MACRO CLEAVAGE ENERGY TO MICRO BOND BREAKING MECHANISMS- SHORTER IS TOUGHER

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Abstract
Fracture of brittle solids is ultimately executed by atomistic-scale, discrete, and ultrafast bond-breaking mechanisms along the crack path. Here, we show new fracture behavior and properties of brittle materials, based on macroscopic fracture cleavage experiments of silicon crystal specimens and atomistic-scale semi-empirical model for bond-breaking mechanisms along the curved crack front, to relate micro to macro in fracture.

1. Introduction

Griffith's theory of brittle solids is based on a total energy balance at equilibrium of slow fracture processes. Griffith defined twice the free-surface energy density, $2\gamma_s$ under vacuum, or $2\gamma_{SCC}$ under environmental stress corrosion cracking as the governing material property controlling crack initiation, known as Griffith barrier. By contrast, atomistic scale theoretical models in brittle periodic lattices and atomistic computer simulations at all levels indicate a 'lattice trapping' effect, suggesting that the energy barrier at crack initiation considerably exceeds the Griffith barrier. Continuum-based Freund equation of crack motion in brittle materials defines the dynamic energy-speed relationship.

We incorporated dynamic crack propagation theory and experiments as an essential tool in resolving the energy difference between the former two theories and redefining the definition of the Griffith barrier and the mechanisms occurring during fracture.

In the talk, we will introduce our extended approach to the macroscale, quasi-static, and *critical* Energy Release Rate (ERR), G_0, and the effect of its derivation, $\Theta \equiv dG_0(a_0)/da$. We then present our high-resolution fracture cleavage experiments of silicon crystal specimens and their macroscale fracture properties. Thereafter, we will introduce the energy dissipation by the microscale bond-breaking mechanisms in form of planner kinks. The macro-to-micro approach connects the cleavage energy and the ERR, G_0, and the microscale energy dissipated by kinking mechanisms. We then introduce an additional fracture mechanism we termed quasi-propagation, during which the cleavage energy is increased at short propagation length and at nearly zero speed. Only then, do we connect the macroscale and microscale in fracture.

2. Results

Our experimental, theoretical and numerical evaluations have yielded the following findings discussed in the talk:

1. Evaluations of the energy-speed relationships of cracks propagating along the two LECSs of single crystal silicon specimens (**Fig. 1a**) yielded increasing cleavage energy, Γ_0, for decreasing precrack length, a_0. We choose to use the gradient of the ERR, $\Theta \equiv dG_0(a_0)/da$ as the key parameter controlling fracture-related processes and material properties. Hence, $\Gamma_0=\Gamma_0(\Theta)$.

2. It will show that while the Griffith barrier of $2\gamma_{SCC}$ is the lower bound for crack initiation energy, while the lattice-trapping barrier is the upper bound for that energy. Both are linearly dependent on Θ (**Fig. 1b**).

3. While it is widely accepted that fracture processes include initiation and propagation, we indicate the existence of a third mechanism, that of a short propagation of several microns only at zero speed (**Fig. 1a**). It is spent to increase the cleavage energy from the Griffith barrier of $2\gamma_s$ (or $2\gamma_{SCC}$) to that dictated by the

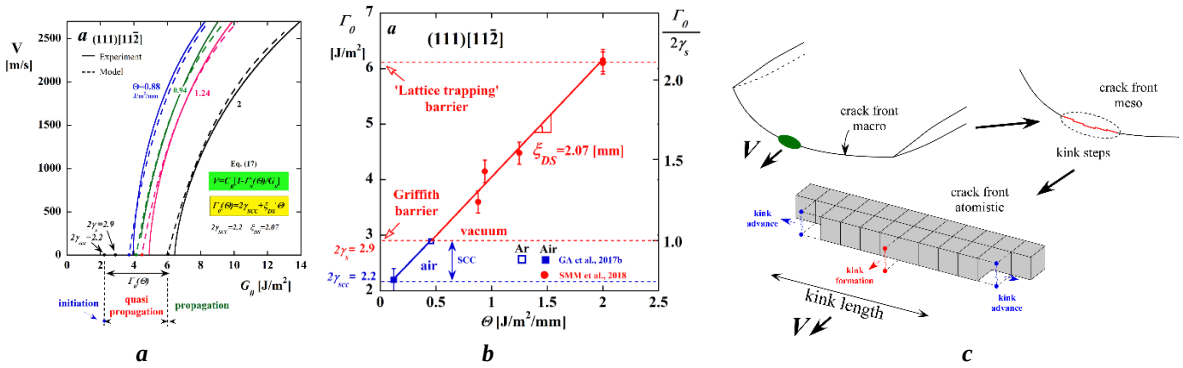
energy flow to the crack front, $\Gamma_0(\Theta)$. It is also intended to change the bond-breaking mechanisms along the crack front from kink advance dominated mechanisms to kink formation ones.

4. We defined 2 new material properties that are atomistic arrangement dependent: ξ_{DS} and Γ_{form} (**Fig. 1b**) is the energy density required to form a new kink. Γ_{form} is to be found by experiments.

5. The suggested bond-breaking mechanisms are based on in-plane step-like kinks (**Fig. 1c**). While the energy density dissipated by kink advance mechanisms is somewhat higher than $2\gamma_s$, we evaluated here the kink formation energy density, Γ_{form}, to be ~6 and ~5 J/m^2 for the (111)[11$\bar{2}$] and (110)[1$\bar{1}$0] LECSs of silicon crystal, respectively, by experimental results.

6. An important result of this investigation is that the strength of a material may increase significantly compared to Griffith's prediction, due to $\Gamma_0=\Gamma_0(\Theta)$. For short precracks, this increase may be tens of percent.

$$\sigma_{cr} = \sqrt{\frac{\Gamma_0(\theta)E}{\pi a}}$$



a ***b*** ***c***

Fig.1 – ***a*** The energy speed relationships of cracks propagating on (111)[112] low energy cleavage plane of silicon with increasing Θ. Note $\Gamma_0(\Theta)$ and the new fracture mechanism, quasi-propagation. ***b*** Γ_0 vs. Θ for the same cleavage system, its slope ξ_{DS}, and the maximum value, Γ_{form}. ***c*** The macroscopic curved crack front, the mesoscopic kink steps, and the atomistic kink advance (in yellow) and kink formation (in red).

3. Conclusions

Brittle single crystal silicon specimens have shown Preudo-R-Curve behavior as in metals. This is due to bond-breaking mechanisms along the crack front in form of low-energy kink advance (migration) and high-energy kink formation (nucleation) mechanisms in vincreasing number of the latter. The change in the kinking mechanisms is attributed to the increase value of G_0 and its gradient Θ, both are increased by decreased initial crack length, a_0. While this investigation is based on long-range order materials, i.e. crystals, we believe that similar general behavior may apply also to other types of brittle materials.

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