Lattice instability at a fast moving crack tip

Y. W. Zhang[a] and T. C. Wang
LNM, Institute of Mechanics, CAS, Beijing 100080, People's Republic of China

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A molecular dynamics method is used to analyze the dynamic propagation of an atomistic crack tip. The simulation shows that the crack propagates at a relatively constant global velocity which is well below the Rayleigh wave velocity. However the local propagation velocity oscillates violently, and it is limited by the longitudinal wave velocity. The crack velocity oscillation is caused by a repeated process of crack tip blunting and sharpening. When the crack tip opening displacement exceeds a certain critical value, a lattice instability takes place and results in dislocation emissions from the crack tip. Based on this concept, a criterion for dislocation emission from a moving crack tip is proposed. The simulation also identifies the emitted dislocation as a source for microcrack nucleation. A simple method is used to examine this nucleation process. © *1996 American Institute of Physics.* [S0021-8979(96)01420-X]

I. INTRODUCTION

In recent years, much experimental, theoretical and numerical investigation has been carried out to study the instability of crack propagation. These researches have gained many insights into the understanding of many baffling problems, such as that (1) the experimentally observed crack velocities are much lower than the Rayleigh wave velocity c_r, (2) the crack velocity oscillates during crack propagation, (3) instability of crack tip occurs, and that (4) a critical condition for crack branching exists during rapid growth. Recent experiments on dynamic fracture by Fineberg *et al.*,[1,2] by Gross *et al.*,[3] and by Sharon *et al.*[4] showed that when the crack velocity exceeded a certain critical value which was far below the theoretical value, a dynamic instability took place, causing oscillation in the crack propagation velocity and the fractured surface morphology. They suggested that the governing mechanism for the crack instability was local crack branchings, which results from the initial defects ahead of the main crack tip.

A wavy-crack model for the lower velocity of crack propagation was proposed by Gao.[5] With this model he could explain why the apparent propagation velocity was much lower than the Rayleigh wave velocity. Washabaugh and Knauss[6] proposed that the fracture propagation was associated with multiple flaws or microcracks preceding the main crack and that these multiple cracks coalesced to form the main crack. They believed that a crack should propagate at a higher velocity, possibly the Rayleigh wave velocity, if micro-cracks were suppressed.

Several analytical models of crack propagation, in which dissipative terms were introduced, were investigated by Langer,[7,8] by Langer and Nakanishi,[9] and by Ching.[10] In their work, they incorporated detailed physical mechanisms into a number of phenomenological parameters, and shed much light on the crack instability. Langer[7] found that the crack-opening displacement underwent underdamped oscillation, and suggested that further study was needed to verify whether the appearance of such oscillations in the steady-state solution involved periodical motion or even irregular motion of the crack tip itself.

Molecular dynamics (MD), which describes atomic lattice characterization and nonlinear effects, has been used to study dynamic fracture. A 2D triangle solid with the Johnson potential was used by Dienes and Paskin[11] and by Sieradzki *et al.*[12] to investigate the energy balance during the crack extension, the dislocation emissions from a moving crack tip and the stress fields near a moving crack tip. Dynamic fracture simulations using large-scale MD with 2D triangle solid were carried out by Holian and Ravelo[13] and by Abraham *et al.*[14] Holian and Ravelo showed that dislocations could be emitted from the crack tip, could climb and become nucleation sites for additional microcracks. Abraham *et al.* showed that the onset of the crack instability resulted in a pronounced zigzag tip motion and dislocations provided the signature for crack oscillation. The origin of erratic velocity oscillation was related to stair-step branching and connecting of failure regions at and preceding the crack tip.

An idealized lattice model has been used by Marder and Liu[15] and by Marder and Gross[16] to study the instability of crack tip. Their results showed that the constant velocity crack solution obtained from continuum elastodynamics did not exist. When the propagation velocity was larger than a certain critical value, the crack became unstable with respect to a nonlinear microcracking.

