

MACRO TO ATOMISTIC EXAMINATION OF DYNAMIC CLEAVAGE IN SINGLE CRYSTAL SILICON

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ABSTRACT

A set of cleavage experiments with strip-shaped single-crystal silicon specimens subjected to three-point bending will be presented. The experiments enabled examination of the relationships between crack velocity, the crystallographic orientation, and the cleavage plane of propagation.

Dynamic crack propagation experiments show that when a [001] silicon single crystal is fractured under three-point bending at measured velocity of up to 1500 m/sec, it prefers to cleave along the vertical (110) plane, while when the specimen is fractured under the same conditions but at a velocity higher than 2900 m/sec, it cleaves along the inclined (111) plane. At intermediate velocities, the crack will deflect from the (110) plane to the (111) plane.

The deflection phenomenon presents an excellent opportunity to examine the upper crack tip's velocity limit. Analysis of the experimental results showed that the normalized crack tip velocity in the (110) plane with the Rayleigh surface wave speed yields ratio of up to 0.65 (in the $[1\bar{1}0]$ direction), which reduces to as low as 0.01 (in the [001] direction).

It is suggested that the cause of the deflection phenomenon and the reasoning for the low limiting crack tip velocity is the anisotropic, velocity dependent, irreversible cleavage energy, resulted phonon radiation caused by anisotropic, velocity dependent lattice vibrations.

1. INTRODUCTION

The microstructure of brittle materials, and in particular the bonding potentials, dictate the fracture processes, initiation and propagation. While amorphous and polycrystalline brittle solids behave isotropically, brittle single crystals provide noteworthy challenges due to their anisotropy. In the current contribution we focus on the cleavage behavior of a brittle single crystal, and a Si single crystal in particular. When a brittle single crystal is loaded to fracture, it usually tends to cleave along one of a family of favored crystallographic planes, generally those with the highest in-plane atomic density and maximal inter-plane separation, similar to the conditions dictating dislocation mobility in metallic single crystals.

We raise a fundamental question: Are Irwin's (Irwin, 1958[1]) and Freund's (Freund, 1990 [2]) criteria sufficient to predict the (cleavage) plane of propagation or is an additional criterion required? As is shown below, both criteria are in some cases insufficient to predict the cleavage plane of propagation, and another criterion is required.

From the conventional point of view, Γ_0 , the (quasi-static) cleavage energy of a certain plane, is independent of the cleavage direction, since it only involves a bond breaking mechanism. The dynamic cleavage energy, however, is defined by two variables: the cleavage plane and the cleavage direction. Since the atomic distribution of many cleavage planes is different for different directions, the energy barriers are different, too. This phenomenon, known as 'molecular crack arrest' or 'lattice barrier', is believed to be the source of directional anisotropy, which was first observed in cleavage experiments with tungsten single crystals (Riedle et al., 1996 [3]), and later in silicon (Perez and Gumbsch, 2000 [4]).

In the present paper, we describe the cleavage system of propagation as a function of crack tip velocity and fracture energy. We then discuss the fundamental aspects of propagation and suggest criterion that govern the selection of the cleavage system.

2. EXPERIMENTAL PROGRAM

Commercial 4" silicon wafers, 525 μm thick, with their surface normal to the $[001]$ and $[1\bar{1}0]$ directions, were cut into $25 \times 45 \text{ mm}^2$ strips. An edge notch was introduced in each specimen using a 150 μm thick diamond saw (Fig. 1). The load to fracture, and therefore the maximum velocity and the stored energy, was varied by varying the notch depth between 0.1 mm to 1 mm. The notched strips were loaded to fracture using fully articulated three-point bending (3PB) apparatus having a span of 40 mm, Fig. 1. The (110) cleavage plane is shown in Fig. 1 as the plane of propagation, while the (111) plane, which is inclined 35.26° to the $[001]$ direction, is shown for clarification. The tension/compression stress profile typical of bending, although more complicated to analyze than that in pure tension geometry, has the advantage of confining the crack front to the shape of a quarter ellipse.

