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Consistent formulation for the Discrete-Continuous Model: Improving complex dislocation dynamics simulations

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ABSTRACT

A new and efficient formulation of the Discrete-Continuous Model (DCM) for the simulation of 3D dislocation dynamics in complex finite or periodic volumes is presented. As in previous versions, the improved model is based on a coupling between a Dislocation Dynamics (DD) code and a Finite Element (FE) code through eigenstrain theory. Short-range interactions are now handled more properly. Specifically, in the continuous limit the stress field driving the dislocation dynamics is now reconstructed consistently. Furthermore, the DCM can now handle nonstructured meshes, and free surface and interface handling does not depend on having a structured mesh anymore. Also numerical experiments shed some light on the influence of the choice of the FE quadrature. Some approximations are proposed and justified, and the use of advanced algorithmic techniques are used for time integration and the homogeneisation procedure to reach a high computational efficiency. Basic tests demonstrate the validity and the efficiency of the proposed strategy. Remarkably, it is demonstrated that for a periodic domain the DCM with a very fine FE mesh is actually faster than a corresponding classical DD simulation.

1. Introduction

Three-dimensional Dislocation Dynamics (DD) simulation has become an essential tool in materials science during the last few years because of the many investigations into the mechanical properties of micro- and nano-objects and because of the need for more physically justified crystal plasticity constitutive rules. In its most standard formulations, DD simulations use analytical expressions for the stress field of dislocation segments which are part of discretised dislocation loops. However those expressions are valid only for isotropic elasticity and in an infinite continuum (Hirth and Lothe, 1982; Devincre, 1995; Cai et al., 2006). In order to handle more complex boundary conditions and to take the effects of free surfaces or internal boundaries into account, alternative numerical solutions have also been developed (see for instance (Devincre et al., 2003) for a description and comparison of the main methods). In the following such solutions are called hybrid methods, as opposed to classical methods defined in infinite domains.

Most of the hybrid methods depend on a coupling between DD and Finite Elements (FE). The most widely used approach is the superposition method in which the mechanical problem is decomposed into a DD problem in an infinite medium and a

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dislocation-free complementary boundary value problem, solved by a FE elastic solver (Van der Giessen and Needleman, 1995; Fivel and Canova, 1999; Zbib and Diaz de la Rubia, 2002; Weygand et al., 2002; Tang et al., 2006; Leiter et al., 2013). The Peach-Köhler forces driving the dislocation dynamics are then calculated, at line segments, from the stress obtained by adding the stress from the dislocation-free complementary FE problem to the analytical stress as calculated in the standard DD simulation in an infinite medium, so that the boundary conditions are taken into account properly. This approach was extensively used and optimised in the past years to simulate mainly plasticity of micro- and nano-objects (see for instance (Weinberger and Cai, 2007; El-Awady et al., 2008; Takahashi and Ghoniem, 2008; Weinberger et al., 2009; Akarapu et al., 2010; El-Awady et al., 2011; Zhou and LeSar, 2012; Crone et al., 2014)).

An alternative hybrid approach is the Discrete-Continuous Model (DCM) (Lemarchand et al., 1999, 2001; Liu et al., 2009; Vattré et al., 2014; Cui et al., 2015). Here only the short-range dislocation–dislocation interactions are treated analytically and all other interactions including those due to external loads and free boundaries are calculated numerically by FE. Mixed calculations in which the DD responses in one set of regions are combined with phenomenological constitutive laws in other regions of the structure then become almost trivial. The DCM is based on a regularisation of the atomic displacement jump across the slip plane into a plastic strain inclusion following the eigenstrain theory (Mura, 1991). It was successfully applied to several practical problems, such as anisotropic thin films (Groh et al., 2003; Liu et al., 2011), metal-matrix composites with long fibres (Groh et al., 2005), micro-pillars (Liu et al., 2009) and single-crystal $\gamma-\gamma'$ Ni based superalloys (Vattré et al., 2010). Nevertheless, several limitations have appeared in the past years:

- The calculations were restricted to simple geometries due to the need for regular structured meshes made out of hexaedron elements.
- The procedure for regularising slip near domain boundaries was restricted to and optimised for such structured meshes (Vattré et al., 2014).
- Calculations of the dislocation self-stress field at distances around the boundary of the eigenstrain volume suffered from a sharp discontinuity and therefore could be at the origin of an artificial jump in the velocity of two approaching dislocations (Groh et al., 2004).
- The coupling algorithm between the two codes was general and not optimised for the DCM.