Hence in dynamic fracture, the appearance of a problem may be greatly different from the local or the microscopic one. Crack velocity oscillation, branching and dislocation emission from crack tips are generally related to local or microscopic phenomena. Therefore quantitative characterization of the crack instability requires the consideration of the characteristic parameters and the mechanisms related to these phenomena.

In the next section we shall use a MD method to analyze dynamic processes at a fast moving crack tip to examine the variation of lattice configuration and lattice instability of the crack tip. In section III we discuss the relations among lattice configuration, lattice instability, velocity oscillation and dislocation emission from the crack tip, then discuss the crack tip opening displacement around a fast moving crack tip

[a]Electronic mail: zhangy@isaac.engin.brown.edu

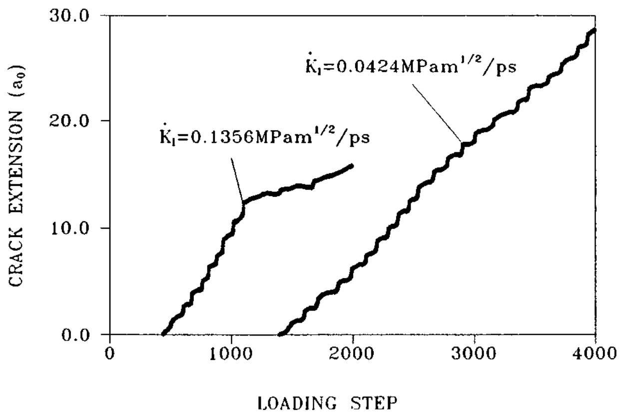

FIG. 1. Crack extension vs loading step.

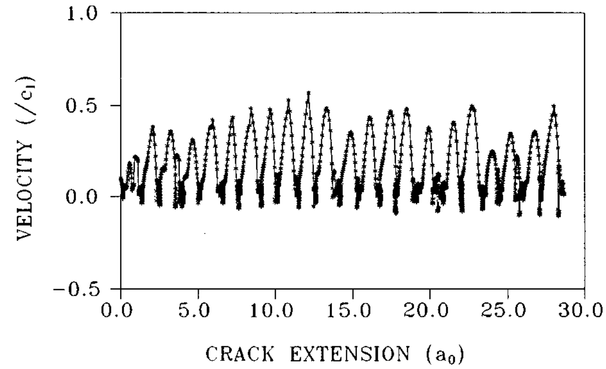

FIG. 2. Crack propagation velocity vs the crack extension for $\dot{K}_I=0.0424$ MPa $\sqrt{\text{m}}$/ps, c_l is the longitudinal wave velocity. When the crack extension reaches approximate $12a_0$, dislocations are emitted from the crack tip.

based on continuum elastodynamics. We then propose a criterion for lattice dislocations emitted from a fast propagating crack tip based on the crack-tip-opening-displacement (CTOD), and then analyze the microcrack nucleation processes from an emitted dislocation. Finally we present the summary.

II. ATOMISTIC SIMULATION

Details of the MD formulation can be found in Ref. 17, 18. Here we only describe it briefly. The ''N-body'' potential proposed by Finnis and Sinclair[19] is used to simulate the dynamic fracture processes. This has the form

$$E_{\text{tot}}=-\sum_i \rho_i^{1/2}+\frac{1}{2}\sum_i \sum_{j(i\neq j)} V_{ij}\,. \tag{1}$$