Velocity measurements of the crack on the specimens' surfaces were made using the 'potential drop' method (Stalder, 1983 [5]), involving coating one or both surfaces of the specimens with 200 nm of a brittle metal (Ta or Cr) and measuring the increase in resistivity as the advancing crack is cutting the metal layer.

3. RESULTS

The profile of the crack front in the currently used thin specimens under 3PB has previously been analyzed (Sherman and Be'ery [6], Be'ery et al., 2003 [7]). While the so-called 'crack front' (Fig. 2) was shown to have a quarter-elliptical shape with a straight long 'tail', we postulate that this 'front' is actually only a virtual entity constructed from a set of ridges that are advancing in the material, initiating at the bottom surface, Point A, and progressing towards the upper portion of the specimen, Point B, Fig. 2, for an individual, isolated ridge, and described elsewhere (Be'ery et al., 2003 [7]). The velocity of propagation of an individual ridge, designated V_n , is normal to the local crack front, Fig. 2. This normal velocity is the actual velocity at which the bonds between atoms along the crack tip's path are breaking and is therefore the physically meaningful velocity.

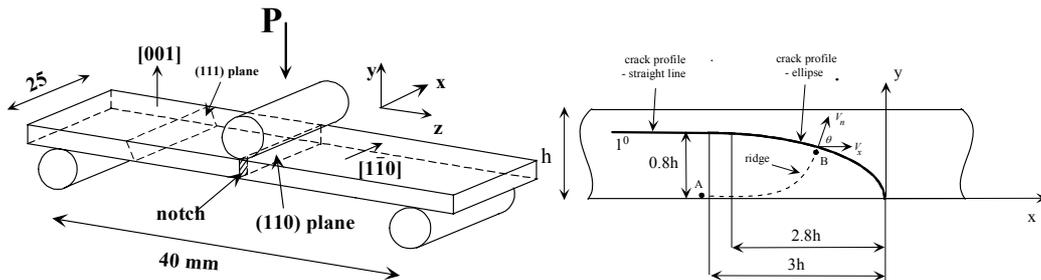


Fig. 1: The 3PB specimen geometry and definition of the main axes, directions, and planes.

Fig. 2: The quarter elliptical crack front shape and its velocities

At steady state of the parallel velocity, V_x , which occurs over most of the specimen's width, the crack front moves at almost constant velocity (V_x) in the x direction. The physically significant growth velocity of a ridge, V_n , coincides with the parallel velocity, V_x , in the lower portion of the cross-section (see Fig. 2). In the upper portion of the specimen the growth velocity is very low and

almost normal to the parallel velocity. For specimens with smooth surfaces, the normal velocity at any point on the crack front is given by $V_n = V_x \sin \theta$, where θ is the angle between the local normal to the crack front and the x-axis, Fig. 2.

The most fascinating experimental result in the current experimental program is the gradual deflection of the preferred cleavage plane from (110) to (111) in the [001] specimens subjected to bending (Sherman and Be'ery, 2003 [8], 2004 [9]). This behavior is schematically shown in Figs. 3a to c. At the measured steady state crack front velocity, V_x , of up to 1560 m/sec, the cracks propagated solely on the (110) plane, (Fig. 3a). On the other hand, at velocities higher than 2900 m/sec, the cracks propagated entirely on the (111) plane (with a small transition zone at the beginning) (Fig. 3c), although the geometry and the loading were the same. Deflection from the (110) plane to the (111) plane can be seen when the crack velocity is moderate (Fig. 3b). An important observation is that the deflection zone, namely the border between the (110) and the (111) plane, has a shape distinct from that of the crack profile, which suggests that this border is presumably dictated by the local velocity of the bond-breaking mechanism, and not by the crack profile.

