NANO-SCALE PLANAR FIELD PROJECTION OF ATOMIC DECOHESION

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ABSTRACT An atomistic cohesive zone of a crack tip is characterized by a nano-scale planar field projection of the elastic field of a crack tip, analyzing the near-tip deformation field with a molecular statics simulation of gold. A general form of planar elastic field projection is derived to identify cohesive-zone constitutive relations from the elastic field of a cohesive crack tip sitting on an interface between two anisotropic solids. The cohesive traction, the interface separation and the surface-stress caused by gradual variation of surface formation within the cohesive zone can be obtained by the nano-scale planar field projection.

INTRODUCTION

When atomistic simulations or atomic resolution experiments are carried out to analyze deformation energetics of atomic lattices near a crack tip, the results of the atomic positions and the total energy of the system have not been systematically converted to field quantities such as stresses or tractions near the crack tip. In this paper, we introduce a mathematically consistent way of defining and measuring the cohesive tractions, separations and surface stresses in an atomic decohesion process zone using the atomic displacement data at some distance away from the crack tip. The method is called "nano-scale planar field projection method." This is a generalization of the method developed for isotropic homogeneous solids by Hong and Kim (2003). The formulation introduced here is applicable to interface cracks between anisotropic solids as well as to cracks in homogeneous solids whether they are anisotropic or isotropic. The field projection method is then applied to a crack tip field in gold, simulated atomistically. The atomistic simulation is made with an embedded atom method (EAM) potential for a crystal decohesion along $[\bar{1}\bar{1}2]$ direction in a (111) plane. Then, the details of energy partition in various modes of nano-scale separation processes are analyzed with the field projection method.

PLANAR FIELD PROJECTION METHOD FORMULATION

The field projection method uses interaction J integral (Chen and Shield, 1977) between the atomistic field of interest and a configurational-work-conjugate eigenfunction field of an interface cohesive crack tip. Therefore, a complete set of the eigenfunction fields is constructed with the Stroh formalism (Stroh, 1959) for which the displacement field $\boldsymbol{u}$ of a two dimensional elastic deformation in anisotropic bimaterials is represented in terms of a complex column matrix function $\mathbf{f}(z)$ as $\{\boldsymbol{u}\} = 2\,\mathrm{Re}\left[\mathbf{A}\mathbf{f}(z)\right]$. Here $\mathbf{A}$ is the Stroh eigenvector matrix and z a reduced representation of complex variables $z_j = x_1 + p_j x_2$ with the Stroh eigenvalue p_j for $j = 1,2,3$. Then, the cohesive crack tip field can be expressed in terms of an eigenfunction expansion as

$$\mathbf{f}'_{<\mu>}(z) = \frac{1}{2}\mathbf{B}^{-1}_{<\mu>}\left[\mathbf{I} - (-1)^{\mu} i\boldsymbol{\beta}\right]\left\{\mathbf{Y}\left[(z+c)^{-i\varepsilon}\right]\sqrt{z+c}\,\mathbf{g}(z) - \mathbf{Y}\left[(z-c)^{-i\varepsilon}\right]\sqrt{z-c}\,\mathbf{h}(z)\right\}$$
$$+\frac{i}{2}\mathbf{B}^{-1}_{<\mu>}\left[\mathbf{I} - (-1)^{\mu}\boldsymbol{\alpha}\right]\left[\sqrt{z^2-c^2}\,\mathbf{q}(z) + \mathbf{r}(z)\right],$$

for $\mu = 1$ or 2 referring to the materials 1 or 2 respectively, where $\mathbf{B}$ is another Stroh matrix, and $\mathbf{g}(z)$, $\mathbf{h}(z)$, $\mathbf{q}(z)$ and $\mathbf{r}(z)$ are analytic real matrix functions. The symbols $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ represent the generalized Dundurs-parameter real matrices, ε the bi-material oscillatory index, and $\mathbf{Y}\left[\eta(z)\right]$ for an arbitrary function $\eta(z)$ is the bi-material real function matrix for anisotropic bi-materials (Choi and Kim, 2004). In this expression, terms of $\{\mathbf{g}(z), \mathbf{h}(z)\}$ and $\{\mathbf{q}(z), \mathbf{r}(z)\}$ are interaction J-integral work conjugate pairs respectively, and the power series of the analytic functions can be arranged to construct J-orthogonal sets for the two function pairs. Interaction J integral between an eigenfunction field and the atomistic field of interest provides the magnitude of the conjugate term included in the atomistic field.