The inner atoms follow Newton's law and boundary atoms are placed at the fixed locations given by the mode I anisotropic elastic K displacement field.[20] Incremental loading is used with variation of loading rates. The leapfrog algorithm is used in the calculations. The time step is taken to be 1.18×10^{-14} s. In all simulations, the initial ground state of a copper crystal is assumed. A parallelepiped with a slit is used as the simulation cell. The crack growth direction along $\langle 110\rangle$, the crack plane normal along $\langle 111\rangle$ and the crack front along $\langle 112\rangle$ are assumed to be the x, y and z axes, respectively. Since the simulation temperature is near 0K and the Schmid factors in all slip systems are low, the crack in the copper crystal may propagate in a brittle way under mode I loading and higher loading rate. The length and width of the cell are $180\sqrt{2}a_0/4$ and $101\sqrt{3}a_0/3$, respectively (a_0 is the lattice constant). The separation between the crack tip and the left boundary is $60\sqrt{2}a_0/4$. The separation of the upper and lower crack planes is taken to be $\sqrt{3}a_0$ which is larger than $1.22a_0$, the cutoff distance of the potential. The number of atoms used in the present simulations for each case is 18342. Since periodic conditions are used along the $\langle 112\rangle$ direction, the atomic movement is three dimensional. The treatments of boundary conditions are important to the accuracy of the final results.[21] Fixed boundaries suffer serious deficiencies when the waves emitted from crack tip are reflected by the boundaries. Our calculations show that when the moving crack tip is far from the boundaries, such influences are relatively small and do not modify the qualitative results of the present article. The location for an atomistic crack tip is taken to be the position where the separation of the upper and lower atomic planes of the crack is equal to the cutoff distance of the potential.

For a loading rate of $\dot{K}_I=0.0424$ MPa$\sqrt{\text{m}}$/ps, the crack extension versus the loading steps is given in Fig. 1 and the crack propagation velocity versus the crack extension is given in Fig. 2. From Figs. 1 and 2, it can be seen that the crack velocity oscillates violently. Such a velocity oscillation is caused by a repeated process of opening and closing at the fast moving crack tip. This opening-closing process can clearly be seen from atomic configuration figures shown in Figs. 3(a) and 3(b). Although the average velocity during crack growth is only about $c_r/6$ (c_r is the Rayleigh wave velocity), the maximum velocity of crack growth on a microscopic scale is not limited by this theoretically predicted velocity based on the continuum elasticity. The negative propagation velocities in Fig. 2 result from the crack tip configurations changing from blunt to sharp. For this loading case, no dislocation emission and crack branching take place.

For $\dot{K}_I=0.1356$ MPa$\sqrt{\text{m}}$/ps, the crack extension versus the loading steps is also shown in Fig. 1 and the crack propagation velocity versus the crack extension is shown in Fig. 4. Figures 1 and 4 demonstrate a violent oscillation in the crack velocity. The apparent crack velocity is about $c_r/4$, while the maximum crack velocity on a microscopic level exceeds the Rayleigh wave velocity but is less than the longitudinal

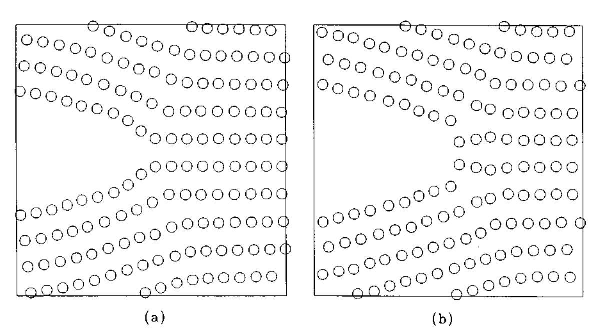

FIG. 3. The simulated opening-closing lattice configuration at a fast moving crack tip, from an atomistically sharp crack tip (a) to a blunted one (b).

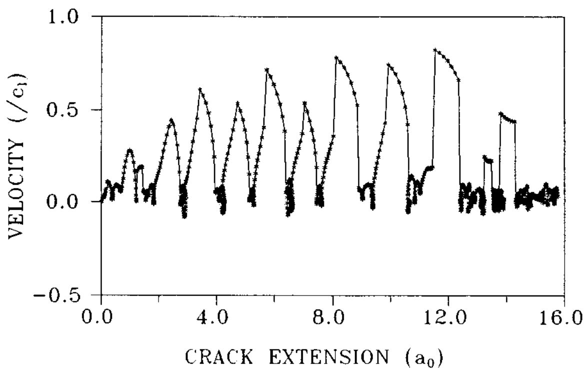

FIG. 4. Crack propagating velocity against the crack extension under $\dot{K}_I = 0.1356$ MPa $\sqrt{m}$/ps.

