Atomic Scale Origin of Crack Resistance in Brittle Fracture

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We investigate the physical meaning of the intrinsic crack resistance in the Griffith theory of brittle fracture by means of atomic-scale simulations. By taking cubic SiC as a typical brittle material, we show that the widely accepted identification of intrinsic crack resistance with the free surface energy underestimates the energy-release rate. The strain dependence of the Young modulus and surface energy, as well as allowance for lattice trapping, improve the estimate of the crack resistance. In the smallest scale limit, crack resistance can be fitted by an empirical elastoplastic model.

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A basic result of fracture mechanics for brittle materials is represented by the Griffith theory for crack stability [1], which describes a planar crack in a homogeneous medium as a reversible thermodynamic system. The total energy of the system is written as the sum of a mechanical contribution due to the strain energy absorbed from the external work, and a crack resistance term, originating from the material resistance to create new free surface by breaking bonds. A crack of given length is stable at the critical value of load for which the total energy of the system is stationary. Once the load exceeds such a critical value, the energy-release rate for unit area of crack advance G becomes larger than the intrinsic crack resistance and therefore the crack propagates. In a perfect homogeneous solid in vacuum the crack resistance energy per unit surface is, in fact, identified with the (unrelaxed) free surface energy γ [2,3]. The Griffith criterion was extensively verified in glass specimens containing cracks of controlled length and it is still adopted to estimate the surface energy of a brittle material [2,4].

At a more fundamental level it is known that, even for a perfectly brittle material, some modification of the Griffith theory has to be taken into account in order to describe the atomistic nature of the interactions [3]. As already indicated by Griffith in his original study, this turns out to be particularly relevant for microcracks of very short length. First of all, it was shown by means of a simple lattice model of brittle crack propagation in a two-dimensional crystal [5] that the discreteness of the lattice may increase the effective crack-tip force necessary to break a bond across the surface, therefore causing crack arrest for some range of loads above the theoretical Griffith value. Such a phenomenon was termed *lattice trapping* and was subsequently studied in a number of atomic-scale simulations [6–9]. However, the results are sometimes difficult to generalize. Second, the effective crack resistance could include terms beyond the mere energy of the unrelaxed cleavage surface. Formally, G is defined [10] as $G = 2\gamma_s$ where the material parameter γ_s is the integral of the stress versus separation curve for the atomic planes undergoing separation during the fracture process. While γ_s may ideally coincide with the energy γ of the cleavage surface, it could include also other atomic-level details. Moreover, the maximum σ_f of such a curve defines the critical fracture stress, i.e., the value at which a brittle crack starts propagating. However, the actual maximum stress at the crack tip could overcome σ_f before propagation because of various features, including lattice trapping, nonideal sharpness of the (finite-size) crack-tip, anharmonic, and many-body effects in the atomic-level forces. While the Griffith theory does not depend on σ_f but only on the integral γ_s, other theories tried to also include the role of the maximum stress at the crack tip [8,11,12].

Atomistic simulations offer the opportunity to study the fundamental issues underlying the Griffith theory in ideally pure, perfect single-crystal materials. In this Letter we present an atomic-scale investigation of brittle fracture addressing the relationship among the critical load to fracture, intrinsic crack resistance, and surface energy, in the framework of the Griffith theory. We find that the identification of crack resistance with the surface energy provides only a lower limit to the energy-release rate. By including the strain dependence of the Young modulus and surface energy, a large part of the discrepancy between the atomistic results and Griffith theory may be recovered. Moreover, we set an upper bound for the role of lattice trapping in increasing the effective crack resistance. Finally, for the shortest microcracks of length of a few lattice spacings, we give an empirical fit to an elastoplastic model, asymptotically merging into the Griffith theory at longer crack length. We focus our work on cubic silicon carbide (β-SiC) since it is the prototype of an ideally brittle material up to extreme values of strain, strain rate, and temperature, and because of its technological relevance as a structural and nuclear material. The available data [2] for β-SiC are accurate enough (despite the microstructural heterogeneities of experimental samples) to suggest that its intrinsic crack resistance in vacuum is, indeed, higher than the theoretical, ideal-crystal surface energy.

