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Dynamic fracture instabilities in brittle crystals generated by thermal phonon emission: Experiments and atomistic calculations

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A R T I C L E I N F O

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A B S T R A C T

Dynamic cleavage fracture experiments of brittle single crystal silicon revealed several length scales of surface and path instabilities: macroscale path selection, mesoscale crack deflection, and nanoscale surface ridges. These phenomena cannot be predicted or explained by any of the continuum mechanics based equations of motion of dynamic cracks, as presumably critical energy dissipation mechanisms are not fully accounted for in the theories. Experimentally measured maximum crack speed, always lower than the theoretical limit, is another phenomenon that is as yet not well understood.

We suggest that these phenomena depend on velocity dependent and anisotropic material property that resists crack propagation. The basic approach is that the bond breaking mechanisms during dynamic crack propagation vibrate the atoms at the crack front to generate thermal phonon emission, or heat, which provides additional energy dissipation mechanisms. This energy dissipation mechanism is a material property that resists crack propagation. To evaluate this property, we combined the continuum based elastodynamic Freund equation of motion with molecular dynamics atomistic computer "experiments".

We analyzed the above experimental dynamic fracture instabilities in silicon with the obtained velocity dependent and anisotropic material property and show its importance in cleavage of brittle crystals.

1. Introduction

Dynamic crack instabilities refer to deviations of the propagating crack from smooth and straight, self-similar crack; surface features in the form of roughness or undulations are surface instabilities and deviations of the crack from its main course or branching refer to path instability. The instabilities in dynamic fracture have been studied during last decades primarily in brittle isotropic materials such as frozen rubber, glasses, and brittle polymers, all having short range order atomistic structure. Andrews (1959) was the first to identify the surface roughness occurring during dynamic crack propagation in brittle frozen rubber as mirror, mist, and hackle, and manifested the increased amplitude of the surface features with crack speed. Ravi-Chandar and Knauss (1984) showed that these surface features in brittle plastic (Homalite-100) progressively grow in size. Fineberg et al. (1991) were the first to correlate the oscillations in crack velocity with surface features in brittle amorphous polymer (PMMA) and in soda lime glass (Gross et al., 1993), and to term the effect 'instabilities in dynamic fracture'. At velocities lower than $0.4C_R$ (C_R is the Rayleigh free surface wave speed, the theoretical

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limit for Mode I cracks), the surface is featureless, mirror like. At increased crack velocity, the surface instabilities increase to the well-known mist and hackle, and then crack branching phenomenon occurs. The maximum crack velocity in these brittle solids never attains C_R, as the surface undulations become an additional source of energy dissipation mechanism (Ravi-Chandar, 1998). Yoffe (1951) has analytically analyzed crack propagation in finite length crack moving in isotropic material and noticed that crack branching occurred at relatively high speed due to bifurcation of the high stress fields at the crack front. Over the last decade, large scale atomistic simulations of rapidly propagating cracks in brittle materials models have shown the existence of dynamic instabilities in the form of crack surface undulations (Abraham et al., 1994; Buehler and Gao, 2006; Cramer et al., 2000). It was shown recently (Goldman et al., 2010) that crack speed instability occurred in brittle sol–gel thin specimens as a result of reflected stress wave from the boundaries of narrow specimens.

Different phenomena, in contrast to those observed in brittle isotropic materials, were evident during dynamic crack propagation in brittle single crystals, owing to the long range atomistic structure and directional anisotropy of these materials. For example, low speed surface instabilities were reported recently (Kermode et al., 2008; Sherman et al., 2008), while the surface became mirror-like smooth at high speeds (Sherman and Be'ery, 2004; Sherman et al., 2008). Crack propagated initially on the $(1\,1\,0)[1\,\bar{1}\,0]$ (crack plane and crack direction of propagation) low energy cleavage system of silicon was progressively deflected to the $(1\,1\,1)[1\,1\,\bar{2}]$ cleavage system with increased maximum crack speed (Sherman, 2005; Sherman and Be'ery, 2003b, 2004), a phenomenon that has not been observed in isotropic materials. In addition, and similar to the phenomenon observed in glasses and plastics, the maximum crack speed measured in cleaving brittle crystals is always lower than the limiting crack speed, C_R.

