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Improving 3D mechanisms used in mechanism-based discrete dislocation plasticity by considering Periodic Boundary conditions

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ABSTRACT

Dislocations are the primary carriers of crystal plasticity and their collective dynamics define material's response to variety of loading conditions. Several computational approaches were developed on the structure and motion of single dislocations [1]. The method of 2D or 3D Dislocation Dynamics (DD) was designed for collective motion of many dislocations. In a 2D model, dynamics of dislocation lines is reduced to the motion of points confined to the glide planes. This model captures some of the physics of crystal plasticity, however, in reality dislocations behaviour is strongly affected by line tension and dislocation interactions in three dimensions. 3D DD simulations, using large computing resources, have begun reveal more realistic, but still limited because they are very computationally intensive. Published 3D DD studies have been limited to strains of fractions of 2% and relatively low dislocation densities, even for simple problems such as tension of a periodic cell [2]. By considering these limitations for 2D and 3D DD simulations, mechanism-based discrete dislocation plasticity (2.5D DD) has been developed [3]. The dislocations are modeled as line defects in a solid so that the long-range interactions between them are directly accounted for. The short-range interactions are incorporated into the formulation through a set of constitutive rules that allow for approximate representations of key 3D dislocation mechanisms in a 2D framework, for the purpose of computational efficiency. These rules account for junction formation and destruction, dynamic source creation and line tension. The Frank–Read (F-R) source is one of the dislocation glide multiplication sources. When the resolved stress is applied on the glide plane of two-end-fixed dislocation line, the dislocation line bowed out and in semi-circular shape it is in equilibrium. This equilibrated resolved stress is known as critical nucleation stress τ_{nuc}. It can be shown that τ_{nuc} takes the general form $\tau_{nuc}=\beta\mu b/L$, where β depends on poisson's ratio ν, the inner cutoff radius ρ and the line character, μ is the shear modulus, b is the magnitude of burgers' vector and L is the initial dislocation line length [4]. τ_{nuc} is calculated in the infinite domain assumption without any other dislocation remote stress field effects; however, in reality this source is located in the domain with other sources. We propose that coefficient β should be modified by considering other dislocation sources effects. For considering these effects, τ_{nuc} should be determined for an F–R source in periodic

array. For this end a recently developed non-singular continuum elastic theory of dislocations is employed that requires positional continuity only and is capable of describing the forces acting on all points in the discrete network of dislocations [5]. The F–R source in the finite cell with periodic boundary conditions (PBC cell) is simulated. Three aspects of periodic boundary conditions are: (a) line connectivity, (b) initial dislocation arrangements compatible with PBC and (c) treatment of image stresses [6, 7]. For example fig. 1 shows the effect of periodic boundary conditions for Frank-Read source generation in an FCC Material (such as Cu).

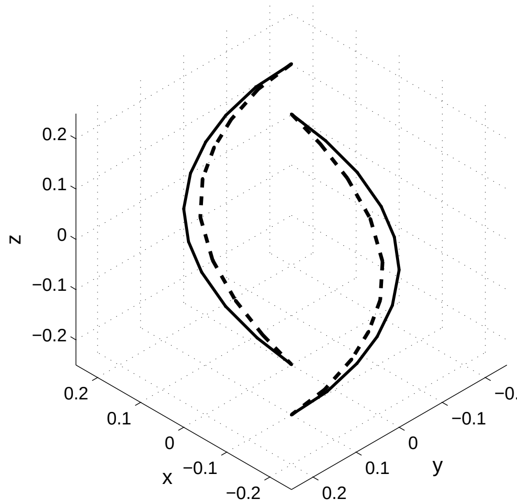

Fig. 1: Frank-Read source in an FCC Material; solid line: the critical shape of F-R source in infinite domain which is produced by τ_{nuc}, dashed line: the shape of F-R source in PBC cell which is produced by the same τ_{nuc}. (Because of second aspect of periodic boundary conditions, two dislocation lines with opposite dislocation senses in different glide planes are simulated.).

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