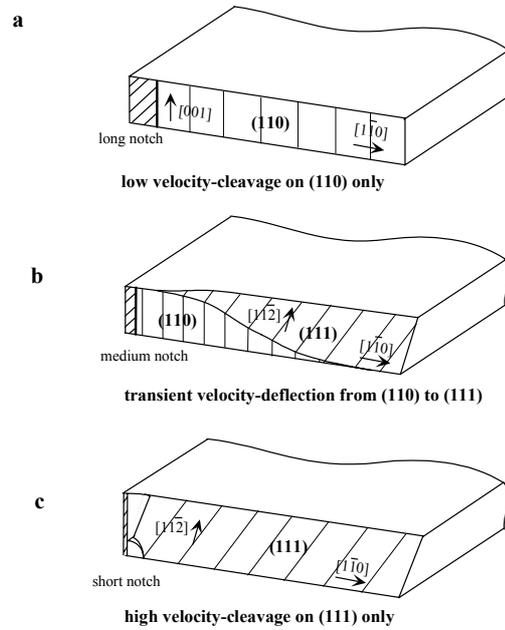


Fig. 3: Schematic representations of the deflection phenomenon: the transition from the propagation along the (110) plane only (a), to propagation along the (111) plane only (c), and the deflection from (110) to (111) (b), when the crack length and the crack velocity are intermediate.

The combination of the velocity profile with the calculated critical normal velocity, V_n , and the precise crack shape yield a description of the deflection velocity as a function of the crystallographic orientation, as shown in Fig 4a. Analysis of the experimental results showed that a crack, propagating in the (110) $[1 \bar{1} 0]$ system will deflect to the (111) $[1 \bar{1} 0]$ system at a velocity of nearly 2900 m/sec. This velocity reduces to less than 30 m/sec if the crack system is (110)[001]. The variation in the deflection velocity is nearly linear depending on the crystallographic orientation

on the (110) plane. Normalizing these velocities with C_R yields ratios of up to 0.65, which reduces to as low as 0.01, which means that the maximum velocity a crack can attain is only about 1 percent of the Rayleigh surface wave speed (Fig. 4b). The reason C_R is far from predicting the limit of the crack tip velocity in certain crystallographic orientations lies in the continuum versus atomistic approach, see below.

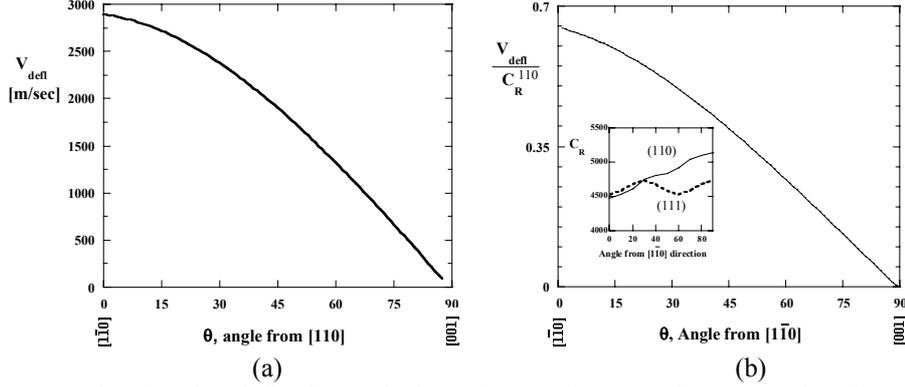


Fig. 4: The deflection velocity (a) and the normalized velocity (b) as a function of the direction of the crystallographic orientation with respect to the $[1\bar{1}0]$ direction.

4. DISCUSSION

The most significant result of our experiments, as stated above, is the discovery of the macroscopic change in the preferred cleavage plane from (110) to (111) when the crack velocity increases above a certain critical value, as shown in Fig. 4. The reason for the change in the preferred cleavage plane is fundamental, and requires a thorough analysis.

In this regard we refer the reader to two important parameters in our investigation. The first is the quasi-static surface energy, respectively Γ_0^{110} and Γ_0^{111} , obtained lately by full-density functional molecular dynamic simulations (Perez and Gumbsch, 2000 [4]), and calculated to be 3.46 and 2.88 J/m². However, when the crack is propagating on the {111} plane, which is inclined 35.26° to the {110} plane, the total energy dissipated is $\bar{\Gamma}_0^{111} = 2.88 / \cos(35.26) = 3.52$ J/m². In these circumstances, the {110} plane becomes the low-energy cleavage plane. Therefore, in the following discussion, G and Γ refer to a unit area of the specimens' cross-section, not to the crack surface.