These phenomena in brittle crystals cannot be explained by any of the continuum mechanics based equations of motion of dynamic crack propagation. An additional energy dissipation mechanism, anisotropic in nature and velocity dependent is thus missing in the theories to describe the phenomena occurring in dynamic crack propagation in brittle crystals. Incorporating such a term to the existing theories may explain the experimental findings.

The energy balance during crack propagation formulated by Freund (Freund, 1998) using continuum elastodynamics for isotropic materials, defines the net energy, $\Gamma(V)$, necessary for the bonds-breaking mechanisms at speed V, as equal to the net energy transferred to the crack front, $G(V)$, as follows:

$$\Gamma(V) = G(V) = G_0 g_d(V) \tag{1}$$

where G_0 is the quasi-static strain energy release rate (SERR) for a stationary crack of certain length and is considered the driving force for cracking, appropriate for isotropic as well as for anisotropic materials. The complex universal dynamical function $g_d(V)$ is well approximated by a linear function, $(1-V/C_R)$, which depends on crack speed only and scales with C_R. Eq. (1) was defined for semi-infinite bodies, avoiding the effect of reflected stress wave from its boundaries.

There is no theory to define $\Gamma(V)$, the velocity dependent material property that resists crack propagation, or, alternatively, the energy required to propagate a crack at velocity V. It should primarily be evaluated by experiments. Such a property for material with varying internal structure was suggested (Freund, 1998), but the adaptation to atomistic structure of brittle crystals has not been shown yet.

The main theme of this contribution is to suggest a velocity dependent and anisotropic energy dissipation mechanism in an attempt to explain the experimental findings observed in silicon crystal. Here we suggest that this energy dissipation mechanism is the phonon emitted during rapid bond breaking mechanisms occurring when the crack cut through the material. The bond breaking mechanisms vibrate the atoms at the crack front vicinity. These vibrations are characterized by low amplitude and high frequency vibrations and termed thermal phonon, translated to increased temperature at the crack front vicinity, which is practically the heat generated during propagation. As this thermally activated process consumes energy, it can be transformed to the additional energy release rate (ERR) required to propagate a crack. We chose to add it to the material property, and termed it G_{Ph}, the phonon emission ERR. In addition to being velocity dependent, G_{Ph} is strongly depend on the anisotropy of the crystal, namely, by the atomistic arrangement at the crack front. Considering now the velocity-dependent material resistance to crack propagation more explicitly as the sum of the quasi static and the dynamic parts, one can obtain:

$$\Gamma(V) = 2\gamma + G_{\text{Ph}} = G_0\left(1-\frac{V}{C_R}\right) \tag{2}$$

where 2γ is twice the free surface energy of the plane of propagation, used by Griffith (1921) as the criterion for slow crack propagation in ideally brittle materials, and considered the lower limit of Γ. Phonon emission is a velocity-dependent property, thus it can be considered either as a part of the material property side of Eq. (2) or as a part of the driving force side of this equation that is represented by the total ERR, which contains all forms of energy exchange with the surroundings. The term phonon emission ERR is used to describe specific contribution of phonon emission to the total ERR. In this contribution, however, we consider phonon emission as the mechanism increasing the material property that resists crack propagation.

An exact definition of G_{Ph}, and, therefore, of $\Gamma(V)$ in Eq. (2) is beyond the ability of continuum mechanics to provide, as continuum mechanics does not account for atomistic scale events. We therefore turned to extract G_{Ph} by means of atomistic computer calculations "experiments" combined with the continuum mechanics based Freund equation of motion, in an attempt to rationalize the experimental results.