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Local lattice instability analysis on mode I crack tip in β-SiC: Characteristics in binary covalent crystal

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ABSTRACT

Local lattice instability analysis based on the atomic elastic stiffness (AES), $B_{ij}^{\alpha} = \Delta\sigma_i^{\alpha}/\Delta\varepsilon_j$ ($i,j = 1$—6 in Voigt notation), is applied to mode I crack tip in covalent binary crystal β-SiC of Tersoff interatomic potential. The application limit of the AES is disclosed at the discontinuous local energy surface of disordered broken bonds in the discrete binary system; however, we also captured interesting results with the 1st eigenvalue $\eta^{\alpha(1)}$ of B_{ij}^{α} as follows, (1) the atomic stress of C atoms coincides with the stress singularity in the linear fracture mechanics, when the minimum eigenvalue of C atom shows the first sudden drop or the first instability, (2) but the crack doesn't propagate nor there is no remarkable change in the stress–strain curve, (3) bond breaking and reconstruction occurs in the vicinity of crack tip at the second instability in the eigenvalue, (4) C atoms in the disordered configuration show extraordinary large negative eigenvalue (possibly due to discontinuity of energy surface), while Si atoms show third drop in the eigenvalue just before unstable crack propagation, (5) linear fracture mechanics fails to predict the stress singularity at the crack propagation, (6) the principal axes of the eigenvector of $\eta^{\alpha(1)} < 0$ atoms reveal the deformation mode for local slip and cracking on the multiple (1 1 1) planes in the unstable domain at the forefront of the propagating crack.

1. Introduction

Wang et al. [1,2] proposed the stability criteria (B-criteria) for crystal under finite strain and temperature, based on the elastic stiffness coefficients which relate the stress and strain in the nonlinear elasticity [3]. Ignoring subtle asymmetry in the original form of elastic stiffness coefficients, the 4th order tensor $B_{ijkl} \equiv \Delta\sigma_{ij}/\Delta\varepsilon_{kl}$ ($i \sim l = 1,2,3$ or x,y,z in the Cartesian coordinate) could be rewritten as 6×6 matrix $B_{ij} = \Delta\sigma_i/\Delta\varepsilon_j$ in the Voigt notation [3], $i,j = 1$—6 or xx, yy, zz, yz, zx, xy. Wang discussed the stability limit with the principal minor determinant of the matrix B_{ij} to check the positive definiteness of the stress–strain relation. It is much easier to understand the criteria by using the eigenvalue of the solution of eigenequation, $B_{ij}\Delta\varepsilon_j = \eta\Delta\varepsilon_i$. The negative eigenvalue implies the existence of the unstable deformation path with the straightforward interpretation of $\Delta\sigma_i = B_{ij}\Delta\varepsilon_j = \eta\Delta\varepsilon_i$, and corresponding eigenvector $\{\Delta\varepsilon_i\}$ gives the deformation path in the 6-dimensional strain space.

Although the B-criteria is defined for the whole system or crystal, we have applied this concept to evaluate the local stability by defining atomic elastic stiffness (AES) B_{ij}^{α} at each atom [4–8]. Here, the B_{ij} can be evaluated with the elastic coefficients C_{ij} and stress σ_i at current state $\{\mathbf{x}\}$ such as $B_{11} = C_{11} + \sigma_1, B_{12} = C_{12} - (\sigma_1 + \sigma_2)/2$ and $B_{44} = C_{44} + (\sigma_2 + \sigma_3)/2$. The σ_i and C_{ij} are defined as the first and second order derivatives of the internal energy per unit volume, $E(\mathbf{x})$, against strain [3]. Atomic simulations based on the central force approximation assume the potential function for atom–atom interaction, and the system energy E^{tot} is given by the sum of the each atom contribution, E^{α}. Thus we can easily derive the mathematical form for $\sigma_i^{\alpha} = (\partial E^{\alpha}/\partial\varepsilon_i)/\Omega$ and $C_{ij}^{\alpha} = (\partial^2 E^{\alpha}/\partial\varepsilon_i\partial\varepsilon_j)/\Omega$ (Ω; atomic volume) for potential function adopted, and evaluate the B_{ij}^{α} only with the current configuration as same as force calculation. In the latest report on mode I crack in hcp-Mg [8], we visualized the unstable deformation mode with the principal axis of the strain tensor $[\Delta\varepsilon_{ij}]$ of which components are those of the eigenvector $\{\Delta\varepsilon_i\}$ for the unstable atoms with large negative 1st eigenvalue $\eta^{\alpha(1)}$.