wave velocity c_l (The longitudinal wave velocity c_l used here is 5480 m/s, which is calculated by the present MD method). The oscillation for this case diverges gradually. The large bluntness of the crack tip at high velocities results in a lattice instability, in which two dislocations are emitted symmetrically from the crack tip (Fig. 5). These dislocations are the Frank partial dislocation with the Burgers vector $b=\sqrt{3}a_0/3$. Before the emitted dislocations move away from the tip, two microcracks are nucleated at the cores of the dislocations as shown in Fig. 6. The emission angle is about 70° inclined from the crack plane and the nucleation site is at about $2a_0$ from the crack tip. Hence for the fast propagating crack, dislocations may be emitted from crack tip by the lattice instability and may be taken as the nucleation sites for microcracks. During the processes of dislocation emission and microcrack nucleation, the main crack propagating velocity decreases drastically (Fig. 1).

III. ANALYSIS AND DISCUSSION

One of the main simulation results is that although the crack propagates along a straight line even without dislocation emission, its propagation velocity oscillates violently.

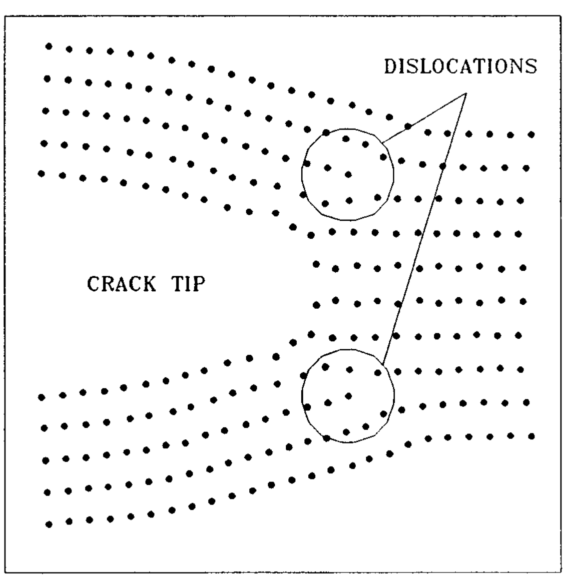

FIG. 5. A pair of dislocations are emitted symmetrically from the crack tip.

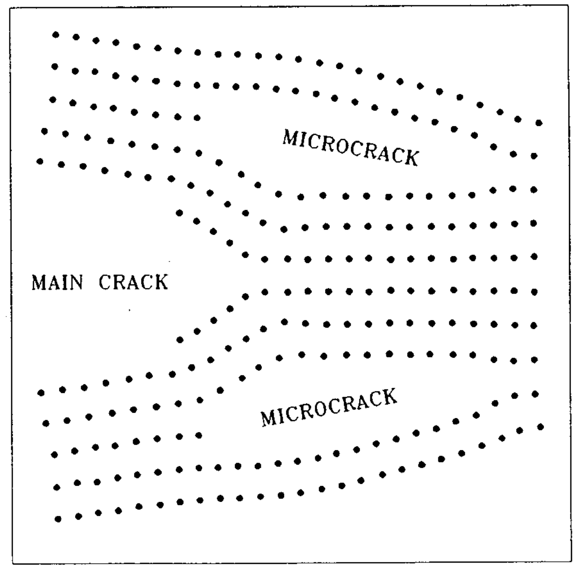

FIG. 6. Microcracks are nucleated at the cores of the emitted dislocations.

