IMPULSIVE NUCLEATION AND FRACTURE OF BRITTLE MATERIALS BY NONLINEAR SURFACE ACOUSTIC WAVES

P. Hess, A.M. Lomonosov, and T. Lucza
Institute of Physical Chemistry
University of Heidelberg
Im Neuenheimer Feld 253
D-69120 Heidelberg, Germany

ABSTRACT

Nonlinear surface acoustic wave (SAW) pulses with shocks were used to nucleate cracks in brittle materials such as single-crystal silicon, quartz crystals, and fused quartz. The strongly nonlinear elastic surface pulses were excited with pulsed laser radiation and detected with a continuous-wave (cw) laser employing the probe beam deflection method. These SAW pulses with finite amplitudes develop steep shock fronts and spikes during propagation with strains in the 10^{-3}–10^{-2} range that break most chemical bonds. The resulting impulsive nucleation of dynamic fracture occurs without an artificial seed crack, and therefore the technique can be used to study the intrinsic initiation of failure in materials. A single SAW pulse generates a large field of small surface cracks with similar shape. Crack extension along the surface was detected by scanning force microscopy (SFM) and optical microscopy. The penetration of cracks into the solid was studied by the focused ion beam (FIB) technique in silicon and confocal laser microscopy (CLM) in transparent fused and crystalline quartz. In anisotropic crystals the nucleation process launches cracks propagating along the weakest cleavage planes of the crystal. In isotropic materials crack evolution depends on the temporal and spatial variation of the stress field, controlling the movement of the crack tip. By taking into account the stress field of the elliptically polarized SAWs and the tendency of the crack tip to maintain pure tensile stress conditions, crack propagation in fused quartz can be explained.

1 INTRODUCTION

Laser-generated nonlinear surface acoustic wave (SAW) pulses provide a novel tool for studying the nonlinear elastic and mechanical properties and mechanical failure of materials, such as brittle isotropic solids and anisotropic crystals. During propagation, finite-amplitude SAWs develop steep shock fronts or spikes due to the elastic nonlinearity of the material. If the locally applied internal stress exceeds the mechanical strength, dynamic fracture is observed. This localized initiation of impulsive cracking deviates from previous experiments, in which a global constant force was applied by external loading of macroscopic specimens. For this reason, only short cracks are expected in the present experiments, not complete destruction of the sample. In addition to the spatial localization of the applied stress there is a temporal localization due to the fact that the duration of the steep shocks and spikes is on the (sub)nanosecond time scale.

To initiate fracture processes with a pulsed laser no artificial notch or precrack is needed on the sample to achieve impulsive dynamic fracture of brittle materials. In fact, it is not the laser-induced excitation process but the bond disruption process that ultimately limits the achievable nonlinear SAW amplitudes to acoustic Mach numbers or strains of about 10^{-3}–10^{-2}. For this reason

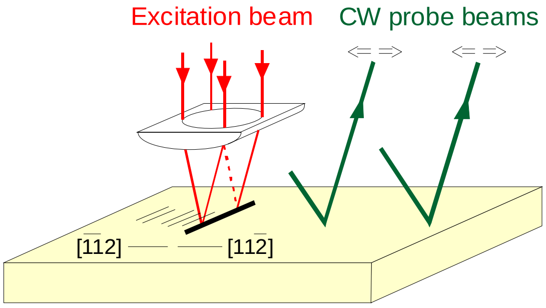

Fig. 1 Experimental setup used for detecting the effects of nonlinear SAWs propagating in the opposing directions [-1-12] and [11-2] on the Si(111) plane after pulsed excitation.

the initiation of fracture in many materials can be studied. The constant force technique, on the other hand, provides information on crack propagation and allows the measurement of the crack velocity to be compared with the limiting speed of tensile cracks, the Rayleigh velocity. Since it seems to be extremely difficult to reproduce the microscopic nature of the tip of an artificial seed crack, control of the initiation process at a molecular level may not be possible with this technique.

The intrinsic localized nucleation process is an important advantage of the impulsive method. A single SAW pulse can easily generate tens of crack nuclei during propagation. Obviously the nucleation conditions are satisfied at many locations and because the extension of the cracks is nonzero a whole crack field or pattern can be observed. The nucleation process leads to spontaneous fracture along preferred cleavage planes in anisotropic crystals or the cracks react dynamically to the transient stress field in homogeneous materials.

