FROM CONTINUUM TO QUANTUM MECHANICS STUDY ON THE FRACTURE OF NANOSCALE NOTCHED BRITTLE MATERIALS

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Abstract
The fracture of nanoscale notched brittle materials is investigated using the multi-scale analysis of cohesive zone modeling and first-principles calculations based on the notched nano-cantilever bending experiment. first-principles calculations are performed to investigate the inherent fracture properties of single-crystal silicon from atomic and electronic viewpoints. The fracture surface energy and critical bond length for the break of atomic bonds during the fracture are compared with the cohesive energy and failure length parameter, which indicates that the consumed energy is an effective linkage to quantify the fracture of brittle materials at different scales.

1. Introduction
Brittle semiconductors, such as silicon (Si) and gallium nitrides (GaN), have been widely applied in small-scale devices of modern technological applications due to their rich variety of exquisite functionalities, including electrical, piezoelectric, electro-mechanical, and optica properties at the nanoscale. Despite the wide applications, the mechanical failure of nanoscale brittle materials usually leads to a critical reliability issue and thus prevents the further miniaturization of small-scale devices. Thus, the precise evaluation of fracture properties of nanoscale brittle materials is highly important for the reliable design of small-scale components in advanced devices.

2. Results
Figure 1 shows the load-time curve and in situ observation of notched nano-cantilever specimen C1 during fracture experiment. As shown in Fig. 1(a), the applied load starts to linearly increase when the diamond indenter touches the free end of the cantilever. In addition, after the applied load reaches a maximum value, a sharp drop occurs and subsequently becomes zero, which indicates the total fracture of the specimen. From the in situ TEM observation in Fig. 1(b), it can be confirmed that the crack emerges at the tip of the nano-notch and immediately propagates through the lower part of the specimen, leading to the complete fracture of the specimen. Moreover, the deflection at the cantilever free end is precisely measured from the recorded videos in TEM. Similar fracture behaviors are observed in the other three specimens as well.

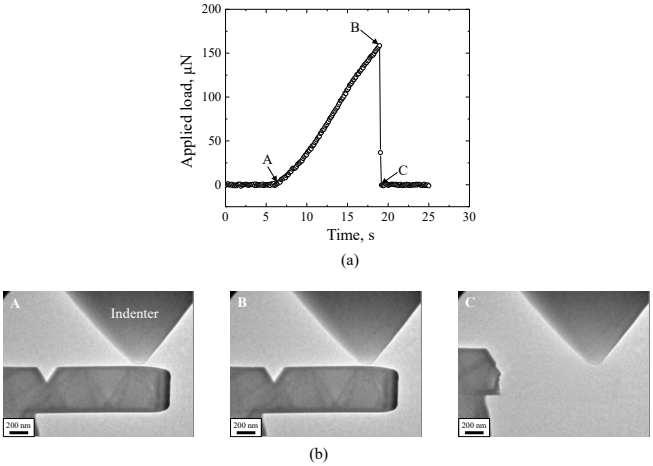

Fig. 1 (a) Load-time curve of specimen C1 during the experiment, and (b) in situ TEM observation of fracture behavior of notched nano-cantilever specimen.

The driven energies for fracture of small-scale and bulk single-crystal silicon obtained by current CZM simulation and previous conventional fracture mechanics are compared in Fig. 2. It should be noted that the fracture energy in previous and current studies was derived from the fracture experiment from the pre-crack and the nano-notch tips, respectively. Thus, the dimensions of concentration factors of stress fields near the crack and notch tip are completely different. However, the driven energies derived from CZM and conventional fracture mechanics of single-crystal silicon from nanoscale to macroscale are very close to each other. This indicates that the energy consumed during fracture of brittle materials can be an effective linkage to quantify the brittle fracture behaviors at different scales due to its closely physical relation to atomistic fracture process.

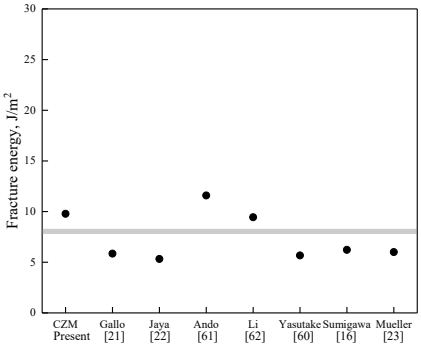

Fig. 2 Comparison of the driven energy for fracture of single-crystal silicon of nano- and macro-scale.

3. Conclusions

In summary, we investigated the fracture of nanoscale notched brittle materials with in situ TEM fracture experiments and multi-scale simulations including CZM simulation and first-principles calculations. The fracture behaviors of nanoscale single-crystal silicon were experimentally investigated using notched nano-cantilever specimens. By calibrating with the experimental load-deflection curve of one specimen, the parameters of bilinear CZM were precisely determined. In addition, the CZM parameters solely determined from one specimen accurately predicted the fracture in all other specimens regardless of geometric sizes, indicating the applicability of CZM for describing the fracture due to extremely small stress concentration. on the other hand, the inherent fracture properties of single-crystal silicon were obtained by first-principles calculations, which provided a lower limit of driven energy for the fracture by breaking the atomic bond. Finally, the cohesive energy was compared with fracture energy determined from fracture mechanics of nanoscale and bulk single-crystal silicon, and the fracture criterion of energy concept shows a universal validity for the fracture of brittle materials due to its close relation to the atomic bond strength.

This work provides critical insight into the fracture of nanoscale notched single-crystal silicon and offers an applicable experimental and analytical scheme to investigate the fracture of other brittle materials.

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