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Interfacial elastic fields of a 3D polygonal prismatic dislocation loop in anisotropic bimaterials of spherical shells

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A B S T R A C T

By combining the new superposition principle of linear elasticity used in discrete dislocation plasticity and the recently available solution of the elastic displacement and stress fields due to a polygonal dislocation loop within an anisotropic homogeneous full-space, the anisotropic elastic fields induced by a 3D polygonal prismatic dislocation loop (PPDL) in bimaterials of spherical shells are obtained. The location and orientation of the PPDLs with respect to the fixed reference coordinate system are arbitrary. Factors influencing the interfacial elastic fields, such as the size of the PPDLs, the thickness of the inner-layer and lastly the mismatch of crystallographic orientations of the adjacent layers are investigated in detail. The present model has two distinct features of easy extensibility to planar or nonplanar multilayered polycrystalline models and the ease of numerical implementation for parallel programming.

1. Introduction

Polycrystalline thin films are important structural components in a wide variety of nanofabricated equipment in order to meet the great demand for miniaturization of products [1–2]. These metal films are widely utilized as electrical conductors and resistors, magnetic layers, and structural elements. On account of differential thermal expansion between film and substrate, appreciable stresses may be induced on the interfaces. These stresses will then give rise to inevitable failure of different mechanisms, such as undue elastoplastic deformation, stress voiding, fracture, or interfacial delamination. Thus, considerable effort has been made to theoretically and experimentally predict and investigate the mechanical behaviors of multilayer films and films on substrates [3–12]. Interfacial stresses will be generated owing to several detrimental factors, including the presence of elastic modulus mismatch and crystallographic misorientation across the interface of multilayer materials and grain boundaries in polycrystalline materials, which constitute essential information in fully predicting and understanding the mechanical behaviors and intricate interaction nature between dislocations and interfaces [13–15]. Interface image stress seems to be an influential element preventing dislocation motion from one layer to the abutting layers.

Green's function method has been finding a wide and effective application in obtaining elastic stress and/or displacement fields induced by dislocation loops in homogeneous full-space, half-space, bi- and tri-materials [7,8,16–22]. The elastic stress fields induced by prismatic and glide circular dislocation loops, which are located on a plane parallel to the interface in a bimaterial of two isotropic half-spaces, were calculated by employing Green's function method, respectively, by Salamon and Dundurs [23] and Dundurs and Salamon [24]. Also using Green's function method, Ohr [25,26] calculated the displacement fields of a prismatic dislocation loop in anisotropic cubic crystals, and elastic fields of a shear dislocation loop in an anisotropic hexagonal crystal, respectively. Explicit expressions for the 3D full-space anisotropic Green's functions were obtained by Ting and Lee [27] following the formalism of Stroh [28,29]. Elastic displacement and stress fields due to an arbitrary polygonal 3D dislocation loop in a homogeneous and anisotropically elastic 3D full-space [20], 3D half-space [21] and bimaterials [22] were efficiently calculated by firstly performing analytical integration with respect to the radial variable over the decomposed sub-triangles and then numerically carrying out the integration within the angular interval of $[0, \pi]$ for the circumferential variable. These numerical procedures and results obtained will greatly facilitate the theoretical investigation based on elastic deformation fields due to dislocation loops in anisotropic medium, such as imaging simulation of dislocations in thin films employing theory of dynamics diffraction by TEM [30]. Recently, adopting analytical continuation technique, Gao and Larson [31] developed a novel approach to calculate displacement fields and self-energies of circular and polygonal dislocation loops in homogeneous and layered anisotropic solids.

Discrete dislocation dynamics (DDD) has been attracting the attention of researchers in the community of materials science and now

