8.3 SINGULARITY-FREE DISLOCATION DYNAMICS WITH STRAIN GRADIENT ELASTICITY - G. Po, M. Lazar, D. Seif, N.M. Ghoniem (University of California, Los Angeles)

EXTENDED ABSTRACT *- paper published in JMPS 68 (2014) 161-178.*

The discrete Dislocation Dynamics (DD) method is one of the fundamental tools for the numerical investigation of the mechanical properties of defects in irradiated materials. For example, massive atomistically-informed DD simulations have been performed to study the phenomenon of plastic shear localization and formation of defect-free channels in irradiated materials [1]. Based on the classical theory of elasticity, the method allows to compute the elastic interaction between dislocations and other defects and to predict the evolution of the defect microstructure. However, because the classical theory of elasticity predicts singular elastic fields of dislocations, the DD method suffers both theoretical limitations and practical complications when computations are performed in the proximity of dislocation cores. One way to avoid singularities is to assume that the strain energy density of a certain material depends not only on strains but also on their gradients. This assumption, which models a weak non-locality of the energy density, allows to obtain a physically-based regularization of the singularities in the elastic fields of defects, and in particular of dislocations. In fact, in gradient elasticity, the issue of singularity is removed at the outset and smooth elastic fields of dislocations are available.

In this work [2] we consider theoretical and numerical aspects of the non-singular theory of discrete dislocation loops in gradient elasticity of Helmholtz type, a particular version of Mindlin's gradient elasticity with only one characteristic length scale parameter. Emphasis is focused on the application of the theory to three-dimensional DD simulations. The gradient solution is developed and compared to its singular counterpart in classical elasticity using the unified framework of eigenstrain theory. The fundamental equations of curved dislocation theory are given as non-singular line integrals suitable for numerical implementation using fast one-dimensional quadrature. These include expressions for the interaction energy between two dislocation loops and the line integral form of the generalized solid angle associated with dislocations having a spread core. The single characteristic length scale of Helmholtz elasticity is determined from independent molecular statics (MS) calculations (Fig 1). The gradient solution is implemented numerically within our variational formulation of DD, with several examples illustrating the viability of the non-singular solution. The displacement field around a dislocation loop is shown to be smooth (Fig 2), and the loop self-energy non-divergent, as expected from atomic configurations of crystalline materials. The loop nucleation energy barrier and its dependence on the applied shear stress are computed and shown to be in good agreement with atomistic calculations (Fig 3). DD simulations of Lomer–Cottrell junctions in Al show that the strength of the junction and its configuration are easily obtained, without ad-hoc regularization of the singular fields (Fig 4). Numerical convergence studies related to the implementation of the non-singular theory in DD are presented.

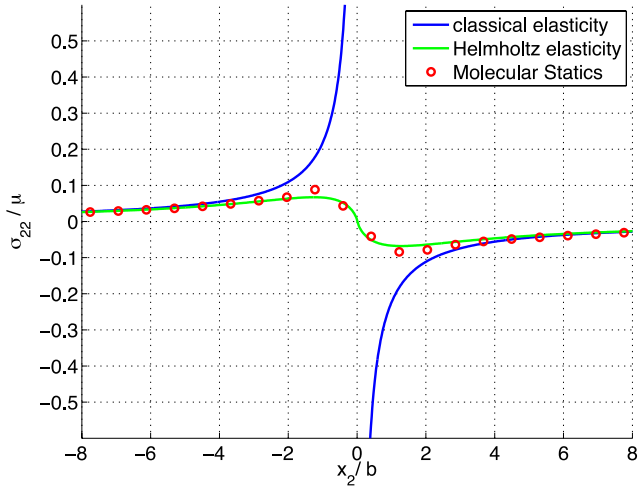

Figure 1. Comparison between virial stress and Cauchy stress (singular and non-singular). The gradient parameter L of the non-singular theory was chosen as a fitting parameter.