We carried out damped-dynamics atomistic simulations with the aim of reproducing the macroscopic conditions of a quasistatic (or adiabatic) crack loading process at $T = 0$ K. External loading was represented in terms of surface forces, or *tractions* [13], applied at the nonperiodic borders of the simulation cell (see below). Atomic positions were relaxed according to the local values of the forces and by constantly damping velocities to zero, until the maximum force was less than 0.0001 eV/Å.

Atomic forces were calculated according to the Tersoff model [14]. Such an empirical interatomic potential has already been applied [15] to the study of mechanical properties in β-SiC and it is able to describe the experimentally observed brittle behavior [16] of cubic β-SiC. Furthermore, the same force model has been applied to investigate the static mechanical response of nanostructured β-SiC to uniaxial tensile loading [17].

The simulation cell is represented schematically in Fig. 1. The lowest unrelaxed surface energy of β-SiC is that of the (111) shuffle plane [16], having the lowest density of dangling bonds. As a consequence, (111)-plane cracks are the most likely to form in experimental conditions, and we therefore focused our theoretical analysis on such a crack arrangement. The simulation cell has the x, y, and z Cartesian axes parallel to the $[11\bar{2}]$, $[\bar{1}10]$, and $[111]$ crystallographic directions, respectively. Therefore, the crack front lies parallel to the $[11\bar{2}]$ direction; i.e., the crack arrangement is $(111)[11\bar{2}]$.

We took special care in order to avoid finite-size effects. The size of the simulation cell was chosen so as to get in any case a ratio of $L/c > 10$ (see Fig. 1) as indicated by previous molecular dynamics studies [7]. The resulting number of atoms ranged from 30 000 up to ~250 000.

The external load was applied according to the constant traction method [13]. To this end, the three-dimensional periodic simulation box is initially deformed along the z direction according to a given strain value $\epsilon = \epsilon_{[111]}\delta_{zz}$, while keeping $\epsilon_{xx} = 0$ and $\epsilon_{yy} = 0$ (plane-strain condition). Periodicity is then removed along z and surface tractions are calculated, in order to preserve the state of deformation. At this stage a microcrack of given length is introduced by mathematically cutting the interatomic bonds across a segment of a central (111) plane. The interbond distance along $[11\bar{2}]$ is $c_0 = 2.644$ Å. The actual minimum-energy atomistic configuration is eventually obtained by the above specified damped-dynamics procedure. After crack opening, interatomic forces are fully restored and the microcrack reaches its equilibrium shape following stress relaxation.

When applying tensile loads, one can reach a strain state such that the Si-C bond length at the crack tip lies in the range of values for which the cutoff function of the Tersoff potential operates. Notably, the Tersoff potential was not originally intended for being used under such extreme deformations. To overcome artifacts due to the cutoff, Tang *et al.* [15] shifted the cutoff distance to larger values as a function of the applied deformation. At variance with that work, in the present study the system is deformed nonhomogeneously since the crack acts as a stress concentrator [17]. Therefore, we set a local criterion to adjust the cutoff distance, instead of globally changing the cutoff for all the atoms. In practice, a list of the original neighbors is kept during microcrack relaxation. As far as the neighbor distance is increased, the cutoff around each crack-tip atom is varied so as to retain the interaction with all the original neighbors in the list. With such a choice, atoms undergoing bond breaking can explore the proper Tersoff curve (i.e., no smoothing function is at work), while all the bulk properties are unchanged.