The particle displacements and stress field of a nonlinear SAW are characterized by a strong decay (essentially exponential) from the surface into the bulk. Crack nucleation is therefore expected to occur at the surface. Usually crack initiation takes place at the strongest defects at the surface, which could be surface steps, voids, impurities, or other disturbances in the surface region. After nucleation, the crack embryos simultaneously grow along the surface and into the bulk of the solid. Assuming that the cracks quickly accelerate to a reasonable fraction of the Rayleigh velocity, they can travel distances of several micrometers on the nanosecond time scale.

2 EXPERIMENT

Nonlinear plane SAWs were launched with a pulsed laser by the absorption-layer method. The absorption of laser radiation leads to explosive evaporation of the strongly absorbing layer and efficient excitation of elastic surface waves. The launched SAW pulses were detected at two different distances from the source by continuous-wave (cw) laser probe beam deflection, monitored with a position sensitive detector. The setup with pulsed laser excitation and cw laser detection is shown schematically in Fig. 1. By using the velocity waveform measured at the first probe spot as input, the SAW profile at the second probe spot was calculated and compared with the experiment. During nonlinear evolution of SAWs, frequency-up (pulse shortening) and frequency-down (pulse lengthening) conversion processes take place. In finite amplitude waves the stress increases and spikes or shock fronts are formed in the nonlinear waveforms during propagation due to the elastic nonlinearity of the material. In crystals such as silicon or quartz the magnitude of these nonlinear effects varies with the crystallographic plane and direction of SAW propagation and is described theoretically by nonlinear evolution equations. The theoretical treatment of nonlinear SAWs yields the configurations with the shortest shock formation distances, which are usually selected for dynamic fracture experiments.

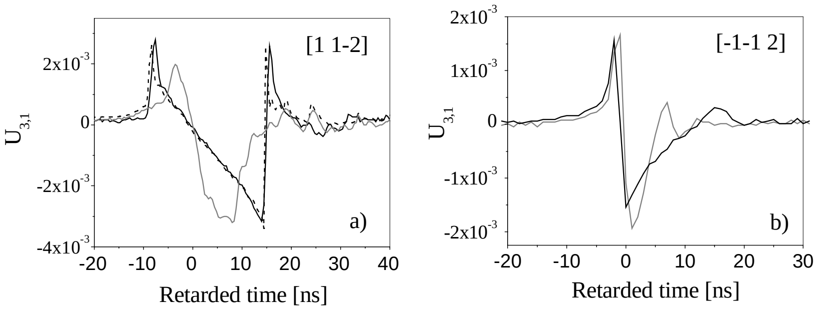

Fig. 2 Shear strain $U_{3,1}$ of the nonlinear SAW profiles on Si(111) for pulses propagating in a) the [11-2] direction and b) the [-1-12] direction. Gray solid lines: waveforms measured at 3 mm from the source; Black solid lines: waveforms measured at 18 mm; dotted line: calculated waveform.

The extension of the nucleated nanocracks into the micrometer range under the influence of the transient SAW stress field was detected at the surface by scanning force microscopy (SFM) in silicon and optical microscopy in the transparent samples. Crack penetration into the depth of the solid was studied by the focused ion beam (FIB) technique in silicon and by confocal laser microscopy (CLM) in the transparent samples.

3 RESULTS

3.1 Single-crystal silicon

The Si(111) plane and the <112> directions were selected for a series of experiments with silicon because of the high value of the coefficient of nonlinearity and the suppression of diffraction in this geometry. Moreover, the evolution of the SAW pulse can be accurately calculated, since the second- and third-order elastic constants are well known for silicon. Figure 2 shows the development of the velocity profiles measured for SAW propagation in the [11-2] and [-1-12] directions on Si(111) at the two probe spots. The surprising effect of very different pulse shapes generated in the two opposing directions is explained by the symmetry properties of the selected plane and directions in the anisotropic silicon crystal, without referring to the fracture process itself. As one can see from Fig. 2, nonlinear evolution leads to the formation of short spikes in the vicinity of the shocks. Their duration was comparable to the sampling rate of the detection technique applied, or, in other words, the finite bandwidth of the setup limited the accurate evaluation of the spike magnitude, and therefore the peak values of stress realized experimentally could be significantly larger than estimated from the measured waveforms.

SAW-induced cracks were detected at the surface by SFM, as shown in Fig. 3. A strongly nonlinear SAW pulse generates a whole series of cracks extending along <110> perpendicular to the direction of SAW propagation. The characteristic sawtooth-like surface displacements observed are in the range of 10–30 nm with a separation of the individual cracks of 15–30 µm. As can be seen, the elliptically polarized SAW pulse introduces not only tensile stress (opening, mode I, fracture) but also in-plane shear stress (sliding, mode II, fracture). Penetration of the crack into the bulk occurs along the {11-1}-cleavage plane, as shown by FIB experiments.