The present study is the first report on the application of our AES analysis to mode I crack in the binary covalent crystal β-SiC. On the cleavage cracking in small β-SiC system, Tang and Yip [9] performed B-criteria analysis on the perfect β-SiC periodic cell with 216 atoms under hydrostatic tension, just after Wang's paper since they are the member of same research group. They demonstrate

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the validity of the *B*-criteria and report the cleavage cracking in the shuffle-set (1 1 1) plane. Then the research group shifted stability analysis from elastic stiffness to dynamical matrix of the lattice dynamics or phonon soft mode analysis and insist on that they captured the initiation of cleavage cracking in the same 216 atoms of SiC by using local participation fraction (LPF) [10]. Furthermore they proposed the following Λ-criteria by considering the displacement of $\mathbf{u}(\mathbf{x}) = \mathbf{w}\exp(i\mathbf{k}\cdot\mathbf{x})$ excited by long elastic wave in homogeneous crystal [11],

$$\Lambda(\mathbf{w},\mathbf{k}) \equiv (C_{ijkl}w_i w_k + \sigma_{jl}|\mathbf{w}|^2)k_j k_l > 0. \tag{1}$$

They also define the $\Lambda_{\min}$ at each atom position as "micro-stiffness" and report they can capture the defect nucleation under indentation at the site where $\Lambda_{\min}$ vanishes [12]. It is of interest they start the discussion from phonon mode analysis for system but the final form quite resembles to our scheme based on the local stress and elastic coefficient. Their discussion for phonon mode analysis still continues for monatomic less-inhomogeneous system [13], however, their formulation is quite complicated even for simple EAM potential and it is unclear the applicability to mixed atom species and crack problem which might have reflection of elastic wave. As another approach to local instability, Kitamura, Umeno and Shimada propose the direct calculation of system Hessian [14–16]; that is, they evaluate near $3N \times 3N$ Hessian matrix for whole system with *N* atoms and find negative eigenvalue and corresponding 3*N*-dimensional eigenvector $\{\Delta x_i^\alpha\}$ as directions of motion of all atoms in the unstable deformation mode. However, the enormous matrix calculation restricts their application to small system of few thousand atoms. Contrary to these strict analysis, our scheme requires the eigenvalue calculation only for 6×6 matrix of all *N* atoms, and the computational cost for B_{ij}^α calculation is almost similar to the force calculation in molecular dynamics (MD) simulation.

Referring to crack simulations of β-SiC, Kikuchi et al. [17] performed MD simulations on the (1 1 0), (1 1 1) and (1 0 0) crack and reported the orientation dependence and discussion with the energy release rate. Yang et al. [18] studied crack propagation behavior at Cu/SiC interface for the strength of the ceramics reinforced metal matrix nanocomposite (MMNC) and discussed with Rice–Thomson model [19]. On the other hand, some DFT calculations report the significant difference between DFT and empirical potentials for the crack tip problem [20,21]. That is, MD simulations based on the interatomic potential function have more or less deviations from real material. However, as insisted on in our previous report [7], our main purpose is *not* to discuss the crack propagation of the real β-SiC but to seek the physical meaning of our AES. Today many researchers can easily use the open MD code such as LAMMPS [22], however, there is no research to spotlight the second order derivatives of the potential function adopted. Even though the adopted empirical potential is not correct as real β-SiC, the obtained results for model material would give new insight that nobody studies.

In the present study, the (0 1 0) and (1 1 1) through cracks are subjected to mode I loading by MD simulation, and the propagation behaviors are discussed with the eigenvalue and eigenvector of B_{ij}^α. Different from our previous studies for monatomic systems, the application limit is also disclosed for C atoms at disordered broken bonds in the dynamic crack propagation.

2. Atomic stress and elastic constants

The interatomic potential adopted is the modified Tersoff potential for Si and C [23]. In the Tersoff potential, the energy contribution of atom α, E^α, and atomic stress σ_{ij}^α and elastic coefficients C_{ijkl}^α are defined as follows;

$$E^\alpha = \frac{1}{2}\sum_{\beta\neq\alpha}[f_R(r^{\alpha\beta}) + b^{\alpha\beta}f_A(r^{\alpha\beta})] \tag{2}$$

$$\sigma_{ij}^\alpha = \frac{1}{\Omega}\frac{\partial E^\alpha}{\partial \varepsilon_{ij}} = \frac{1}{2\Omega}\sum_{\beta\neq\alpha}\left[\{f_R' + b^{\alpha\beta}f_A'\}\frac{r_i^{\alpha\beta}r_j^{\alpha\beta}}{r^{\alpha\beta}} + b_{,ij}^{\alpha\beta}f_A\right] \tag{3}$$