This velocity oscillation results from the CTOD oscillation. This means that the steady-state solution obtained by the continuum elastodynamics does not exist. Whether the CTOD oscillation maintains a periodic or a divergent variation depends on the loading conditions. The crack tip might involve a periodic motion without the dissipation by plasticity or a divergent motion with dislocation emissions. A one-dimensional model with viscous dissipation has been used to analyze a steady-state motion by Langer.[7] He found that the crack-opening displacement underwent underdamped oscillations. This is consistent with the present simulation result. The present simulation also shows that even for a propagation crack in a perfect crystal, its moving velocity is much lower than the Rayleigh wave velocity. This is because, at a higher velocity, the crack tip cannot maintain its stability and the lattice at its tip becomes unstable. Accompanying the crack instability, dislocations are emitted from the tip. Dislocation emission from a fast moving crack tip has also been observed by Dienes *et al.*,[11] by Holian *et al.*,[13] and by Abraham *et al.*[14] Hence the instability of a fast moving crack tip is closely related to dislocation emission from its tip. Consider a crack propagating along a straight mode I fracture path with velocity v in a linear elastic isotropic crystal. The near tip singular stress and displacement distributions[22] can be written as

$$\sigma_{ij}=\frac{K_I}{\sqrt{2\pi r}}\Sigma_{ij}^I(\theta,v), \tag{2}$$

$$u_i=\frac{K_I\sqrt{r}}{2E\sqrt{2\pi}}\Omega_i^I(\theta,v), \tag{3}$$

where K_I is the dynamic stress intensity factor, r and θ are polar coordinates centered at the crack tip, E is the elastic modulus, and $\Sigma_{ij}^I(\theta,v)$ and $\Omega_i^I(\theta,v)$ are angular distribution functions which can be found in Refs. 22 and 23. With these equations, the crack tip opening profiles, normal stress σ_{yy} (y along the crack plane normal) are plotted in Figs. 7(a) and 7(b). From Fig. 7(a), it can be seen that with an increase in

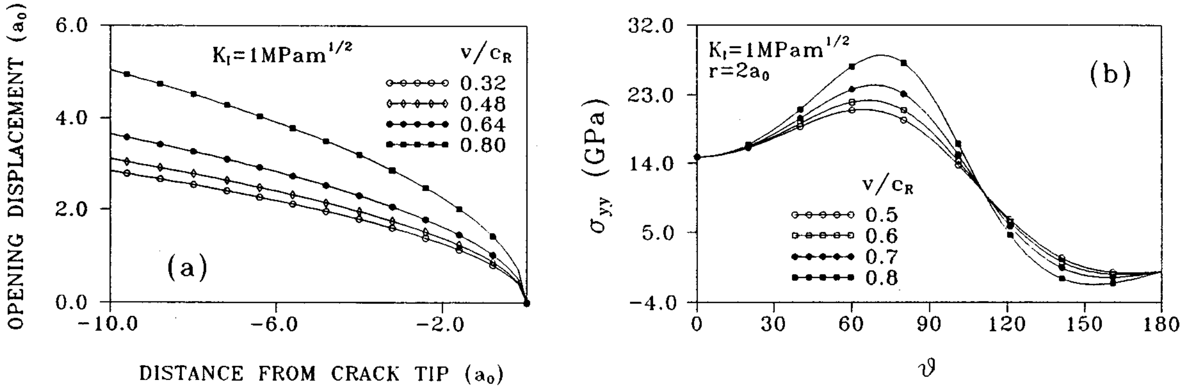

FIG. 7. Elastodynamics results with variation of crack velocity under mode I loading in copper crystal, (a) profiles of crack tip, (b) σ_{yy} distributions.

the crack velocity, the opening of the crack tip increases. Since these analytical results are based on elastodynamics and a small strain formulation, such an opening process is purely elastic and does not involve any dislocation activity. However, when a crack propagates at higher velocity, the crack tip opens wider. If the CTOD exceeds a critical value δ_{us}, the atomic stacking lattice becomes unstable and dislocation emission from the fast moving crack tip takes place. Based on this concept, a criterion based on the CTOD for a fast moving crack tip is proposed, i.e.,

$$\delta(\sigma,a,v)=\delta_{us}, \tag{4}$$

where the $\delta(\sigma,a,v)$ is the CTOD, which is related to the loading stress, the crack length and the crack velocity, and δ_{us} is the critical CTOD value for lattice instability or dislocation emission from a fast moving crack tip, which should be a material parameter.

