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Crack initiation behavior in single crystalline silicon

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ABSTRACT

In this article, we report special fracture initiation behavior of (110) cleavage in silicon single crystal. It is found that the static energy release rate always exceeds the material toughness upon crack initiation. According to high-speed imaging measurements and fractographies, it is found that the crack has an important initial velocity, i.e. up to 3000 m/s, and then reaches the steady-state propagation regime very quickly. The experimentally revealed initial crack velocity is in good agreement with estimation from the energy flux at crack initiation.

Single crystalline silicon is very actively used in microelectromechanical (MEMS) and photovoltaic (PV) industries. The understanding of the material failure is always a major concern for both manufacturers and users in order to ensure the structural integrity and satisfactory performance during service [1].

The fracture of single crystalline silicon is a dynamic process due to the brittle behavior of the material [2,3,4]. The fracture takes place preferentially on crystallographic planes (111) and (110) where the material toughness is the lower [5,6,7–9,10]. In dynamic fracture investigations, the crack propagation velocity is of first importance since many material properties and abnormal phenomena in silicon are related to velocity such as the dynamic toughness [11] and the presence or not of crack surface instabilities [12,13]. Silicon cracking has been widely investigated by means of the 'potential drop' measurement method [14]. It consists in pasting an ultra-thin conductive film on the specimen's surface and correlating the resistance variation with the crack length. Thanks to this method, it has been shown that slow steady-state crack velocity ($\ll$2000 m/s) is never observed in silicon [2,11,3,6]. This velocity gap is contradictory to the classical continuum fracture theories which predict a continuously increasing steady state velocity with increasing load. Numerical simulations based on continuum mechanics fail systematically to elucidate this phenomenon. Nevertheless, molecular dynamics (MD) simulations provide fundamental insight of the atomistic fracture scenario. In particular, the simulation of silicon cracking necessitates quantum mechanical precision [15,16,12]. Based on a multiparadigm simulation hybrid ReaxFF-Tersoff model [17], the occurrence of localized phase transformation of silicon lattice from 6-membered rings to 5–7 double rings has been highlighted [18]. The same finding has been reported with a modified embedded atom method (MEAM) [19] in MD scheme analysis [20]. This phase transformation actively blunts the crack tip and leads to the velocity gap by delaying the crack initiation.

In the literature when measurements are performed using the 'potential drop' method, a moderate acceleration until the maximum speed is reached is systematically observed, either for tensile [11,3] or bending [4] tests. This phase begins by a very slow initial crack velocity, then the crack velocity increases until the crack length goes as far as 5 to 10 mm before to reach the steady-state speed. However, the results with this measurement technique should be considered with caution. In one hand, one can imagine that a ductile cracking (with a material like Ta or Cu) cannot strictly follow a brittle cracking since the deformation over cracking is very small. In the other hand, a fast cracking within metals might undergo a hysteresis due to plasticity. In the numerical framework, molecular dynamics allow to gain results for a very small time length, which is ideal to capture the crack initiation onset. According to MD simulations [18], a very high crack initial velocity was highlighted, conversely to experimental data until now. Yet, this incoherence has never been addressed properly within an experimental framework since most of these previous studies only focused on the steady-state stage of the fracture to highlight velocity correlated properties and related phenomena, while the initiation behavior was rarely concerned.

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In fracture mechanics, it is widely admitted that the crack initiation and propagation obey the Griffith criterion [21] and the Freund condition [22], respectively, as recalled in the two following equations:

$$G_s = \Gamma_0 = 2\gamma \tag{1}$$

where G_S is the static energy release rate (SERR), and Γ_0 stands for the material toughness which equals to 2 times the surface energy of the fracture plane γ.

$$G_S\left(1-\frac{v}{C_R}\right) = \Gamma_D \tag{2}$$

where Γ_D denotes the dynamic toughness which depends on the crack velocity v, and C_R is the Rayleigh velocity. Indeed, if the Griffith criterion is met at initiation, the initial crack velocity would be zero and the crack will accelerate until it reaches the steady-state speed. However, if the crack tip is blunted by phase transformation during loading, then the local material resistance will be more important than the normal cleavage toughness, i.e. 2γ, and the Griffith condition is no more valid. To initiate the cracking, bigger SERR is then required. In addition, the crack would have a finite rather than null initial velocity in this case.

Our motivation is here to investigate more precisely the crack initiation behavior of (110) cleavage in silicon, especially the relationship between the SERR and the initial velocity v_0. Our specimens are thin square plates (50 × 50 × 0.2 mm) obtained from silicon ingot with diamond wire sawing. A chemical etching was carried out to eliminate a small layer of the damaged surface. Nevertheless, the sawing lines were intentionally kept in order to have a sufficient roughness to generate Wallner lines [23] on the fracture faces. A pre-crack was introduced with a Vickers indent at the center of one edge of each specimen. In order to have distinguished crack velocities for different specimens, two strategies were used to control the pre-crack's dimension. The first one was to indent the specimen on a rigid flat support so that a sharp notch could be obtained (around 200 μm). The second one consisted in indenting the specimen edge into a shallow hollow support so that a relatively long pre-crack was generated (around 1000 μm).

