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Dynamic crack path selection in brittle crystals under mixed mode loading

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ABSTRACT

We studied, experimentally, the conditions required to deflect a dynamic crack from the low energy cleavage planes of propagation under in-plane mixed mode loading, and the path selected by the crack afterwards, where the shear stress, crack speed, and crystal structure were the governing variables. Silicon crystal, which shows cleavage along the {1 1 0} and {1 1 1} families of planes, was used as a model material. The experiments were carried out by our recently developed coefficient of thermal expansion mismatch (CTEM) method. Finite element analysis was used to compute the quasi-static mode-mixity and energies release rate, and Freund equation of motion was used to estimate crack speed.

Deflection occurs due to the competition between the propensity of the crack to propagate on the low energy plane and the requirement to reduce the shear energy. This energy balance depends on crack speed and crystal structure. It is shown that when the crack speed increases, higher shear mode stresses are required to deflect the crack macroscopically from the low energy cleavage plane. Our work indicates that crack path selection in single crystal silicon at the macro-scale can vary between nearly perfect cleavage on the {1 1 1} low energy cleavage planes and nearly isotropic path selection on the {1 1 0} planes. Finally, we postulate that in mixed mode loading, the tensile mode is the driving force for crack speed while the shear mode is responsible for crack deflection.

1. Introduction

The material resistance for crack initiation can be described in terms of the fracture toughness, e.g., K_{IC}, the Mode I critical stress intensity factor (SIF), or the critical energy release rate (ERR), G_{IC}, which is also the fracture energy, both of which are interrelated. In isotropic materials, the external loading and geometry alone determine the fracture behavior. The crack will initiate when the ERR at the crack tip, G_0, is equal to the material property that resists initiation [1], Γ_0, i.e.,

$$G_0 = \Gamma_0. \tag{1}$$

The accepted lower bound for G_0 is the Griffith barrier energy [2], which is twice the free and relaxed surface energy, 2γ. It is therefore commonly accepted that crack initiation in brittle materials obeys:

$$G_0 = \Gamma_0 \geqslant 2\gamma. \tag{2}$$

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In case of loading under tension and shear, crack initiation and path selection are more complex. Three main criteria for quasi static crack path selection in isotropic homogenous materials include: Maximum tensile stress or zero shear stresses [3], maximum energy release rate, G_{max} [4,5], and principle of local symmetry, $K_{II} = 0$ [6]. These criteria predict that a crack loaded under mixed-mode loading will *immediately* deflect in the direction described by these criteria. These three main criteria generally predict similar crack paths. Finite element analysis (FEA), can be used to compute the direction of crack deflection of a mixed-mode crack based on the calculated SIF [7].

The energy-speed relationship for a propagating crack was formulated via elastodynamic equation of motion [8] for time independent loading in semi-infinite body. State of equilibrium prevails among the various energies in the system. It was shown that the energy available for the bond breaking mechanisms, G(V), is the product of G_0 and the universal dynamic function, $g_d(V)$, which can be approximated as a linear function. Under Mode-I loading the energy-speed relationship can be expressed as:

$$G(V) = G_0 g_d(V) \approx G_0\left(1 - \frac{V}{C_R}\right) = G_0 - G_K(V), \tag{3}$$

where C_R is the Rayleigh free surface wave speed of the material, which is the theoretical upper limit for Mode-I crack speed in solids. In the continuum relation and due to energy equilibrium, the quasi-static ERR, G_0 (for V = 0), is consumed by the energy required to create new surfaces, G(V), and by the energy dissipated by elastic wave, or the kinetic energy $G_K(V)$, Eq. (3), where V is the crack speed. In ideally brittle materials, $G(V) = 2\gamma$. From Eqs. (1) and (2) the relationship between these two energy consumption mechanisms can be written as,

$$2\gamma \approx G_0\left(1 - \frac{V}{C_R}\right) = G_0 - G_K \tag{4}$$

Most importantly, the quasi-static ERR can be determined by static FEA, for isotropic and anisotropic materials [9]. In addition, Freund described the energy-speed relationship for each individual, pure mode [8] and thus, this equation can be utilized to determine the dynamic crack speed when describing the path of dynamic mixed-mode cracks by FEA [10,11]. Notably, Freund equation of motion was formulated for semi-infinite continuum, where reflected stress waves from the boundaries back to the crack tip are not considered.

With linear elastic fracture mechanics concepts, developed from the study of crack path selection in isotropic materials, it is possible to describe crack path selection in BSCs. Several authors have utilized these concepts, such as $K_{II} = 0$ or G_{max}, to produce theoretical descriptions of crack path selection. Lawn [12] proposed that the path of fracture in crystals is controlled by competing forces to propagate along the cleavage plane and to reduce shear at the crack tip. This was based on observations of crack deflection from the low energy cleavage plane of silicon during indentation fracture. Other authors have described this competition in terms of ERR at the crack tip and the anisotropic fracture energy [13–16]. This description is analogous to crack path selection criteria based on proposed energy concepts [17]. These theoretical descriptions of crack path selection do not include the effect of crack *speed* in crystals. Rather, they assumed that crack propagation is quasi-static and the fracture energy can be described as $\Gamma(\theta) = 2\gamma(\theta)$, where θ is the orientation on the cleavage plane. An experimental investigation to evaluate crack path selection in crystals under mixed-mode loading has not previously been performed.

Fundamentally, cleavage in crystals is a dynamic process of bond breaking mechanisms at the crack tip. Energy-speed relationship, bond breaking mechanisms, and role of other cracks dynamics phenomena were thoroughly described by atomistic simulations in the last 3 decades. Atomistic simulations at all levels, under pure mode I [13,18–22] or under Mode II and combined loading [23–25] have demonstrated the importance of the atomistic aspects of fracture.

In the present work, the effect of crack speed and mode-mixitiy on crack path selection in silicon crystal will be evaluated experimentally and by means of numerical analysis (FEA) and theoretical considerations through Freund equation of motion. The current study aims to measure the conditions for macro scale deflection from the cleavage plane, where the shear stress, crack speed, and crystal structure are the governing variables.

2. The experimental method

Single crystal silicon was used here as a model material. The cleavage plane and direction of crack propagation corresponds to the $(1\,1\,0)[1\,\bar{1}\,0]$ and $(1\,1\,1)[1\,1\,\bar{2}]$ low energy cleavage or crack systems (the first bracket denotes the cleavage plane of propagation, the second-crack speed direction). The experimental method for Mode I loading has been extensively described elsewhere [26,27].

2.1. The specimen

Single crystal silicon [0 0 1] or [1 1 0] wafers, 6″ in diameter and 680 μm thick were used in this investigation. Rectangular specimens were diced from these wafers to a dimension of 25.00 by 42.00 mm (Fig. 1c), where the $(1\,1\,0)[1\,\bar{1}\,0]$ and $(1\,1\,1)[1\,1\,\bar{2}]$ cleavage systems were inclined by $15.00 \pm 0.05^\circ$ relative to the wafer's flat. The wafer's flat alignment tolerance to the crystallographic orientation of the silicon was specified as $\pm 0.5^\circ$ according to the manufacturer's specification. Thus, the effective inclination of the cleavage plane to the specimen's geometry was $15.00 \pm 0.55^\circ$.