A parameter called the unstable stacking-fault energy was recently proposed by Rice[24] and modified by Zhang *et al.*[25] to characterize the resistance to dislocation nucleation from the crack tip. The present criterion is identical to the one proposed by Rice when the slip plane is along an inclined plane with the prolongation of the crack plane. For example, for the case that the slip plane is coincident with the crack plane and the slip direction along the crack propagation direction, if the energy release rate is equal to the unstable stacking-fault energy, or equivalently if the CTOD is equal to $b/2$ (where b is the Burgers vector), the dislocation emission will take place. However, for the case that the dislocation is the Frank partial dislocation and its movement involves climbing, its nucleation and emission cannot be characterized by the unstable stacking-fault energy, but still can be described by the CTOD criterion.

With the increase of crack velocity, the σ_{yy} also increases. After dislocation emission, microcracks can be nucleated at the cores of the emitted dislocations. This is due to the strong stress level contributed by near tip stress field [Fig. 7(b)] and the emitted dislocation stress field.[26]

Considering a microcrack produced by an edge dislocation emitted from the crack tip along an inclined plane near a moving crack tip, one can write the total variation of energy for a microcrack of size l under stress, according to Friedel,[27] approximately as

$$\frac{1}{8}\pi(1-\nu)\frac{(\sigma_{yyc}+\sigma_{yye})^2 l^2}{\mu}+2\gamma l, \tag{5}$$

where, ν and μ are the Poison's coefficient and shear modulus, respectively, γ is the surface energy, and σ_{yyc} and σ_{yye} are the stresses of the moving crack and the emitted dislocation, respectively. By using $\sigma_{yye}=Ab/l$, $(A=\mu/2\pi(1-\nu))$ and the conditions that the energy variation (5) is zero and $l\geqslant l_c=\sqrt{2}a_0/4$, ($l_c$ is the separation between the adjacent atomic planes along $\langle 112\rangle$), the critical condition for forming a microcrack from an emitted dislocation can be written as

$$l=(16\gamma-b\sigma_{yyc}+\sqrt{256\gamma^2-32b\gamma\sigma_{yyc}})\frac{A}{\sigma_{yyc}^2}\geqslant l_c. \tag{6}$$

If one takes $\gamma\approx 0.1\ \mu a_0$, μ=40.8 GPa, ν=0.3, σ_{yyc} can be obtained by using Eq. (2) with θ=70°, K_I=1.5 MPa $\sqrt{\mathrm{m}}$ and $r=2a_0$. The result suggests that $l=1.5l_c$, and Eq. (6) is satisfied. Hence, the emitted dislocations may be the sites for nucleating microcracks at a fast moving crack tip.

The experimental results of Fineberg *et al.*,[1,2] Gross *et al.*[3] and Washabaugh *et al.*[6] showed that the fracture propagation resulted from the initial defects ahead of the main crack tip coalescing with the main crack. Our present results, however, suggest that even without initial defects, the main crack can also propagate via the defects emitted from the main crack itself. Hence the crack instability is not necessarily related to the initial flaws. Because the lattice instability taking place at the crack tip results in the dislocation emissions, the crack cannot propagate at a higher velocity even if the zone ahead of the crack tip is initially defect free.