The following discussion attempts to analyze and explain the reasons for the change in the preferred cleavage plane, assuming $C_R^{(110)} = C_R^{(111)}$. We indicate the different variables participating in the dynamic crack propagation and point to the one that governs the deflection. Then we formulate *energy-based* criteria that determines the selection of the cleavage system.

4.1 Crack deflection and the governing variable.

In the following, we show the dependence of the cleavage energy on the velocity. The basic form of the cleavage energy is:

$$\Gamma = \Gamma^R + \Gamma^I \quad (1)$$

where Γ^R and Γ^I are the reversible and the irreversible fracture energies, respectively. This formulation, as will be seen below, is essential to the explanation of the crack deflection mechanism. We postulate that to rationalize crack deflection, additional dissipating mechanisms that increase the energy dissipation as the crack's velocity increases, must be added to the main, ideally brittle bond-breaking mechanisms. We further postulate that Γ^I is only velocity-dependent parameter, namely, $\Gamma^I = \Gamma^I(V)$, and is our reasoning for the deflection phenomenon; A crack tip, as much as a dislocation line, moving in a perfect crystal lattice dissipates energy by radiating phonons. The lattice barrier (Spence et al., 1993 [10]; Perez and Gumbsch, 2003 [4]) is expected to act in a manner very similar to that of Peierls barriers that radiate phonons from a moving dislocation (Lawn, 1993 [11]). It is therefore reasonable to explain the transition from one cleavage system to another as the result of a stronger phonon dissipation of the $\{110\}$ plane. The change by two orders of magnitude between V_{defl} of the $[001]$ and that of the $[110]$ direction along the (110) plane, shown in Fig. 4, is explained by the difference in lattice trapping between the (110) - $[001]$ and the (110) - $[110]$ systems, and the stronger phonon dissipation in the former. In our specimens, where the crack is propagating along a quarter-elliptical path, the cleavage energy is also a function of direction, thus: $\Gamma^I = \Gamma^I(V, \theta)$, and Eq. (1) becomes, more rigorously,

$$\Gamma = \Gamma(V, \theta) = \Gamma^R + \Gamma^I(V, \theta) \quad (2)$$

4.2 Criteria for crack deflection

The problem of selecting a cleavage system in the fracture of single crystals has not yet arisen. We presume that the dynamic cleavage energy, $\Gamma(V)$, **Fig. 5**, depends on velocity (assuming $C_R^{(110)} = C_R^{(111)}$). Referring to **Fig. 5**, initiation and propagation starts when G_0 gradually increases with increasing external load until Irwin's criterion, $G_0 = \Gamma_0$, is met (point A, Fig. 5). As the crack propagates, G_0 increases, and the crack continues to propagate along the (110) plane (line AB). It

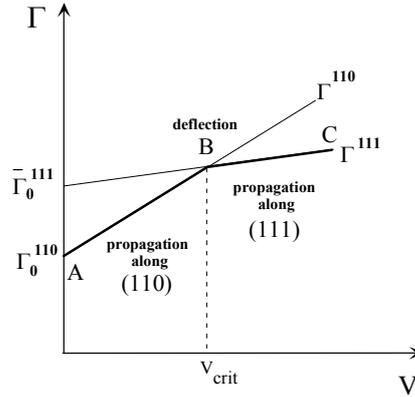


Fig. 5: Schematic diagram suggesting $\Gamma = \Gamma^R + \Gamma^I(V)$ as a linear function of the velocity (for a certain crystallographic orientation) assuming equal values of C_R for both planes. Note that $\partial\Gamma^{(110)}/\partial V > \partial\Gamma^{(111)}/\partial V$, which is presumably due to higher lattice trapping on the (110) plane. The intersection of the functions at point B indicates the deflection.

does so until point B, thereafter it deflects to the (111) cleavage plane, where the rest of the propagation is taking place. With respect to this occurrence we suggest a more general energetic criterion for the selection of the preferred plane of propagation, viz.:

$$G(V) - \Gamma_i(V) = \max. \quad (3)$$

Eq. (3) is similar to Irwin's criterion (Irwin, 1958 [1]) for crack initiation. That criterion states that propagation occurs on the lowest-energy plane. At point B, deflection to the (111) plane takes place, since it is now the lowest-energy plane.

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