$$\begin{aligned} C_{ijkl}^\alpha &= \frac{1}{\Omega}\frac{\partial^2 E^\alpha}{\partial\varepsilon_{ij}\partial\varepsilon_{kl}} \\ &= \frac{1}{2\Omega}\sum_{\beta\neq\alpha}\left[\{f_R'' + b^{\alpha\beta}f_A''\}\frac{r_i^{\alpha\beta}r_j^{\alpha\beta}}{r^{\alpha\beta}}\frac{r_k^{\alpha\beta}r_l^{\alpha\beta}}{r^{\alpha\beta}} + f_A'\left(b_{,kl}^{\alpha\beta}\frac{r_i^{\alpha\beta}r_j^{\alpha\beta}}{r^{\alpha\beta}} + b_{,ij}^{\alpha\beta}\frac{r_k^{\alpha\beta}r_l^{\alpha\beta}}{r^{\alpha\beta}}\right) + f_A b_{,ij,kl}^{\alpha\beta}\right] \end{aligned} \tag{4}$$

where Ω is atomic volume, Greek superscripts α, β identify atoms while subscript i, j the Cartesian free index x, y and z. The $'$ and $''$ indicates the first and second derivatives of the function f_R and f_A ($r^{\alpha\beta}$ is omitted), $_{,ij}$ and $_{,ij,kl}$ also indicate derivatives by the strain, $\partial/\partial\varepsilon_{ij}$ and $\partial^2/\partial\varepsilon_{ij}\partial\varepsilon_{kl}$. The bond order parameter $b^{\alpha\beta}$ is the power function of other function $\zeta^{\alpha\beta}$ which involves the 3 body effect. The function $\zeta^{\alpha\beta}$ in the original Tersoff [24] has not only internal angle θ between atoms μ-α-β but also exponential term $\exp[\lambda^3(r^{\alpha\beta} - r^{\alpha\mu})^3]$ so that its second order derivative $\zeta_{,ij,kl}^{\alpha\beta}$ results in bothering verbose form [7]. Modified Tersoff omits the exponential term so that the derivatives become rather simple as follows;

$$\zeta_{,ij}^{\alpha\beta} = \sum_{\mu\neq\alpha,\beta}\left[f_c' g(\theta)\frac{r_i^{\alpha\mu}r_j^{\alpha\mu}}{r^{\alpha\mu}} + f_c g'(\theta)\cos\theta_{,ij}\right] \tag{5}$$

$$\begin{aligned} \zeta_{,ij,kl}^{\alpha\beta} = \sum_{\mu\neq\alpha,\beta}\Bigg[&\left(f_c'' - \frac{f_c'}{r^{\alpha\mu}}\right)g(\theta)\frac{r_i^{\alpha\mu}r_j^{\alpha\mu}}{r^{\alpha\mu}}\frac{r_k^{\alpha\mu}r_l^{\alpha\mu}}{r^{\alpha\mu}} \\ &+ f_c' g'(\theta)\left(\cos\theta_{,kl}\frac{r_i^{\alpha\mu}r_j^{\alpha\mu}}{r^{\alpha\mu}} + \cos\theta_{,ij}\frac{r_k^{\alpha\mu}r_l^{\alpha\mu}}{r^{\alpha\mu}}\right) \\ &+ f_c\left(g''(\theta)\cos\theta_{,ij}\cos\theta_{,kl} + g'(\theta)\cos\theta_{,ij,kl}\right)\Bigg] \end{aligned} \tag{6}$$

Table 1
Atomic elastic constants and atomic mean stress at 0 K perfect lattice in 3C-SiC (unit [GPa]).

	Si atom	C atom	Unit cell average
C_{11}^α	311.3	562.1	436.7
C_{12}^α	146.9	89.0	118.0
C_{44}^α	250.5	371.2	310.9
σ_m^α	14.4	−14.4	0.0

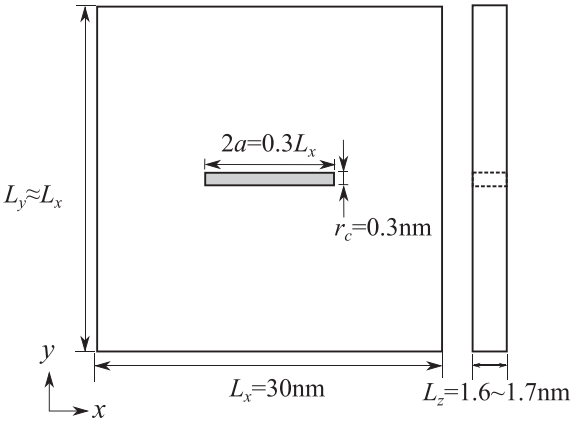

Fig. 1. Dimensions of periodic slab cell with single crack.