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Critical dimensional limit of continuum fracture mechanics for dislocation emission

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ABSTRACT

One major elementary process in ductile failure is the emission of a dislocation from the crack tip, the criterion for which is well established within the framework of fracture mechanics and involves the intensity of the stress singularity appearing near the crack tip. The continuum-media postulate of fracture mechanics, however, might prevent us from predicting the failure of nanoscale materials, such as ultrathin films and nanowires, because the continuum concept becomes less plausible as the size of the region of interest approaches the atomic scale. Here, we examine the applicability and lower size limit of continuum fracture mechanics at the nanoscale in the case of dislocation emission, by conducting computational simulations that were modeling nanometer-scale Cu specimens. We find that fracture mechanics works successfully for singular fields larger than a few nanometers, but fails for singular fields smaller than 1.5–2.0 nm, i.e., the lower size limit of fracture mechanics for dislocation emission. We further demonstrate that this lower size limit is determined by the atomistic nature of the structural instability, suggesting that the limit depends on atomic-level phenomena at the crack tip.

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1. Introduction

The mechanical failure of materials is a physically inevitable phenomenon and industrially critical issue commonly exhibited by structures of all scales, so the fracture of materials is of central importance and interest in a variety of research fields, such as mechanical engineering, materials science, physics, geology, and biology [1–14]. Materials always contain defects and cracks, and the failure of materials usually originates at a crack tip, whose rapid growth and unstable propagation can result in global rupture of the entire structure. It is therefore critical to understand the mechanics of cracks in materials. Fracture mechanics [1], a theory of fracture, is based on the continuum mechanics theory, and can be used to determine when a crack will become mechanically unstable and start to propagate. The stress (or strain) concentrates near the crack tip and forms a singular field proportional to $r^{-1/2}$ (r is the distance from the crack tip), which leads to a strain energy concentration at the crack-tip, which in turn acts as a driving force for propagation. Such divergence of stress at the crack tip does not allow a simple determination of the critical condition as a maximum stress at a certain point, but as the intensity of the stress singular field (i.e., stress intensity factor K_I) has been proposed. A large number of experimental and computational fracture tests have been performed over the past few decades, which have demonstrated that the fracture mechanics concept can be successfully applied at scales ranging from meters to micrometers [1–16]. For instance, Hurford et al. [4] used the

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Nomenclature

a	*crack length*
a_0	lattice constants
C_{ij}	elastic constant
K_I	stress intensity factor
K_I^c	critical KI for dislocation emission
M	applied bending moment
P	applied load
W	specimen width
Λ_K	*K*-dominant region
Λ_d	region of discrete atomic deformation

concept of fracture mechanics to investigate eruptions arising from tidally controlled periodic openings of rifts on Enceladus, where the scale ranges from several to tens of kilometers. Livne et al. [5] performed direct and precise measurements of the near-tip fields of rapid cracks in polyacrylamide gels at meter scale. Beyond metallic and ceramic materials, Nalla et al. [6] demonstrated the application of fracture mechanics concept for the failure of human cortical bone in the range of millimeters. Zhang et al. [7] combined experiment and modeling verify the applicability of the classic Griffith theory of brittle fracture to graphene with the specimen size about several micrometers. Warner et al. [8] considered rate dependence of crack-tip processes to predict twinning trends in f.c.c. metals with sub-micrometer specimens. Investigations on failure mechanisms in a wide range of materials from microscopic to macroscopic scale have been extensively reviewed by Buehler and Keten [9]. Furthermore, fracture mechanics can be applied not only to simple brittle fracture but also to ductile failure, including the emission of dislocations from a crack tip [17–21]. Therefore, the singular stress field based on continuum fracture mechanics dominates phenomena at the crack tip regardless of the size of materials, although the nature of fracture behavior is ultimately determined by discrete events at the atomic scale, such as local bond breaking or switching [22,23].

The applicability of fracture mechanics, however, remains unclear at the nanoscale. It is well known that as the size of a material is reduced to nanometers, the singular stress field also shrinks proportionally to the nanometer scale [21,24–26], which involves only a few atoms. This situation contradicts the facture mechanics concept based on the continuum theory, which assumes a large enough number of atoms to regard even the crack-tip region as a continuum medium. This contradiction suggests the possible existence of a critical size at which the fracture mechanics concept is no longer applicable. To investigate whether or not such a critical size exists, precise computational fracture tests have been performed for nanometer-scale specimens consisting of a simple brittle material (Si). These tests demonstrated that fracture mechanics is rendered invalid when the singular stress field is confined to a region with the dimensions of less than 2–3 nm [27]. The results suggested that this critical size is determined by discrete atomic events in the vicinity of the crack tip (for the Si case: covalent bond breaking just as the crack becomes unstable). The critical size is therefore expected to strongly depend on the materials involved, and in particular, discrete atomic events at the crack tip. Although the previous studies have focused on ideal brittle fracture with a very simple event accompanying bond breaking at the crack tip, the applicability of fracture mechanics to a totally different fracture process with a more complicated atomistic event, e.g., dislocation emission from the crack tip, which is commonly observed in metals [8,28–31], is unclear and remains a major challenge.

Here, we investigate the applicability and lower size limit of continuum fracture mechanics with regard to the dislocation emission event at a crack tip by conducting computational tensile and bending experiments on nanometer-scale Cu specimens. We observed the breakdown of fracture mechanics at the nanoscale and determined the lower size limit to be 1.5–2.0 nm for dislocation emission. We then attempted to understand this lower size limit through a comparison with the characteristic size associated the atomic dislocation emission event.

2. Methodology

To perform ideal loading tests and precisely determine the critical loads for nanoscale to atomic-scale specimens with a pre-existing crack, we used molecular statics (MS) computational tests. We employed Cu as a representative face-centered cubic (fcc) metal because Cu is often used for the study of dislocation emission [8,30,32–35]. To investigate whether fracture mechanics based on continuum mechanics can be applied to dislocation emission from a crack-tip at the nanoscale, the stress distribution and stress intensity factor were analyzed by the finite element method (FEM) using the critical load determined by the MS loading experiments. Furthermore, we used atomistic instability mode analysis to provide atomic-level insight into the lower size limit for fracture mechanics.

2.1. Molecular statics simulations for loading tests in silico

We prepared nanometer-scale specimens of a Cu single crystal for the present fracture testing *in silico*, as shown in Fig. 1 (a). A pre-crack was introduced at the center of each specimen. The central crack length was 2*a*, which is one-third of the

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