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Effect of hydrogen on the collective behavior of dislocations in the case of nanoindentation

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ABSTRACT

Most of the studies reported treats the effect of hydrogen on single dislocation line, while models that describe the collective interaction are missing. In this study, hydrogen-induced softening of metallic materials is studied from a perspective of collective behavior of dislocations. Building on the evolution of dislocation density, a hydrogen-informed expanding cavity model is developed for the first time to predict the dynamic evolution of load-displacement curve obtained from nanoindentation tests. Large-scale molecular dynamics simulations on the mechanical behavior of fcc Ni with and without hydrogen (H) charged are performed to calibrate the proposed continuum model. The results show that the H-induced decrease of indentation force is due to that the energy barrier for dislocation nucleation is lowered by the solute drag of the H atmosphere formed around dislocations. Envisioned as a complex non-equilibrium process, it is found that the power-law exponent of the self-organized criticality of dislocations increases due to the insertion of H atoms. Analysis also indicates that H can reduce the probability of dislocation pile-up, thus promote the delivery of dislocations to the surface of specimens during nanoindentation.

1. Introduction

It is widely known that hydrogen interstitials in metallic lattice can induce damage of infrastructure materials, such as, high-strength steels, titanium alloys and aluminum alloys. Hydrogen embrittlement (HE) is often referred to as the sudden failure of system with H charged at a stress level much lower than the fracture strength, although in numerous studies it has also been used to stand for H-induced blistering, vacancy formation, etc. As to the embrittlement of non-hydride-forming metals [1], one of the most accepted HE mechanisms is the hydrogen enhanced decohesion (HEDE) [2–5], which suggests that the formation of an atomically sharp crack-tip is facilitated due to the H-induced bond weakening. Under the framework of HEDE mechanism, dislocation activity is allowed, but has to be fairly limited so that the crack tip will not be blunted. However, with the development of advanced *in-situ* imaging and characterization techniques, it has been revealed that H can actually promote the multiplication of dislocations, which is precluded in HEDE mechanism. Thus, the so-called hydrogen enhanced local plasticity (HELP) mechanism has been proposed to explain the observed localized slip bands [6,7] and enhanced dislocation motion [8–10] in H-charged specimens. Quote from the original definition by Birnbaum and Sofronis [11], HELP is based on the assumption that the inserted H atoms can shield the repulsive interaction between neighboring dislocations, thus can be used to address the easier dislocation slip behavior [12,13], reduction of yield stress [14–16] and some other softening phenomenon [17,18] under H environment. However, H-induced increase of flow stress experimentally observed in Fe alloys [19–22], Al [23] and Ni alloys [24,25] challenges the validity of HELP. Theoretically, using the nudged elastic band method, Wen et al. [26] studied the effect of hydrogen on the kinking process of a screw dislocation in bcc Fe and found that the activation energy is decreased (increased) by the transition of hydrogen to a stronger (weaker) binding site. This work firstly provides atomistic evidence for the hydrogen-induced softening and hardening behavior. By applying a Monte Carlo procedure to generate equilibrated H atmosphere around an edge dislocation in bcc Fe, Bhatia et al. [27] observed the H-induced increase of Peierls stress. In order to comprehensively understand the

