Journal of the Mechanics and Physics of Solids 83 (2015) 104–128

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

journal homepage: www.elsevier.com/locate/jmps

Displacement fields and self-energies of circular and polygonal dislocation loops in homogeneous and layered anisotropic solids

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ARTICLE INFO

Article history:
Received 24 September 2014
Received in revised form
9 June 2015
Accepted 14 June 2015
Available online 19 June 2015

Keywords:
Dislocation loop
Anisotropic elasticity
Equivalence between dislocation and contact problems

ABSTRACT

There are large classes of materials problems that involve the solutions of stress, displacement, and strain energy of dislocation loops in elastically anisotropic solids, including increasingly detailed investigations of the generation and evolution of irradiation induced defect clusters ranging in sizes from the micro- to meso-scopic length scales. Based on a two-dimensional Fourier transform and Stroh formalism that are ideal for homogeneous and layered anisotropic solids, we have developed robust and computationally efficient methods to calculate the displacement fields for circular and polygonal dislocation loops. Using the homogeneous nature of the Green tensor of order -1, we have shown that the displacement and stress fields of dislocation loops can be obtained by numerical quadrature of a line integral. In addition, it is shown that the sextuple integrals associated with the strain energy of loops can be represented by the product of a pre-factor containing elastic anisotropy effects and a universal term that is singular and equal to that for elastic isotropic case. Furthermore, we have found that the self-energy pre-factor of prismatic loops is identical to the effective modulus of normal contact, and the pre-factor of shear loops differs from the effective indentation modulus in shear by only a few percent. These results provide a convenient method for examining dislocation reaction energetic and efficient procedures for numerical computation of local displacements and stresses of dislocation loops, both of which play integral roles in quantitative defect analyses within combined experimental–theoretical investigations.

1. Introduction

Dislocations are fundamental building blocks in understanding the deformation and failure of crystalline materials by interactions among themselves, with other point defects such as solute atoms and vacancies, and with three-dimensional features such as precipitates, cracks, and internal interfaces (Hirth and Lothe, 1982). With decreasing materials microstructure scales and applications under extreme conditions such as high temperature and irradiation, it is imperative for dislocation mechanics analysis to quantitatively examine anisotropic elastic interactions (Norfleet et al., 2008; Kwon et al.,

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http://dx.doi.org/10.1016/j.jmps.2015.06.008
0022-5096/

2013; Xu et al., 2013) and to address the roles of nanostructure features (Hoagland et al., 2006; Zhang et al., 2012; Feng and Freund, 2010). In many cases, analytical solutions are not available for applications that involve complex geometric features and dislocation evolution, so large scale computational investigations based on discrete dislocation dynamics have been routinely used in recent years (Nicola et al., 2003, 2005; Zhang et al., 2014; Cai et al., 2001; Yin et al., 2012). Undoubtedly these calculations are slow because of the larger number of degrees of freedom and the computationally intensive evaluation of individual dislocation segments. The latter becomes more demanding for anisotropic elasticity analysis since closed-form solutions in real space exist only for the isotropic elastic case. Therefore, significant effort has been devoted to addressing the computational efficiency of dislocation dynamics in three-dimensional anisotropic, heterogeneous solids (Nicola et al., 2003; Yin et al., 2012).

The other challenge in dislocation mechanics in three-dimensional anisotropic, heterogeneous solids is the calculation of displacement fields generated by defect clusters. In current dislocation dynamics simulations, stress fields are used in a linear superposition scheme, so that a boundary value problem without dislocations, but subjected to complex traction boundary conditions, is of the central interest. For stress field calculations, the computational cost can be reduced by taking advantage of the homogeneous nature of the Green tensor in Fourier space, such as the use of the fast multipole method (Yin et al., 2012). Stress calculations require the evaluation of a line integral along dislocation segments, and displacement calculations are challenged by a surface integral over the dislocated area. When dealing with anisotropic elasticity in the absence of a closed-form solution in real space, Fourier transformation is required but it introduces another double integral. Complicating performance of the computations further is the fact that displacement fields are discontinuous (by a Burgers vector jump) over the dislocated surface. This is much harder to deal with than the stress singularity near the dislocation core, for which a cutoff radius can be introduced.

