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Study of dislocation reactions and rearrangements under different loading conditions

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Abstract

In this dislocation dynamics study of a single crystal under a loading–unloading sequence, the role of dislocation reaction is presented. The formation of prismatic dislocation loops is observed during the loading–unloading sequence, when allowing for cross-slip. The cross-slip probability strongly affects the microstructure rearrangement.

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1. Introduction

The study of the evolution of the dislocation microstructure using dislocation dynamics simulations is a common way to access small scale plasticity. The current method is based on the approach, first presented by Van der Giessen [1], which allows for a mechanically consistent description of the dislocation microstructure evolution in a finite volume. The basics of the three-dimensional implementation including the handling of cross-slip can be found in ref. [2].

The present paper briefly outlines some recent advances concerning the implementation of the method and exemplary studies of junction formation processes (glissile junction and collinear junction), and massive dislocation behaviour under various conditions.

2. Method

The dislocation dynamics method is computational intensive due to the long-range interaction between dislocations. In order to reduce the amount of calculation a hierarchical scheme has been implemented, where a distinction between local and global contribution to the total interaction is introduced. Furthermore, based on local geometrical informations, e.g. the time to encounter another dislocation segment and the change in curvature, a local time step associated to each segment is determined. The smallest of these local time steps is used for the advancement of the total time and dislocation microstructure. In the employed sub-iteration scheme, only the local interaction for the segments in the neighbourhood of the segments exhibiting the smallest local time step were recalculated. After the interaction recalculation the new local time step for these segments is determined and the structure is advanced in time. This sub-iteration scheme is repeated until the dislocation structure has evolved over a maximal given time interval, which depends on the loading conditions and expected dislocation density. The external conditions are then updated. Using this scheme, the formation and evolution of locks, where the strongest geometrical changes occur, do not excessively slow down the overall computation. Considering Al as model material (with a drag coefficient of the order of 10^{-5} Pa s), the critical segments, e.g. those which are either forming junctions or which belong to the neighbourhood of junctions, allow for a maximal time step between

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10^{-12} and 10^{-13} s. A time step of the order of 1–5 $\times$ 10^{-10} s for the recalculation of the global interaction is sufficient for the chosen material parameters. Under these conditions, the ratio between the global and the sub time step is about 1000. Due to the reduced amount of interaction recalculations in the incremental scheme, a speed up of roughly two orders of magnitude is reached. The calculation of the stability of junctions with and without subincremental scheme, as presented in the next section, lead to identical values, within the numerical accuracy determined by the discretisation.

3. Results and discussion

3.1. Lock formation

The control of the formation of locks in the simulation is crucial for a correct modelling of multi-dislocation configurations [3,4]. The implemented model can handle all dislocation reactions, based on perfect non-dissociated dislocations: in fcc the reaction products are the Lomer, Hirth, glissile [5] and collinear junction [4]. Special attention has been given to the handling of the glissile junction, which can bow out in one of the glide planes of the reacting dislocations. The glissile junction is considered to unzip under smaller stresses compared to a sessile lock [5] or to remain short [6], leading often to the conclusion, that it can be neglected in the discrete dislocation dynamics modelling [6,7]. Note that the glissile lock represents a dislocation source, which can relax a different component of the applied stress tensor. Fig. 1 shows five dislocation configurations taken at different times during the formation and the further evolution of a glissile junction, which will lead to the emission of a new dislocation loop.

The crucial part is the efficient calculation of the interactions of segments sharing the end nodes of the junctions using a reasonably fine discretisation. In this model the glissile junction is realized by adding an extra dislocation in the plane of the glissile dislocation. The end points of the glissile junctions are shared by the three participating dislocations.

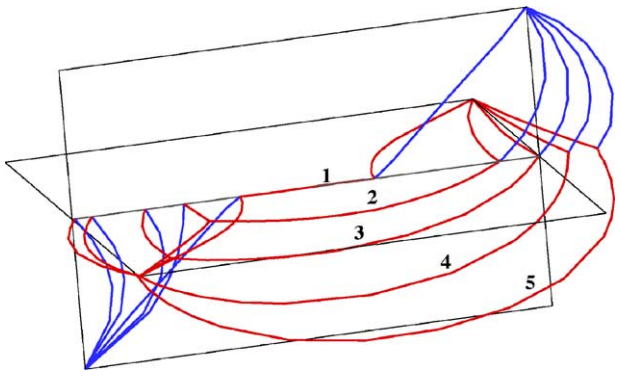

Fig. 1. The formation of a glissile junction close to the starting configuration without applied external load (1) after application of an external stress field (2–5) leading to a Peach–Koehler force on the glissile junction.

3.2. Stability range of the collinear interaction

Fig. 2 shows the stability range of the so-called collinear interaction [4] in absence of an external stress field and with an external stress field. The Peach–Koehler force of the externally applied stress field on both dislocations exceeds the Frank–Read force of the initial segments by 25%. It can be seen that the stability range of the collinear interaction is already considerably reduced due to the external loading.

3.3. Loading–unloading

During the simulation of microstructures evolution the formation of prismatic loops is often observed as a natural consequence of multiple cross-slip and dislocation reaction events. The cross-slip rules and parameters are taken from refs. [8,9]. Fig. 3 shows the final prismatic loops. One of the prismatic loops contains four different sectors, whereas the other contains six different sectors. The two loops are not complementary and cannot annihilate. They will move along the corresponding glide “cylinder”.

The time evolution of dislocation microstructures have been simulated under a loading–unloading sequence. Two

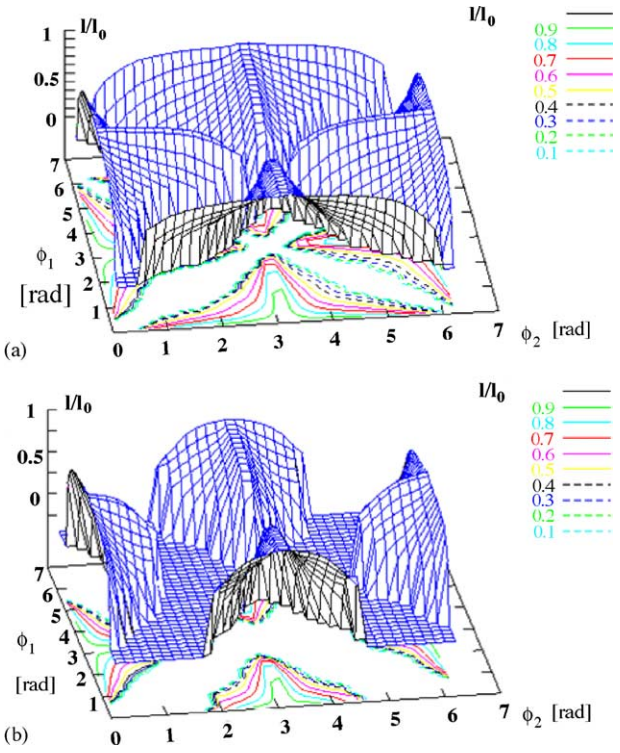

Fig. 2. The stability range for a collinear interaction for two loading conditions. The two dislocations have the same Burgers vector. In the initial position the midpoints of the two dislocations have a distance of two lattice parameters. The angle between the dislocations 1 resp. 2 and the intersection line of the two glide planes of the dislocations is denoted Φ_1 resp. Φ_2. The junction length l is normalised by the initial length of the dislocation l_0 (the distance between the two pinned endpoints): (a) no external stress applied; (b) with external loading ($\tau = 1.25\tau_{FR}$, where τ_{FR} is the critical stress to activate the corresponding Frank–Read sources).