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Elastic interactions between interface dislocations and internal stresses in finite-thickness nanolayered materials

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ABSTRACT

Anisotropic elasticity theory is used to analyze elastic strain interactions between heterophase interface dislocations and four types of internal stresses in finite-thickness nanolayered face-centered cubic materials. The first interaction is related to the mechanical forces acting on semicoherent interfaces, which arise from heterogeneous elastic fields between the neighboring materials with free surfaces. The second interaction is associated with the Peach-Koehler force exerted on lattice dislocations in free-standing bi- and tri-nanolayers, and is compared to the limiting case of infinite bicrystals. The third case yields to the interaction energy balance and the corresponding equilibrium distance between two Shockley partial dislocations. The fourth and last case is dedicated to the elastic interaction forces between vacancies and interfaces using the force dipole moment approximation.

For such cases, the elastic interaction problems are treated by involving the effects of (i) the dislocation characters, (ii) the anisotropic (versus isotropic) elasticity calculations, and (iii) the additional third coherent MgO layer on bilayered Au/Al systems.

1. Introduction

The mechanical properties of high-performance materials require the development of accurate dislocation-based models for understanding the elastic interactions between semicoherent interfaces and internal stresses in confined volumes, e.g., polycrystalline aggregates, single crystal superalloys, semiconductor thin films, multiphase nanocomposites, etc. In particular, interactions between heterophase semicoherent interfaces with various defects play an important role in strengthening of metallic systems [1], crack initiation in metals [2], as well as irradiation embrittlement [3]. It is also desirable to be able to predict these interactions, which may influence materials design as strategies to create and optimize nanolayered structures with desired density of interfaces.

The purpose of the paper is to analyze four mechanical interactions that may occur in anisotropic bi- and tri-layers between semicoherent interfaces and different types of internal stress fields, namely: – the mechanical force acting on heterophase interfaces due to different strain energy densities between adjoining materials (case I), – the Peach-Koehler force exerted on a single lattice dislocation in anisotropic misfit stress states (case II), – the interaction energy balance between two Shockley partial dislocations (case III), and – the elastic interaction of vacancies with heterophase interfaces (case IV) using linear anisotropic elasticity theory in nanolayered materials with different elastic stiffness constants. Thus, all solutions related to the elastically homogeneous and the isotropic elasticity problems, as well as the limiting case of infinite-thickness bicrystals, consist of particular boundary value problems of the present formalism. Each interactions have been individually studied using different computational and theoretical techniques with different boundary conditions [4–18], since such interactions may significantly depend on interface properties, e.g., the type (misfit interfaces, grain boundaries), internal structures, compositions, the characters of the dislocations, the applied and local stress fields, the constraints imposed by the nature of the surrounding interfaces, etc. In the present work, the stress problems are treated by investigating the effects of (i) the dislocation characters, (ii) the anisotropic (versus isotropic) elasticity calculations, and (iii) the additional third coherent layer on bilayered materials.

1.1. Case I

When two oriented single crystals of dissimilar materials are brought into contact, misfit dislocations are created to

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accommodate differences in lattice parameter at the interface between the adjacent crystals [2]. Such interfaces exhibit non-zero short-range elastic distortion fields generated by the superposition of coherency strains and strain fields of dislocation networks, which arise, for example, in epitaxial layers, precipitation, and both diffusional and diffusionless displacive phase transformations. For infinite bicrystals and free-standing bilayers, the associated Burgers vectors of each individual set of misfit dislocations are defined by requiring the condition of vanishing of far-field strains [19–21] and the global force balance on any internal plane perpendicular to the interfaces [22], respectively. Following Eshelby [23,24], the energy-momentum force, arising as a result of inhomogeneous elastic fields between dissimilar materials, may be associated with the configurational and mechanical component that requires the determination of the change in elastic strain energy of the system of interest as the interface is displaced [25,26]. Without taking into account the chemical forces (e.g., due to compositional differences across the interfaces), such elastic force calculations are computed to describe the stability of semicoherent interfaces with pure Lomer edge and out-of-plane 60° misfit dislocations in crystalline systems.

1.2. Case II

A whole range of interaction forces arise from the interaction between misfit dislocations and other lattice dislocations in crystals due to the elastic interaction of mutual stress fields [27–30]. In general, an interface between two dissimilar layers behave as a complex planar obstacle, which may be very difficult for glissile lattice dislocations to cross because of the strong short-range stress fields generated by the interface dislocations. Moreover, such elastic interaction of dislocations in multilayered structures is significantly affected by the proximity of adjacent phases with different elastic properties and free surfaces. The Peach-Koehler force exerted on a straight lattice dislocation [31] is also used to investigate the interaction force between parallel dislocations with different characters in free-standing materials. Unstable and (meta) stable equilibrium positions, and also the conditions needed to nucleate misfit dislocations, are computed in an anisotropic misfit stress state of interest and compared with the isotropic elasticity solutions.