The stress-strain curve obtained with such a modification of the cutoff agrees with that of Tang *et al.* [15] and is represented in Fig. 2, top panel. The slope at vanishing deformation (dashed line) is related to the Young modulus E through the following equation: [18]

$$\sigma_{[111]} = \frac{E}{1-\nu^2}\frac{(1-\nu)^2}{1-2\nu}\epsilon_{[111]} = E' f \epsilon_{[111]}, \qquad (1)$$

where ν is the Poisson coefficient, $E' = E/(1-\nu^2)$. At

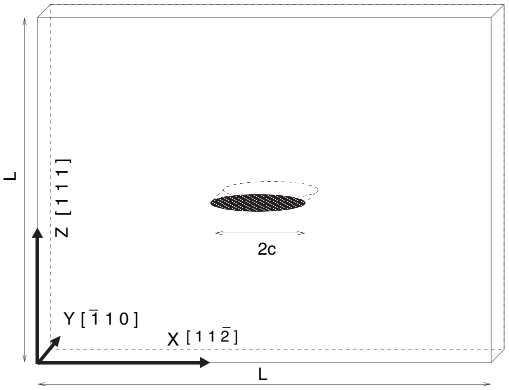

FIG. 1. Geometry and orientation of the simulation cell. In the present simulations 22 nm $< L <$ 88 nm. The shaded area represents the crack position.

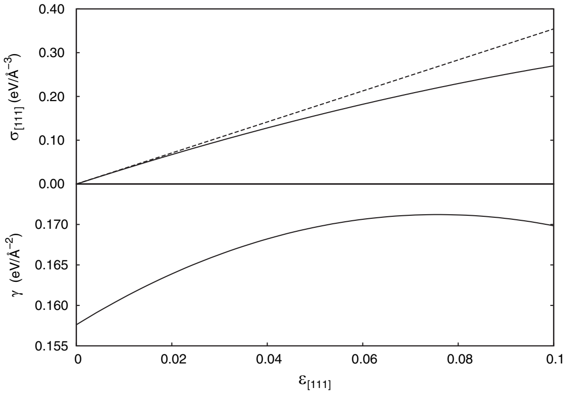

FIG. 2. Top panel: stress-strain curve for SiC (present Tersoff model); bottom panel: unrelaxed surface energy dependence on strain.

deformations $0.02 < \epsilon_{[111]} < 0.12$ the Poisson coefficient is in the range $0.047 < \nu < 0.07$ and $1.0024 < f < 1.0057$. Consequently we can assume $f = 1$ with 0.5% tolerance. In our simulations it is possible to calculate E' by the numerical derivative of the stress at zero strain: $E' = E/(1 - \nu^2) = d\sigma_{[111]}/d\epsilon_{[111]}$. We obtain $E' = 567 \pm 1.2$ GPa in good agreement with previous results [19]. Finally, the value of the unrelaxed (111) surface energy obtained with the present Tersoff model is $\gamma = 0.158\ \mathrm{eV}\,\text{Å}^{-2}$ at vanishing deformation. It is important to stress that the surface energy to use in the Griffith theory is the unrelaxed one, since the newly formed crack surfaces are infinitesimal portions of cleavage surfaces from the bulk crystal.

According to Griffith fracture theory, the critical stress σ_f^G for a sharp planar crack of length $2c$ is a function of the Young modulus E and of the crack resistance γ_s:

$$\sigma_f^G = \sqrt{\frac{2\gamma_s E'}{\pi c}}. \tag{2}$$

As said above, γ_s is usually identified with the free surface energy γ of the cleavage surface.

A series of atomistic simulations was performed with microcracks of length $2c_0 < 2c < 50c_0$. Based on the Griffith formula the critical load increases with decreasing microcrack length. For the Griffith theory to be valid, the limits of applicability of linear elasticity must be respected. Such a requirement implicitly defines the minimum length at which a finite-size microcrack can still be considered a "Griffith crack."

In Fig. 3 we report the values of critical strain ϵ_f as a function of microcrack length, obtained from our atomistic simulations (symbols). The full curve represents the critical strain corresponding to the $\sigma_f(c)$ predicted by the Griffith theory, by using the above defined values at $\epsilon = 0$ condition of E' and γ for the Tersoff potential. The corresponding critical value of the atomistic stress at failure σ_f^{at} is obtained either from the value of the average surface traction which preserves the applied strain or, equivalently, from the asymptotic value of the atomic-level virial stress equation.