The pulse formed in the [-1-12] direction with a single shock is expected to induce fracture more easily along the weakest silicon cleavage plane than the one running in the opposite direction. Indeed, the SAW experiments revealed a significant difference in the conditions needed

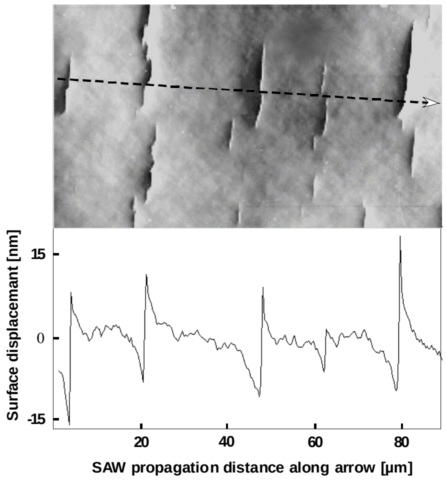

Fig. 3 SFM image of the fractured Si(111) surface. The arrow in the upper image indicates the SAW peopagation direction and the position of the surface profile shown in the lower image.

for crack initiation in these two directions. In the difficult crack direction fracture was observed only for excitation laser pulse energies exceeding 120 mJ, whereas in the opposite direction the threshold was as low as 30 mJ. Under suitable conditions cracks appeared only on one side of the source, namely in the [-1-12] direction and the wave propagating in the [11-2] direction could be used to calibrate the SAW amplitude. Thus the critical amplitude at the cracking threshold could be evaluated, yielding the critical tensile stress for the {11-1}-cleavage plane. From the spatial-temporal distribution of the stress at the cracking threshold, a critical tensile stress of about 1-2 GPa was extracted for the particular silicon wafer used.

This measured fracture stress may be compared with the theoretical strength of 22 GPa calculated for tensile stress oriented in the <111> direction. In the spirit of Griffith's theory this large deviation indicates stress amplifying microcracks located near the surface since crack initiation is expected to occur at the surface. In fact, defects and microcracks are generated predominantly near the surface during wafer production and polishing. For this reason, the possibly damaged surface region will be successively oxidized and removed in future experiments by chemical processing without introducing additional mechanical damage. The goal of these investigations is to find out whether the measured fracture stress approaches the intrinsic strength of silicon because the interior of the crystal possesses fewer defects. In principle, the SAW method allows spontaneous nucleation in defectfree materials, and therefore is suitable for measuring the intrinsic mechanical strength.

3.2 Quartz crystal

The present experiments were performed with trigonal α quartz. The propagation of nonlinear SAWs was investigated theoretically for different directions of the (100) surface (X cut), the (010) surface (Y cut), and the (001) surface (Z cut). Despite the fact that the piezoelectricity of the quartz crystal was neglected in these calculations of the SAW velocity and nonlinear coefficients, good agreement was found between measured and calculated SAW propagation speeds, indicating that the influence of piezoelectricity was relatively small. As an example, we consider the measurements of nonlinear SAW propagation in the [00-1] direction on the quartz (100) plane (X cut). At the first probe spot, about 1 mm from the laser excitation source, a bipolar pulse shape was observed, whereas at the second probe spot, about 15 mm from the first spot, the pulse profile

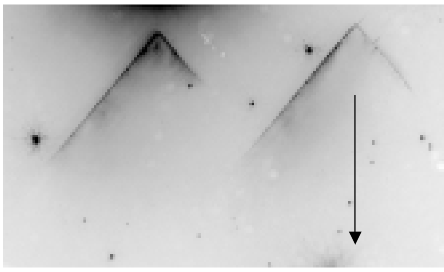

Fig. 4 Impulsive fracture of quartz on the (100) plane (X cut); the arrow indicates the propagation of the SAW pulse in the [00-1] direction.

essentially consists of a single sharp spike. Initiation of fracture occurred at several surface locations and led to V-shaped symmetric cracks propagating symmetrically along cleavage planes in the direction of SAW propagation, as presented in Fig. 4. The nonlinear SAW-pulse shapes, the shock formation distance, and the fracture behavior vary considerably with the particular configuration, namely the crystallographic plane and the direction on this plane.