A 4-point bending equipment was chosen to perform the fracture study. The inner and outer spans are 21 mm and 40 mm for our bending set-up. The specimens were loaded quasi-statically (10^{-6}/s) until cracking. The crack propagation was observed by a high-speed camera thanks to a 45° tilted mirror between the two support rollers (see [10, 24] for more information). The image acquisition frequency was set to 180,000 Hz, the observation zone (512 × 64 pixels) was centered with respect to the pre-crack. Crack length was estimated by performing subtraction between consecutive images. The subtraction results then went through contrast reinforcement as well as denoising (Matlab Wavelet algorithm) processed to highlight the crack tip position. The velocity uncertainty is about 100 m/s when the crack tip position uncertainty is approximately 5 pixels (equivalent to 0.6 mm).

90 tests have been performed which show well repeatable results. When the pre-crack shapes can be precisely obtained, the SERR can be assessed at crack initiation through a finite element analysis. In this work, the pre-crack morphology is identified 'post-mortem' on fractography, as shown in Fig. 1a and b. The pre-crack front presents either an elliptical shape or a tilted straight front with respect to the two indentation techniques. Concerning the elliptical shape, the minor and major semi-axes (a and b) are around 0.8 and 2.8 times the specimen thickness (h). Note that after propagation the trailing edge of the crack (front part behind the 2.8 h semi-axis) is like a straight tail. Thanks to the pre-crack geometry and the measured fracture load, a numerical estimation of the SERR is performed with a finite element model using the commercial FE software Abaqus 6.13-4. The advantage of FE analysis is that the real crack front shape can be accurately taken into account, so the SERR at the crack tip in real experiments can be evaluated. The modeling is schematized in Fig. 1c. In order to limit the computing

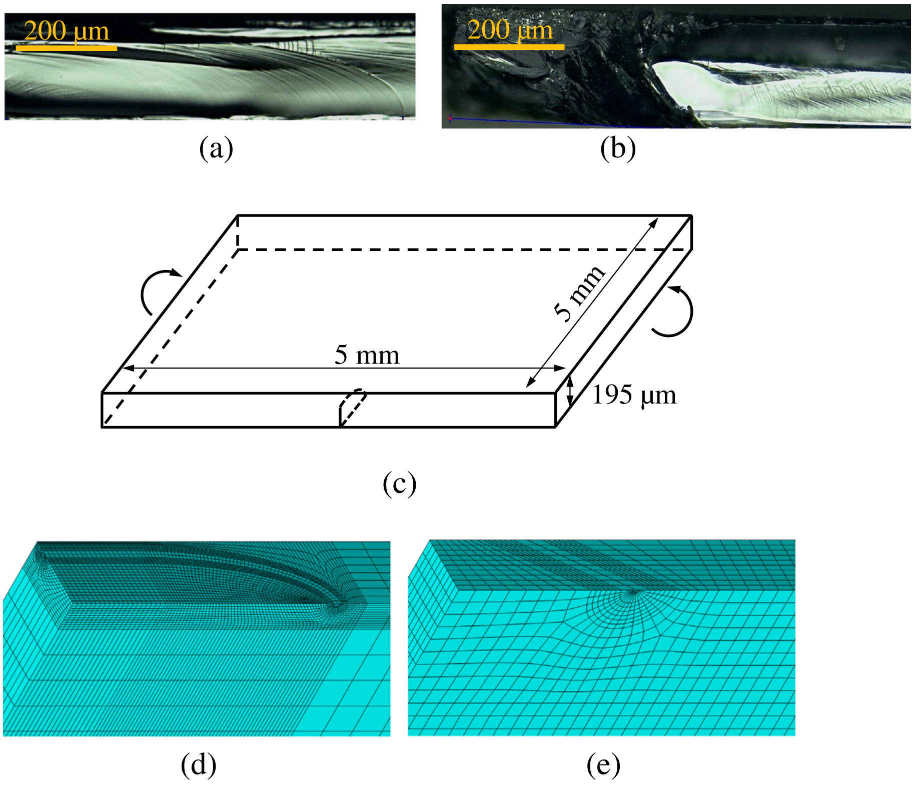

Fig. 1. SERR estimation with finite element analysis taking into account real pre-crack shapes. Crack propagation at a speed lower than 2900 m/s initiates from long elliptical pre-cracks (a), whereas cracks propagate at a speed higher than 2900 m/s from short straight pre-cracks (b), geometry and loading in finite element model for SERR assessment (c), modeling of pre-crack with elliptical front shape (d), and modeling of pre-crack with tilted straight front shape (e), with respect to the revealed pre-crack shapes in (a) and (b).