In this work, these limitations are addressed through the development of a new formulation for the DCM and through numerical improvements. This new formulation is presented in §2 and is said to be consistent because it leads to a proper reconstruction of the stress field driving the DD at the continuous limit for the FE problem. Next, numerical optimisations of the DCM procedures are presented in §3 with some recommendations regarding the choice of the spatial integration in the FE simulation part. The paper is closed with elementary tests presented in §4 to show the new possibilities and performances of the DCM. Large-scale computation tests with high dislocation densities and complex geometries with associated performance analyses will be presented in a forthcoming paper. In the following, all DCM tests use the microMegas DD simulation code (Devincre et al., 2011) and the Z-set FE solver (Z-set, 2015).

2. The new DCM formulation

In the DCM, the stress field $\boldsymbol{\sigma}$ driving the movement of the dislocations is a superposition of a stress field $\boldsymbol{\sigma}^{FE}$ computed numerically by the FE code and a local correction stress field $\boldsymbol{\sigma}^{LC}$. The latter is calculated analytically in the vicinity of the dislocation lines in order to reconstruct a pseudo-singular field close to the dislocation lines. The stress $\boldsymbol{\sigma}^{FE}$ transmits the long-range dislocation–dislocation interactions, the body forces and the loads transmitted through the boundary conditions. However it underestimates dislocation interactions at short distance and their interactions with free surfaces and interfaces, and improving this is the main concern of the present work). $\boldsymbol{\sigma}^{FE}$ takes into account the plastic strains $\boldsymbol{\varepsilon}^{p}$ generated by the movement of dislocations through a regularisation of the displacement jump $[[\boldsymbol{u}]]$ across the slip plane. The regularisation procedure, following the eigenstrain theory (Mura, 1991), introduces a homogenisation length h. The maximum element size of the FE mesh is directly related to this length in order to garuantee that sufficient integration points lie inside each eigenstrain volume. The local correction $\boldsymbol{\sigma}^{LC}$ is computed by the DD code, which then handles the movements of the dislocation lines and their topological contact reactions. These basic principles of the DCM are described in full detail in Vattré et al. (2014) and schematically illustrated in Fig. 1.

The calculation of the local correction $\boldsymbol{\sigma}^{LC}$ is a key point of the DCM to reproduce correctly short-distance dislocation–dislocation interactions and contact reactions between dislocation segments. In the previous DCM formulation, $\boldsymbol{\sigma}^{LC}$ is simply the singular stress field $\boldsymbol{\sigma}^{S}$ as is usually used in standard DD simulations, truncated at a distance h from the dislocation line. This simple solution is precise enough to capture, for instance, the zipping/unzipping process of junctions (Vattré et al., 2014). However it turns out that for small values of h (*i.e.*, <50 nm), large numerical errors may appear in the dislocation dynamics when dislocation lines are at distances around h. This is because the superposition of the two contributions generates a stress discontinuity at the contour of the eigenstrain volume, which becomes significant in those cases.

To overcome this important limitation, a revised local correction is presented in §2.1. This revised local correction is said to be *consistent* because at the continuous limit for the FE solution, *i.e.* at the limit when the element size tends to zero, it leads to an exact reconstruction of the mechanical fields for the problem of an infinite domain. The improved calculation of $\boldsymbol{\sigma}^{LC}$ also implies modifications to the regularisation procedure, *i.e.* the way in which the plastic eigenstrain $\boldsymbol{\varepsilon}^{p}$ is distributed to the