3.3 Fused quartz

In fused quartz (Herasil I), a homogeneous amorphous material, characteristic U-shaped SAW pulses with two spikes develop during propagation, as can be seen in Fig. 5. Note that due to the limited bandwidth of the setup of about 500 MHz the magnitude of the measured spikes may be smaller than the real ones. Since the isotropic material has no preferred cleavage planes, unlike silicon and quartz crystals, fracture is expected to take place perpendicular to the direction of highest stress or strain for the simplest case of modeI behavior. In reality mode I and mode II cracking effects must be taken into consideration in impulsive fracture with elliptically polarized SAWs to rationalize the observed crack patterns with the calculated nonlinear SAW waveforms. Figure 6 shows part of the crack field at the surface generated by a single plane SAW pulse. Obviously impulsive fracture is initiated by an opening stress and initially occurs perpendicular to the SAW propagation direction. Due to the movement of the SAW pulse the stress field changes steadily. The cracks bend forward, symmetrically on both sides, into the direction of SAW propagation, extending into different angles and branches. The reason for this branching effect could be the relatively high stresses, resulting in high propagation velocities, in the impulsive fracture process.

Confocal laser microscopy, probing different depths indicates that crack extension into the solid proceeds with an angle of roughly 30°–35°, with respect to the SAW propagation direction. Theoretically it is expected that the evolution of the crack is stable if mode II loading is zero. Otherwise the growing crack tip changes its propagation direction to minimize the shear load and to maintain purely tensile conditions at the tip (mode I). In order to find the orientations for stable dynamic crack propagation, the angular dependence of the relevant shear stress component of the stress field must be determined. The angle calculated corresponds to a crack tilted inward at 30° from the surface into the direction of SAW propagation, even if initially crack nucleation occurred perpendicular to the surface, in agreement with the experiment.

4 DISCUSSION

The experimental results clearly demonstrate that nonlinear nanosecond SAW pulses allow the nucleation of cracks in isotropic and anisotropic brittle materials without any seed or precrack. This makes it possible to investigate homogeneous nucleation, as well as defect-induced initiation

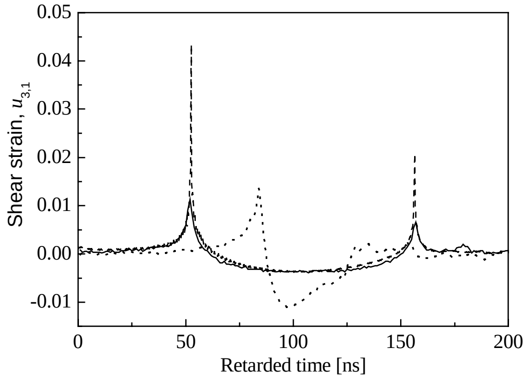

Fig. 5 Shear strain component $u_{3,1}$ of the nonlinear SAW profile for fused quartz at distances of 1 mm (dotted line) and 16 mm (solid line) from the line source. The simulated waveform for the 16 mm location is shown as a dashed line.

of crack propagation according to Griffith's theory. A comparison of the measured critical fracture stress with the calculated ideal fracture strength yields information on the microscopic nature of the nucleation process.

In several cases the tensile opening stress nucleated a crack perpendicular to the propagation direction of the plane SAW pulse. On the Si(111) surface, for a SAW pulse traveling in one of the <112> directions, the crack extended into the <110> direction. In quartz crystals a somewhat different behavior was observed. On the (001) plane (Z cut) in the [100] direction the crack propagated first for some time perpendicular to the SAW pulse but then proceeded at a certain angle along a cleavage plane in the SAW direction.

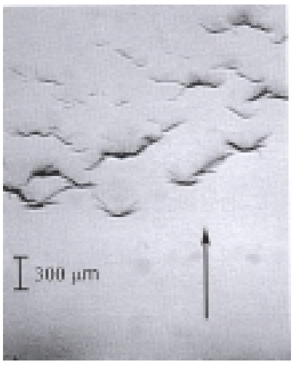

Fig. 6 Optical microscope picture of the characteristic crack pattern at about 2 mm from the SAW excitation line in fused quartz. The arrow indicates the SAW propagation direction.

The fracture behavior of strictly homogeneous materials, where weak paths or bonds of varying cohesive characteristics are excluded, is different. It is well known from remotely applied loading (far-field loading) that, at a crack speed of about 30–40% of the Rayleigh velocity, branching instabilities may be observed, where the initial mode I tip branches in two or even more crack paths. In the present near-field loading case with asymmetric dynamic loading conditions (mode I and mode II) the behavior depends on the temporal and spatial variation of the loading conditions.