between

the two volume fractions $V = 5\%$ and $V = 45\%$ strongly suggest that there is an additional hardening process. By lack of space, the analysis of this effect, which is actually size-dependent, is postponed to a future publication where the in-situ properties of the Al matrix will be investigated in full detail.

Finally, a careful observation of the simulation output reveals the progressive accumulation of a large dislocation density at the interfaces between the fibers and the matrix. In contrast with 2D simulations results, however, no pile-up of dislocation loops is formed around the fibers. This result can be explained in simple terms. In a 3D MMC structure, the dislocations can by-pass the fibers by an Orowan process, irrespective of the volume fraction, whereas this process cannot be accounted for in two dimensions. Hence, if the mean free-path of the dislocations is large enough, a large amount of plastic strain can be produced by each dislocation loop and the sources are much less active in 3D than in 2D. This is why in multi-slip conditions, but also in single slip conditions too, the probability for finding at the interfaces dislocations emitted in the same plane by a dislocation source is rather low.

## 5. CONCLUDING REMARKS

An improvement to the DCM is proposed and tested, which gives access to "massive" simulations of dislocation dynamics accounting for complex boundary value problems. The comparison between conventional DD simulations and the DCM in the case of pure fcc single crystals shows that the interactions of the dislocations at short distances, and especially their reactions, are now quantitatively reproduced.

The first original calculations of this improved version of the DCM have been dedicated to the study of a MMC. It was checked that the DCM, which is a parameter-free simulation, reproduces well the tensile properties of $Al_2O_3/Al$ composites in the longitudinal direction. A simple comparison of 2D and 3D simulation results makes it clear that the hardening processes involved in MMCs are, in essence, three-dimensional.

This first study allows considering many future developments, which, globally, aim at discriminating between dislocation or metallurgical effects and mechanical effects through a coupled analysis of the simulated microstructures and of the stress and displacement fields. A detailed in situ investigation of the strain hardening of the aluminum matrix is under way. Since, however, the stress-strain behavior of $Al_2O_3/Al$ composites deformed along the fiber direction is mainly elastic, size effects can more conveniently be examined by straining along the transverse direction. Lastly, experimental studies suggest the existence of a significant Baushinger effect. Its examination by the DCM could be of interest with reference to kinematic hardening in MMCs.

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