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Improving 3D mechanisms used in mechanism-based discrete dislocation plasticity by considering periodic boundary conditions

***Siamak Soleymani Shishvan[1], Soheil Mohammadi[2] and Mohammad Rahimian[3]**

[1] Ph.D. Student	[2] Associate Professor	[3] Associate Professor
School of Civil Engineering,	School of Civil Engineering,	School of Civil Engineering,
University of Tehran, Tehran	University of Tehran, Tehran	University of Tehran, Tehran
Iran, P.O. Box 11365-4563	Iran, P.O. Box 11365-4563	Iran, P.O. Box 11365-4563
E-mail: sshishvan@ut.ac.ir	E-mail: smoham@ut.ac.ir	E-mail: rahimian@ut.ac.ir

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ABSTRACT

Dislocations are the primary carriers of crystal plasticity and their collective dynamics define materials response to various loading conditions. Several computational approaches have so far been developed on the structure and motion of single dislocations [1]. The method of 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 their glide planes. Despite capturing some of the physics of crystal plasticity, however, the real dislocation behaviour is strongly affected by the line tension and dislocation interactions in three dimensions. 3D DD simulations, using large computing resources, have begun to reveal more realistic (but still limited) results. 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, the mechanism-based discrete dislocation plasticity (2.5D DD) has been developed [3], where dislocations are modeled as line defects in a solid so that the long-range interactions between them are directly accounted for. For the purpose of computational efficiency, 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. 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 shear stress is applied on the glide plane of a two-end-fixed dislocation line, the dislocation line bows out and rests in equilibrium in a semi-circular shape, with an equilibrated resolved shear stress, known as the critical nucleation stress τ_{nuc}. It can be shown that τ_{nuc} takes the general form of $\tau_{\mathrm{nuc}}=\beta\mu b/L$, where μ is the shear modulus, b is the magnitude of burgers' vector, L is the length of the initial dislocation line and β depends on poisson's ratio v, the inner cutoff radius ρ and the dislocation line type [4]. τ_{nuc} is calculated based on the assumption of an infinite domain without any other dislocations stress field effects. In reality, however, the critical nucleation stress is affected by other F-R sources. It is proposed in this paper

that the coefficient β should be modified by considering other dislocation sources effects. For this end, τ_{nuc} should be determined for an F–R source in a periodic array. A recently developed non-singular continuum elastic theory of dislocations is employed, which only requires positional continuity and is capable of describing the forces acting on all points in a discrete network of dislocations [5]. The F–R source in a finite cell with periodic boundary conditions (PBC cell) is simulated. Three aspects of the periodic boundary conditions are: (a) line connectivity, (b) initial dislocation arrangements compatible with PBC and (c) treatment of image stresses [1, 6]. For example, the effect of periodic boundary conditions for an F-R source generation of an initially edge dislocation in an FCC material (such as Cu) is depicted in Fig. 1. Because of the second aspect of periodic boundary conditions, two initially edge dislocation lines with opposite dislocation senses in different glide planes are simulated. This figure shows that the dislocation movement is confined by assuming periodic boundary conditions in the computational cell. Therefore, the greater resolved shear stress is needed for generating the F-R source. By decreasing the periodicity, the confinement of dislocation movement by PBC is increased. Higher levels of straining, generates denser F-R sources and put them closer to each other. As result, individual analyses of mechanisms are likely to affect the estimation of simulated material plasticity behaviour.

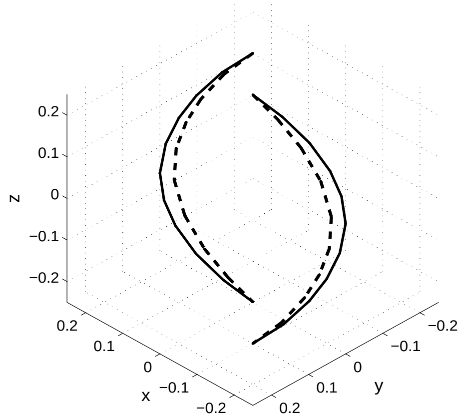

Fig. 1: The Frank-Read source in an FCC material. The solid line represents the critical shape of F-R source in an infinite domain, produced by τ_{nuc}, while the dashed line shows the shape of F-R source in the PBC cell produced by the same τ_{nuc}.

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