IV. SUMMARY

In this article, a molecular dynamics method is used to analyze the dynamic propagation of an atomistic crack tip. The simulation shows that the apparent velocity of crack tip is relatively uniform and well below the Rayleigh wave velocity, while the local propagation velocity oscillates violently, with its maximum value limited by the longitudinal wave velocity. Hence local crack propagation processes are significantly different from macroscopic ones. It is found that such a velocity oscillation results from a repeated process of crack tip blunting and sharpening. Such an oscillation phenomenon cannot be fully analyzed by the continuum elastodynamics theory. The faster the crack moves, the more violently the CTOD and crack velocity oscillate. When the CTOD exceeds a certain critical value, the lattice instability takes place which results in dislocation emissions from the crack tip. Based on this concept, a criterion for dislocation emission from a moving crack tip is proposed. The simulation indicates that the emitted dislocations may be taken as sources for microcrack nucleation. This suggests that at a higher propagation velocity, the instability of a crack tip is inherent and not necessarily linked to the initial defects. A simple energy method is used to examine this nucleation process. It should be noted that the lattice instability at a fast moving crack tip may be closely related to fracture surface morphology, crack bifurcation and velocity oscillations.

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[1] J. Fineberg, S. P. Gross, M. Marder, and H. L. Swinney, Phys. Rev. Lett. **47**, 457 (1991).
[2] J. Fineberg, S. P. Gross, M. Marder, and H. L. Swinney, Phys. Rev. B **45**, 5146 (1992).
[3] S. P. Gross, J. Fineberg, M. Marder, W. D. McCormick, and H. L. Swinney, Phys. Rev. Lett. **71**, 3162 (1993).
[4] E. Sharon, S. P. Gross, and J. Fineberg, Phys. Rev. Lett. **74**, 5096 (1995).
[5] H. Gao, J. Mech. Phys. Solids **41**, 457 (1993).
[6] P. D. Washabaugh and W. G. Knauss, Int. J. Fract. **65**, 97 (1994).
[7] J. S. Langer, Phys. Rev. A **46**, 3123 (1992).
[8] J. S. Langer, Phys. Rev. Lett. **70**, 3592 (1993).
[9] J. S. Langer and H. Nakanishi, Phys. Rev. E **48**, 439 (1993).
[10] E. S. C. Ching, Phys. Rev. E **49**, 3382 (1994).
[11] G. J. Dienes and A. Paskin, J. Phys. Chem. Solids **48**, 1015 (1987).
[12] K. Sieradzki, G. J. Dienes, A. Paskin, and B. Massoumzadeh, Acta Metall. **36**, 651 (1988).
[13] B. L. Holian and R. Ravelo, Phys. Rev. B **51**, 11275 (1995).
[14] F. F. Abraham, D. Brodbeck, R. A. Rafey, and W. E. Rudge, Phys. Rev. Lett. **73**, 272 (1994).
[15] M. Marder and X. Liu, Phys. Rev. Lett. **71**, 2417 (1993).
[16] M. Marder and S. Gross, J. Mech. Phys. Solids **43**, 1 (1995).
[17] Y. W. Zhang, T. C. Wang, and Q. H. Tang, J. Appl. Phys. **77**, 2393 (1995).
[18] Y. W. Zhang, T. C. Wang, and Q. H. Tang, J. Phys. D **28**, 748 (1995).
[19] M. W. Finnis and J. E. Sinclair, Philos. Mag. A **50**, 45 (1984).
[20] G. C. Sih, P. C. Paris, and G. R. Irwin, Int. J. Fract. Mech. **1**, 189 (1965).
[21] B. deCelis, A. S. Argon, and S. Yip, J. Appl. Phys. **54**, 4864 (1983).
[22] L. B. Freund, *Dynamic Fracture Mechanics* (Cambridge University Press, New York, 1990).
[23] M. H. Aliabadi, C. A. Brebbia, and V. Z. Parton, *Static and Dynamic Fracture Mechanics* (Computational Mechanics, Southampton, 1995).
[24] J. R. Rice, J. Mech. Phys. Solids **40**, 239 (1992).
[25] Y. W. Zhang, T. C. Wang, and Q. H. Tang, Philos. Mag. A **72**, 881 (1995).
[26] J. R. Rice and R. Thomson, Philos. Mag. **29**, 73 (1974).
[27] J. Friedel, *Dislocations* (Pergamon, Oxford, 1964).