Engineering Fracture Mechanics 196 (2018) 113–122

Contents lists available at ScienceDirect

Engineering Fracture Mechanics

journal homepage: www.elsevier.com/locate/engfracmech

Unstable cracking behavior in nanoscale single crystal silicon: Initiation, unstable propagation and arrest

Kai Huang[a,b], Takashi Sumigawa[b,*], Licheng Guo[a,*], Yabin Yan[b,c], Takayuki Kitamura[b]

[a] Department of Astronautic Science and Mechanics, Harbin Institute of Technology, Harbin 150001, China
[b] Department of Mechanical Engineering and Science, Kyoto University, Kyoto 615-8540, Japan
[c] Institute of Systems Engineering, China Academy of Engineering Physics, Mianyang 621900, China

ARTICLE INFO

Keywords:
Nanoscale single crystal silicon
Unstable cracking
Fracture toughness
Arrest toughness
Specific surface energy

ABSTRACT

The unstable cracking behavior in nanoscale single crystal silicon, including initiation, unstable propagation and arrest, is experimentally observed by using a nanoscale trapezoidal-double-cantilever-beam method. A well-controlled multi-step cracking experiment is designed for accurately estimating both the fracture toughness K_{Ic} and the arrest toughness K_{Ia}. The experimental results show that the unstable cracking within a short range of hundreds of nanometers leads to an apparent decrease from K_{Ic} to K_{Ia}, i.e., $K_{Ia} < K_{Ic}$, and produces surprisingly clean crack surfaces with negligible energy dissipation. The specific surface energy of (0 1 1) cleavage plane in nanoscale single crystal silicon is accurately evaluated as $\gamma = 1.83$ J/m^2. These results provide a fundamental understanding of the unstable cracking behavior in a brittle material at the nanoscale.

1. Introduction

With the increasing demands for high-density integration, many electronic devices undergo great developments and miniaturization, and a variety of micro- and nano-electromechanical systems (MEMS/NEMS) consisting of small sensors and actuators for multifarious functions have been intensely developed [1–8]. However, fracture, a catastrophic mechanical failure of the components caused by mechanical loading or thermal expansion mismatch, is still a major resistance for further applications [9–11]. In these extremely small components, the sizes of the external structures themselves are approaching the order of nanoscale, while the internal structures are arranged atom by atom. In this case, the internal structures have a direct effect on the fracture mechanism of these nano-components, because the size of intensified stress region governing the fracture is comparable to that of the atomic arrangement. Hence, it is essential to directly explore the fundamental fracture mechanism at the nanoscale.

Based on the continuum mechanics theory, fracture mechanics is well established and succeeds in describing when and how a crack propagates. In the past decades, fracture behaviors in a variety of materials from macroscale to microscale have been widely investigated [12–17], verifying the excellent validity of this fracture mechanics concept. Many different experimental methods have been reported to determine the fracture toughness, such as displacement/load-controlled double cantilever beam (DCB) method [18,19], double torsion method [20,21], and indentation-based fracture method [22,23]. However, it still remains a major challenge as the component size shrinks ultimately down to nanometers.

On one hand, thanks to the remarkable progress made in computer capacities and atomistic calculations, such as molecular

* Corresponding authors.
E-mail addresses: sumigawa@cyber.kues.kyoto-u.ac.jp (T. Sumigawa), guolc@hit.edu.cn (L. Guo).

https://doi.org/10.1016/j.engfracmech.2018.04.014
Received 27 October 2017; Received in revised form 23 March 2018; Accepted 9 April 2018

Nomenclature

a	crack length before the unstable cracking
E	Young's modulus
G	energy release rate
G_a	critical energy release rate at arrest
G_c	critical energy release rate at initiation
K_I	stress intensity factor
K_{Ia}	arrest toughness
K_{Ic}	fracture toughness
M	kinetic energy accompanying the crack propagation
m	kinetic energy acceleration rate
m_a	kinetic energy acceleration rate at arrest
m_c	kinetic energy acceleration rate at initiation
o	energy dissipation
P	load
P_c	critical load
r	distance from the crack tip
U	elastic strain energy
W	external work
γ	specific surface energy
δ	opening displacement
δ_c	critical opening displacement
ΔA	area of new crack surfaces
Δa	crack propagation length
ΔS	absorbed surface energy
ΔU	released strain energy
σ_{xx}	normal stress near the crack tip
φ	diameter of the gold wire
BDT	brittle-to-ductile transition
DCB	double cantilever beam
DFT	density functional theory
FEM	finite element method
FIB	focused ion beam
MD	molecular dynamics
nano-TDCB	nanoscale trapezoidal-double-cantilever-beam
SEM	scanning electron microscope
TEM	transmission electron microscope

dynamics (MD) [24–27] and density functional theory (DFT) [28,29], it enables researchers to reproduce the fracture behaviors at the nanoscale with considerable precision. On the other hand, the fracture experiments at the nanoscale are, however, restricted by the difficulties stemming from specimen gripping and loading and displacement/load measurements. At an early stage, the interface strength of a thin film deposited on a substrate is examined by bending testing [30,31]. Nevertheless, except the thickness, thin films are still large enough in other dimensions. Based on the focused ion beam (FIB) and transmission electron microscope (TEM) techniques, specimens are further scaled down three-dimensionally to the nanoscale [32,33]. It is found that the crack initiation at the interface edge is governed by the nanoscale singular stress field, which means the conventional fracture mechanics is still valid on the order of 10 nm.

Compared with interface delamination, unstable cracking behavior in a brittle material at the nanoscale is undeveloped seriously

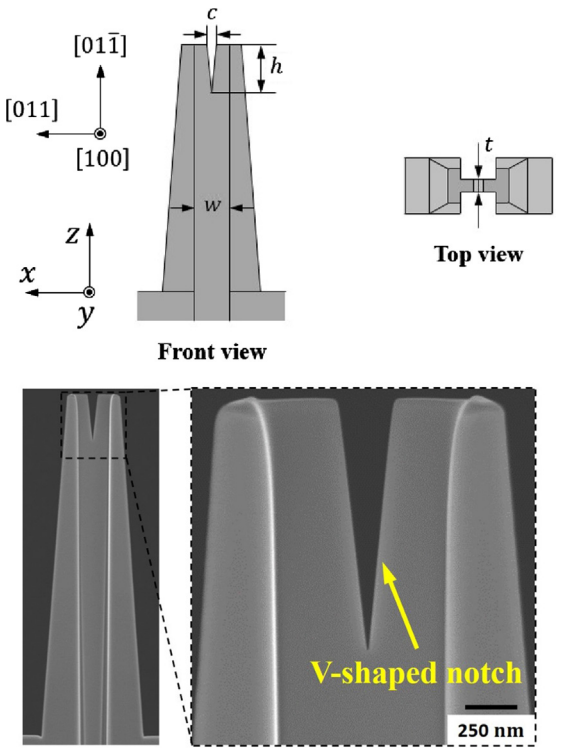

Fig. 1. Schematic of the nano-TDCB specimen and SEM image of Specimen 1.