Consistently with the expected brittle behavior, we found that at loads above the critical strain the microcrack extends in a perfectly brittle way, by preserving atomically smooth (111) cleavage surfaces. Such a result is granted only by the above described modification to the cutoff function: with the original Tersoff cutoff we observed either crack deflection or incipient plasticity, depending on the loading conditions. On the other hand, no rehealing of the microcrack edges was ever observed in our simulations at subcritical values of the load; i.e., the microcrack does not recede back to the perfect crystal. This is due to the relaxation of the free surface created by the microcrack, which entails both a slight energy decrease, and a variation of the optimum bond angles from the perfect tetrahedral arrangement.

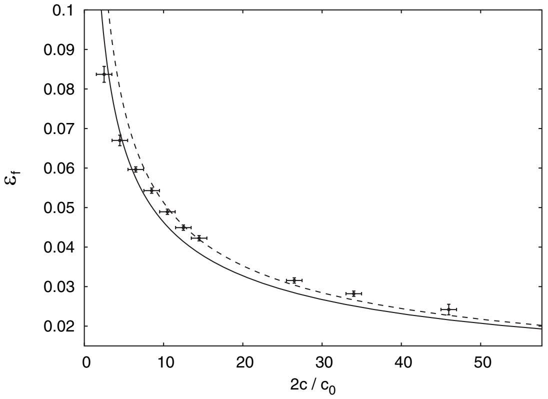

FIG. 3. Critical strain, ϵ_f, as a function of the crack size, $2c$, in units of the $[11\bar{2}]$ interbond distance c_0. Symbols are the data from atomistic simulations; the continuous line is Griffith's theory with constant material parameters and the dashed line is the modified Griffith's theory; see text. The horizontal error bars in the figure are due to the lattice spacing orthogonal to the crack front, while the vertical error bars are due to the steps chosen to vary the strain, $\Delta\epsilon = 0.001$.

Concerning the limits of the Griffith theory, we note that for microcrack lengths $2c < 10c_0$ the critical strain exceeds the value 0.05, i.e., the value at which deviations from linearity start to appear in the Young modulus. As a consequence, this is the minimum crack length for which the Griffith theory is applicable in our model of β-SiC.

For microcracks longer than $\sim 10c_0$ the calculated critical strain is systematically higher than the Griffith theory prediction. It is worth noting that, while atomistic simulations on metallic systems with long-range interatomic potentials reported a substantial agreement with the Griffith theory, [7] Bernstein *et al.* [6] found a similar discrepancy in silicon. According to that study such a discrepancy is by definition the lattice trapping $R = \sigma_f^{\mathrm{at}}/\sigma_f^G$. We believe, however, that the difference between atomistic simulations and the Griffith curve deserves further investigation before getting to firm conclusions. The assumptions of the linear elastic fracture mechanics are, strictly speaking, not correct in the case of a realistic (i.e., anharmonic) force model as is the present case. There are, indeed, at least two possible corrections to the common interpretation of the crack resistance term in the Griffith theory: (i) the surface energy γ depends on the state of strain and (ii) the stress-strain curve is not strictly linear over the range of explored loads; therefore, the Young modulus E' is not constant.

As a matter of fact, the nonlinear dependence of the surface energy γ versus strain $\epsilon_{[111]}$ (see Fig. 2) can also be computed straightforwardly. Accordingly, both the surface energy and Young modulus strain dependence can be introduced into the Griffith curve. The result of such a modified Griffith theory is the curve reported in Fig. 3 as a dashed line. The agreement between atomistic data and the modified Griffith theory is now much better, within the reported error bars. This demonstrates that the common