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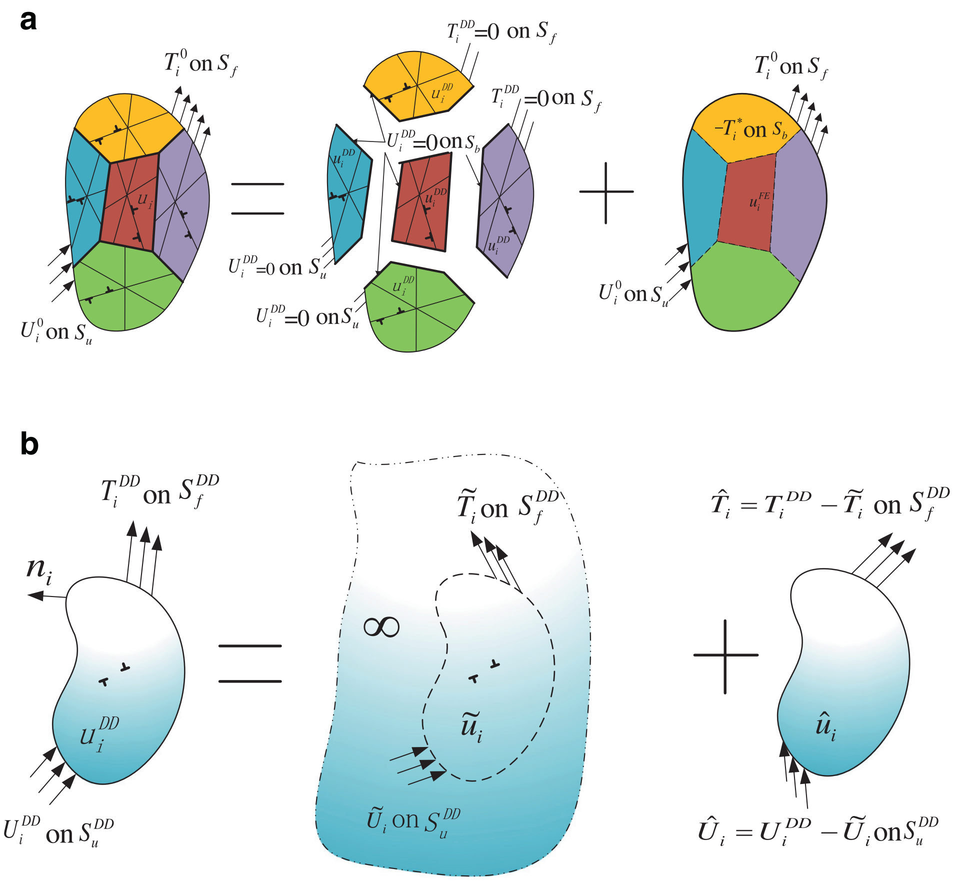

Fig. 1. The setup of polycrystalline model. (a) The entire BVP is made up of two sub-problems: a number of DD sub-problems with general boundary conditions and an FE sub-problem implementing the real boundary conditions and also introducing the interaction between grains (films). (b) Standard superposition framework to solve DD sub-problems by separately dealing with the problem of interacting dislocations in the infinite solid ($(\tilde{\cdot})$ fields) and the complementary problem for the grain without dislocations ($(\hat{\cdot})$ fields). The variables in the figures are described in the following text.

widely used in meso- and nanomechanics [1,32–34]. Jamond et al. [34] propose a new and efficient formulation of the Discrete–Continuous Model (DCM) for the simulation of 3D dislocation dynamics in complex finite or periodic volumes, which is based on a coupling between a Dislocation Dynamics (DD) code and a Finite Element (FE) code through eigenstrain theory. In addition to the above DCM approach, the majority of DDD implementation adopt the principle of superposition due to Giessen and Needleman [32] based on the assumption of linear and isotropic elasticity, de facto standard, to deal with the dislocation problems of finite domains with general boundaries [35,36]. A 3D discrete dislocation dynamics simulation is used to investigate the size-dependent plasticity in polycrystalline, free-standing, thin films [36], in which no crystallographic orientation and anisotropic elastic properties of constituent thin films have been taken into account. To generalize the formalism due to Giessen and Needleman [32] (hereafter called standard principle of superposition) so as to consider and investigate problems of polycrystalline materials containing dislocations and composites with inhomogeneities, O'Day [37] proposed a new principle of superposition, the great advantage of which is its potentiality and capability to investigate the inhomogeneity of materials, such as mismatch of crystallographic orientation and elastic anisotropy of neighboring grains. To the best knowledge of the present authors, there is so far no 3D DDD implementation dealing with finite domain dislocation problems in which to have taken account of the crystallographic orientation and elastic anisotropy of the constituent single crystal grains, i.e., two essential ingredients for describing the mechanical properties of polycrystalline materials. And also there is a scarcity of investigation devoted to the analysis of interfacial elastic fields of multilayered composite shells of anisotropic materials. Gutkin et al. [38] propose a theoretical model to determine the critical conditions for generation of circular prismatic misfit dislocation loops in hollow core–shell nanoparticles, in which however isotropic elasticity is employed. The studies by Shishvan, et al. [39] seem to be the first investigation to have applied the formalism due to O'Day [37] to the analysis of plane-strain discrete dislocation plasticity by incorporating anisotropic elasticity. The purpose of the present study is to calculate the spherical interface elastic fields, including stresses and deformation, of bimaterials crystal layers induced by PPDLs based on the available solution of PPDLs in 3D full-space due to Chu et al. [20,21] and also the new principle of superposition proposed by O'Day [37].

2. Discrete dislocation formulation for polycrystalline materials

Following O'Day [37], the general boundary conditions of the DD sub-problems are specified as $U_i^{DD}=0$ and $T_i^{DD}=0$ on S_u and S_f, respectively, as described in Fig. 1. Additionally, the condition $U_i^{DD}=0$ is enforced on the boundary S_b between the grains or films. Thus, the only necessary information about the full problem that is used in the solution of a DD sub-problem is the geometry of the plastic domain and the specification of whether displacement or traction boundary conditions are imposed on boundaries mutually shared by the DD sub-problems and the full problem. The solution of the DD sub-problem is then obtained by the superposition of solutions for a full-space dislocation problem and for a correcting problem by employing the standard superposition