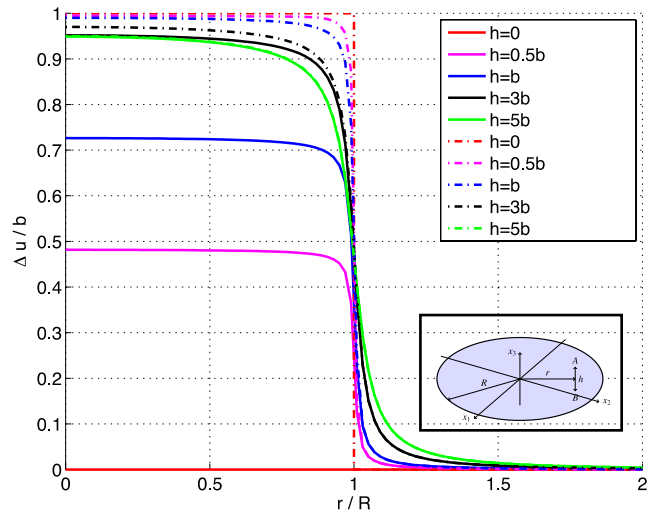

Figure 2. The displacement field of a dislocation loop suffers no jump discontinuity when crossing the loop plane, as a consequence of the regularized solid angle in the non-singular theory.

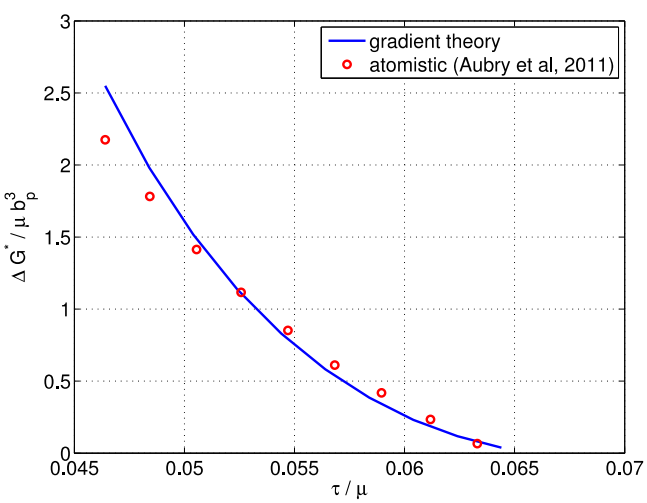

Figure 3. Nucleation enthalpy for a dislocation loop under an applied shear stress τ, according to the non-singular theory. Results compare well with existing atomistic simulations.

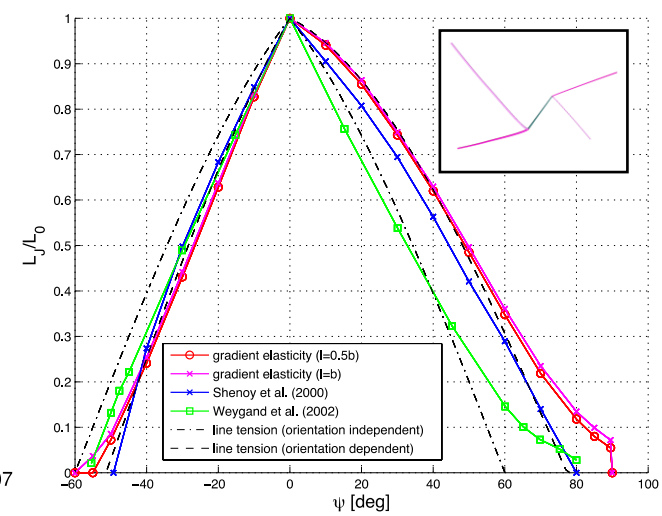

Figure 4. Verification of the strength of a Lomer-Cottrell junction (in insert) in Cu. The choice of the gradient parameter L influences only weak junctions (those with high incident angle ψ).

References

[1] de La Rubia TD, Zbib HM, Khraishi TA, Wirth BD, Victoria M, Caturla MJ. Multiscale modeling of plastic flow localization in irradiated materials. Nature 406 (2000) 871-874.

[2] Po G, Lazar M, Seif D, Ghoniem NM. Singularity-free dislocation dynamics with strain gradient elasticity. JMPS 68 (2014) 161-178.