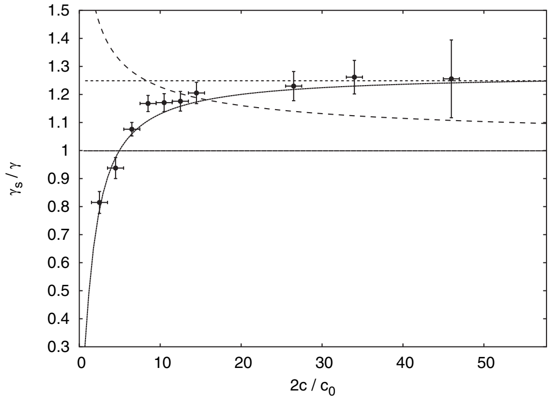

FIG. 4. Crack resistance γ_s as a function of the microcrack length $2c$. Symbols are atomistic simulation data; the horizontal continuous line is the original Griffith theory; the long-dashed line is the modified Griffith theory, with strain-dependent surface energy and Young modulus; the continuous line is the fit to the DBCS elastoplastic model. The horizontal short-dashed line at $\gamma_s/\gamma = 1.25$ represents the asymptotic value for the infinite-crack intrinsic resistance estimated from atomistic simulations.

identification of the crack resistance γ_s with the free energy γ of the cleavage surface provides only a lower bound to the energy-release rate G.

To quantify more accurately the sources of the observed discrepancy, in Fig. 4 we represent our results in a new form. The quantity $\gamma_s = (\sigma_f^{\mathrm{at}})^2 \pi c/2E'$ is the intrinsic crack resistance obtained from atomistic simulations. In the original form of Griffith's theory γ_s does not depend on the crack length and is therefore a constant: a horizontal alignment of the data is expected if Griffith's theory prediction is correct.

We exclude for the moment the first three simulation points from the discussion, since they belong to extremely small microcracks for which the Griffith theory does not apply. In Fig. 4 it can be seen that, although the long-dashed curve corresponding to the modified Griffith theory grossly agrees with the atomistic data, some systematic discrepancy arises asymptotically for macroscopically long cracks. This gives a 25% departure from the classic Griffith theory (horizontal full line at $\gamma_s = \gamma$). However, a substantial part of this discrepancy is due to the lack of strain dependence of the materials parameters. In the modified Griffith theory, these strain dependences are included and provide a $\gamma_s = 1.10\gamma$ as the asymptotic limit. The remaining discrepancy may be attributed to a possible lattice trapping (proportional to the square root of the discrepancy), the value $R = 1.08$ representing an upper bound for such an effect which, however, includes also the statistical error bars of the simulation results.

For very short microcracks, of length of a few c_0, the critical stress σ_f^{at} is so high that it becomes difficult to discriminate between bond breaking and incipient plasticity. A description of this regime can be attempted by a fit to an empirical elastoplastic law, such as the Dugdale-Bilby-Cottrell-Swinden model (DBCS) [12]. In this case, the model fracture stress can be deduced by inverting the expression for the (unknown) crack-tip displacement δ, as:

$$\sigma_f^D = \frac{2\sigma_M}{\pi}\cos^{-1}\left[\exp\left(-\frac{\pi\Delta}{4(1-\nu)}\frac{1}{c}\right)\right]. \qquad (3)$$

The lumped length parameter Δ should be equal to $\Delta = \mu\delta/\sigma_M$, with μ the shear elastic modulus, and σ_M the ideal cohesive strength, in the original DBCS model.

The best fit of the DBCS model to the atomistic data is represented in Fig. 4 by a continuous curve, merging with the atomistically corrected Griffith theory result at longer crack lengths. It is worth noting that, with the fitted values of the parameters, $\sigma_M = 53$ GPa and $\Delta = 2.3c_0$, we obtain an estimate of the crack-tip opening $\delta \sim 0.7c_0$. This means that, for an ideally brittle material, the extent of a "plastic" zone in the incipient microcrack (a "flaw") is, indeed, vanishingly small. However, this analysis also underscores the presence of competing instability modes, e.g., originating from a shear response, for microcracks of atomic-size length under very high stress.

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