We comment also that two-dimensional defects such as cracks can be modeled based on the dislocation density, where the dislocation density field can be solved by differential–integral equations (Suo, 1990; Bower and Ortiz, 1990). The integrands are essentially the displacement fields generated by unit dislocation segments. These problems suffer the same difficulties as the evaluation of displacement fields in dislocation mechanics, *i.e.*, the cumbersome evaluation of double or quadruple integrals with singular kernels. This method becomes computationally intractable for the study of randomly distributed cracks in three-dimensional solids.

While stress components are of central interest in the above mentioned dislocation dynamics computations as well as for defect interaction phenomena, displacement fields associated with dislocations are required to characterize dislocation distributions. For instance, the displacements introduced by the local rotations and elastic strains associated with dislocation loops can be used to compute diffraction contrast (Bullough et al., 1971; Schäublin and Stadelmann, 1993; Schäublin et al., 2000) for direct imaging of loops by both conventional and high-resolution electron microscopy. Similarly, the displacements form the basis for calculating diffuse x-ray diffraction-scattering cross-sections for dislocation loops. These cross-sections in turn make it possible to use x-ray diffuse scattering measurements to determine the loop size, their vacancy-interstitial type, and also the orientations of dislocation loops in neutron and ion-beam irradiated materials (Larson and Schmatz, 1980; Larson and Young, 1987; Ehrhart and Averback, 1989; Nordlund et al., 2000). Diffuse scattering near Bragg reflections provide a non-destructive tool complementary to transmission electron microscopy (TEM) for studying small dislocation loops that are hard to resolve by direct imaging.

An example in which the determination of the orientations and sizes of small and large dislocation loops is required is in obtaining an experimental confirmation of the recently proposed mechanisms of Xu et al. (2013) for the formation and growth of sessile $<100>$ interstitial loops in irradiated bcc Fe and Fe-based alloys through reactions between glissile $\frac{1}{2}<111>$ interstitial loops. The energy gain associated with such reactions (which interestingly do not obey the Burgers geometric relationship) is not large and the small size of interstitial loops in room temperature irradiated Fe samples hampers ambient temperature TEM studies of the evolution of loop orientations and sizes associated with the proposed mechanism. High-temperature *in situ* electron microscopy investigations of ion-irradiation in Fe have reported large, sessile $<100>$ loops (Yao et al., 2010). However, detailed confirmation of the proposed mechanism of Xu et al. (2013) for the growth of sessile $<100>$ loops by interaction of glissile $\frac{1}{2}<111>$ loops at high temperature is just now in progress (Cui and Robertson). Because of the smaller sizes of the loops at room temperature, x-ray diffuse scattering investigations based on numerically calculated displacement fields for $<100>$ and $\frac{1}{2}<111>$ dislocation loops in Fe can be used in conjunction with TEM for analyzing the dislocation loop orientations and evolution.

Yet another important application of three-dimensional anisotropic elastic analysis of dislocation loops is the dislocation energy (Bower, 2009). For line dislocations, the two-dimensional elastic analysis gives rise to the following self-energy density:

$$W_{edge}^{line}=\frac{Eb_{edge}^2}{8\pi\left(1-\nu^2\right)}\ln\left(\frac{R}{\rho_0}\right),\quad W_{screw}^{line}=\frac{Eb_{screw}^2}{8\pi(1+\nu)}\ln\left(\frac{R}{\rho_0}\right) \tag{1}$$

where E is the Young's modulus, ν is Poisson's ratio, b_{edge} and b_{screw} are Burgers vectors, and ρ_0 and R are core and faraway cutoff radii, respectively. For dislocation loops with radius of a, the self-energies are