Since interaction J integral is path independent, the integral can be carried out at far field, and the magnitudes of the conjugate fields obtained in this way determine the cohesive zone characteristics.

RESULTS ON MOLECULAR STATICS SIMULATION

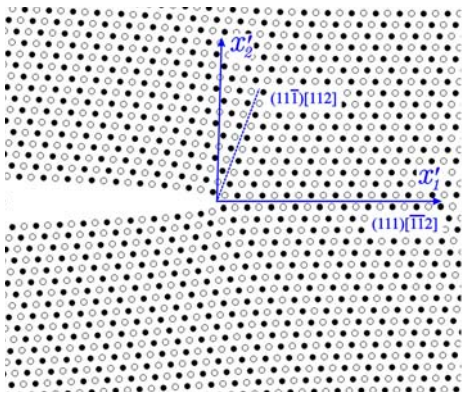

Fig. 1. Atom positions in a crack tip field in gold, simulated with an EAM potential

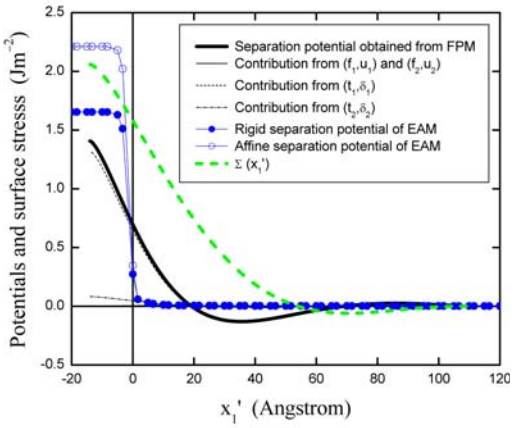

Fig. 2. Cohesive zone potentials measured by the field projection method

Figure 1 shows an equilibrium position of gold atoms relaxed from linear elastic K field positions, holding the linear elastic positions of two atomic layers at the outer boundary with $K_I = 0.38\, MPa\sqrt{m}$ and $K_{II} = -0.10\, MPa\sqrt{m}$. EAM potentials of Foiles et. al. (1986) were employed for this simulation. Then, the atomic positions are used to extract the cohesive zone characteristics applying the field projection method. Figure 2 shows various cohesive zone potentials. The open circle indicates the affine-deformation separation potential of the (111) inter-atomic plane ahead of the crack tip, while the solid dot denotes rigid separation potential. The solid and dashed lines represent the separation potential and the surface stress determined by the field projection method respectively. Here two times of the surface energy, 2γ, of gold (111) is measured $1.41\, J/m^2$ and that of the surface stress $2.06\, J/m^2$.

CONCLUSION

A general formulation of a planar elastic field projection is derived for identifying cohesive zone constitutive relations from the elastic field of a cohesive crack tip sitting on an interface between two anisotropic solids. The formulation is also applicable to the elastic field of a cohesive crack tip in a single isotropic or anisotropic solid. The field projection using the interaction J integrals provides the cohesive traction, the interface separation as well as the surface energy and surface-stress gradients caused by gradual variation of surface formation within the cohesive zone. Therefore, the cohesive traction, the surface-energy and the surface stress could be measured as functions of the interface separation. Molecular statics simulation is performed for crystal decohesion along $[\bar{1}\bar{1}2]$ direction in gold (111) plane with an embedded atom method (EAM) potential, and the field projection method was successfully used to measure the nano-scale cohesive zone characteristics.

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