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The structure and energetics of, and the plasticity caused by, Eshelby dislocations

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ABSTRACT

The structure of coaxial, or Eshelby, dislocations are computed using isotropic elasticity for arrays of up to 500 dislocations. The energies of these arrays are determined in order to predict the lowest energy configuration and multiple meta-stable configurations are often found. The energy from these elasticity predictions shows good agreement with molecular statics simulations of aluminum. From these simulations, the torque-twist curves are predicted and compared with molecular dynamics simulations.

1. Introduction

Eshelby was the first to consider the mechanics of a screw dislocation lying along the axis of a wire (Eshelby, 1953). He postulated that the dislocation was a grown in defect and computed the mechanical properties of the dislocation including the plastic twist caused by the dislocation, now termed the Eshelby twist. Many experiments have confirmed that wires will twist when screw dislocations lie along their axes (Uebach and Bradaczek, 1982; Sears, 1959; Sears et al., 1961), including the recent fabrication of chiral branched nanowires (Bierman et al., 2008; Zhu et al., 2008).

The mechanics associated with these dislocations, which will be called Eshelby dislocations in this article, have been used as deformation mechanisms in several contexts. A single Eshelby dislocation was used by Gao et al. (1999) as the basis for a mechanistic relationship between geometrically necessary dislocation densities and the twist per unit length of wires in torsion. The present author has recently shown (Weinberger and Cai, 2010a,) that, for properly oriented defect free FCC nanowires in torsion, Eshelby dislocations will be the favored mechanism of plastic deformation and will be spatially homogeneous. Finally, Kaluza and Le (2011) have recently developed a solution to the continuum theory for the torsion of a rod with these types of dislocations.

The purpose of this paper is to compute the properties of collections of Eshelby dislocations including their structure, energy, and twist. Eshelby (1953) computed these properties for the case of a single dislocation and Zhu et al. (2008) began the analysis for two dislocations. In this paper, I proceed to look at these properties for 1–25 dislocations as well as 30, 40, 50, 100, 200, and 500. Since Eshelby dislocations provide a plastic twist, it is interesting to see how the energy and twist provided by these dislocations compare against that for grain boundaries.

In addition, since Eshelby dislocations are formed through torsion of properly oriented single crystal wires, I investigate the plasticity of these wires using a hierarchical multiscale modeling approach. I use molecular dynamics (MD) and two dimensional discrete dislocation dynamics models (DD) to compute the torque-twist relationships of wires with these types

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