1.3. Case III

By means of transmission electron microscopy, the dissociation of 60° misfit dislocations have been observed at the interfaces of small-mismatch semiconductor heterostructures [32], e.g., SiGe/Si and InGaAs/GaAs systems. Consequently, dislocation nucleation occurs predominantly at the dissociated interface structure [33], for which the dislocation spacings have been identified as an important role in the emission of partial dislocations from the interface [34]. In accordance with a detailed Burgers vector analysis, such 60° dislocations may also be dissociated into 90° and 30° Shockley partials. The corresponding equilibrium dissociation widths have been predicted using theoretical approaches based on a force balance between two competing terms, i.e., one contribution is related to repulsive elastic interaction force between the leading and trailing dislocations, while the other term arises form the attractive stacking fault energy force between both partials [27,29]. Here, the separation distance of partial dislocations is consistent with the global force balance on any internal plane perpendicular, the constraints on the crystallographic character of semicoherent heterophase interfaces (i.e., misorientation and interface plane orientation), and the traction-free condition on the free surfaces.

1.4. Case IV

The elastic interaction force between vacancies and perfect misfit dislocations is determined using the strain state generated by the dislocation network and force moment approximation to compute the elastic fields induced by a point defect in cubic crystals [35,36]. Such interactions may control the dislocation climbing process and occur as a fundamental mechanism of deformation in diffusion creep [29]. In addition, heterophase interfaces provide a high density of defect trapping sites for vacancies, for which these radiation-induced defects may be rapidly removed in engineering materials [37]. Recent calculations using object kinetic Monte Carlo have shown that the enhancement in sink strength is highly sensitive to the detailed character of interfacial stress fields, such that the coherency stresses in pure misfit interfaces play an important role in predicting the preferential drift of vacancies towards interfaces [38]. The influence of the finite thicknesses on the interaction forces of point defects with interfaces is investigated in bilayers.

Without loss of generality, all cases I, II, III, and, IV, which are displayed in Fig. 1, are illustrated on Au/Al semicoherent heterostructures, widely used in the microelectronics and semiconductor industries [39], with an additional third coherent and ultrathin layer of magnesium oxide in order to describe the trilayered MgO/Au/Al case. Because backscattering spectroscopy studies of compound formation in the Au/Al systems have clarified the role played by the layer thicknesses in influencing the formation of voids, microcracks, and interface decohesions, an investigation of the interaction forces between semicoherent interfaces and free surfaces in elastically stressed bilayers is vital for a better understanding of the mechanical behavior of such thin heterostructures.

2. Problem formulation

Face-centered cubic (fcc) crystals are considered in the cube-cube orientation relationship with $\boldsymbol{x}_1 = [10\bar{1}]$, $\boldsymbol{x}_2 = [010]$, and $\boldsymbol{x}_3 = [101]$. MgO, Au, and Al are three linear anisotropic elastic crystals, where the elastic constants c_{ij} are given in Table 1 from Ref. [29], with the corresponding Zener anisotropy ratios A, and, with finite thicknesses: h_{MgO}, h_{Au}, and, h_{Al}, respectively. Interestingly, Au is strongly anisotropic and MgO gives rise to a hard elastic behavior. The system is constrained against bending and buckling, but is unconstrained against compression for Au and extension for Al, with lattice parameters, $a_{\mathrm{Au}} = 0.4078$ nm and $a_{\mathrm{Al}} = 0.4050$ nm [40]. For all cases I, II, III, and, IV, as schematically illustrated in Fig. 1, the semicoherent and coherent interfaces are coplanar to each other with the common unit vector normal $\boldsymbol{n} \parallel \boldsymbol{x}_2$ and coplanar to two flat free surfaces, located at $x_2 = h_{\mathrm{MgO}} + h_{\mathrm{Au}} > 0$ and $x_2 = -h_{\mathrm{Al}} < 0$, where $h_{\mathrm{MgO}} = 0$ for the bilayered case. An orthogonal network of edge dislocations is needed to accommodate the pure misfit Au/Al interface (with zero misorientation) within which the interaction energy between both sets is zero [20]. Thus, due to the symmetry of the in-plane crystallographic orientationship between Au and Al, the following elasticity calculations are therefore reduced to a single set of infinite, straight, and parallel dislocations along the $\boldsymbol{x}_3$-axis in anisotropic elastic heterostructures. Without loss of generality, the small lattice mismatch between the adjacent crystals, which is frequently met in the heteroepitaxial growth of semiconductors, offers convenient basis for comparison with solutions from classical theory of single dislocations in elastically isotropic materials. Furthermore, both commonly observed dislocation types in such mismatched-lattice structures are also treated, i.e., arrays of pure edge dislocations with individual interface Burgers vectors $\boldsymbol{b}_{\mathrm{e}}^{\mathrm{int}} \parallel \boldsymbol{x}_1$, and mixed 60° dislocations with $\boldsymbol{b}_{60^\circ}^{\mathrm{int}}$, for

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