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atomistic mechanism of HELP, Song and Curtin [28] performed large-scale atomistic simulations to study the hydrogen-dislocation interaction in bcc Fe. Their results show that the Cottrell atmospheres are generated around moving dislocations, thus the dislocation mobility is reduced in contrast with the core assumption of HELP. It can be found that contradictory conclusions about whether the dislocation mobility is enhanced or reduced by hydrogen emerge from a large number of experimental and simulation studies. In a recent kinetic Monte Carlo study of the HELP mechanism, Katzarov et al. [29] have demonstrated that the effect of hydrogen on the velocity of screw dislocation in bcc Fe is sensitive to the external environment, i.e. the applied stress, temperature and hydrogen concentration. This study may shed a new light to finally understand the effect of hydrogen on dislocation mobility and subsequent influence on the mechanical response of materials. It should be noted that all these theoretical studies have been dedicated to investigate the effect of H atmosphere on the motion of single dislocation line, and no related researches have been performed to explore the H influence on the collective behavior of dislocation networks after hydrogen atoms are charged. As demonstrated by Zhu et al. [30], for the laboratory experiments with specimen size at or even larger than sub-μm scale, the large activation volume will lead to the commonly observed rate-insensitive collective behavior of dislocation networks. Envisioned as a complex non-equilibrium process, recent experimental and theoretical studies [31–35] have demonstrated the intermittent and *power-law* behaviors caused by *avalanches* of dislocations motion in plastic deformation. The *power-law* distribution is reminiscent of *self-organized criticality* (SOC), which is a property of dynamical systems displaying the spatial and/or temporal scale-invariance characteristic. The well-known Abelian sandpile model (also known as the Bak-Tang-Wiesenfeld model) [36,37] has been proposed to provide a phenomenological explanation for the SOC phenomenon observed in a wide range of dynamical systems from stock markets to sand dunes. While extensive studies [31,38] have been performed to study the dislocation avalanches in pure metals, no studies have been reported to illustrate the SOC behavior of dislocations under H environment. This work aims to capture the effect of H atoms on the power-law feature of small-scale plasticity.

Due to the characteristic length of the specimen beneath a nanoindenter is on the magnitude of the mean distance between dislocations, nanoindentation experiment can provide deep insight about the small-scale plastic behavior after elastic instability. The basic procedure of a nanoindentation process can be described as following: (a) elastic stage, an indenter with given geometry is pushed into the specimen surface, during which the maximum shear stress beneath the contact interface is lower than the critical resolved shear stress at any slip systems; (b) plastic stage, the dislocation emission is activated, and a characteristic phenomenon is the occurrence of sharp drop on the force-depth curve. While the traditional Hertzian model [39] can be used to describe the elastic response as a function of indentation depth, no corresponding model can be applied to predict the plastic response. In the study of nanovoid, Krasnikov and Mayer [40] have proposed a dislocation density based method to evaluate the void growth through the generation and slipping of dislocations. First established from Hill's solution for the quasi-static expansion of an internally pressurized spherical shell [41], the expanding cavity model (ECM) [39] has been proposed to describe the indentation deformation by considering a hemi-spherical core beneath the indenter. It is assumed that this core is surrounded by a hemi-spherical plastic region outside. Thus, it is reasonable to draw a parallel between the growth of nanovoid and evolution of nanoindentation process, and a similar dislocation density based model [42] can be developed for nanoindentation with a spherical indenter. Furthermore, it is shown that H atoms can facilitate the homogeneous nucleation of dislocation loops [43]. Unlike a straight dislocation line, the dislocation loops formed beneath the indenter do not have a long-range stress field and can only trap H atoms near plastic deformation zone in the ECM model. Without doubt, the distribution of H atoms around a dislocation will affect its energetics and core structure, and thus the mobility [27,28,44–49]. As reviewed above, the effect of hydrogen on the mobility of dislocations is still under controversy, while the hierarchical multiscale modelling [50] has illustrated that, even low H concentration of ~1 at-% in Ni single crystal will lead to a large reduction of HDN energy barriers. Therefore, in this study we will avoid to involve the dislocation mobility explicitly under hydrogen environment, but rather use the nucleation dynamics to drive the evolution of dislocation networks.

Specifically, we developed a theoretical framework based on the evolution of dislocation density to directly predict the elastic-plastic response of metallic materials under nanoindentation, simultaneously considering the kinetic diffusion of H interstitials from region far away from the contact surface. The basic assumption is that the diffused H atoms will finally be trapped in the plastic zone in Fig. 1, and contribute to lower the energy required for the formation of the dislocation loop emitted from the contact surface. The main goal of this paper is to understand the effect of H atmosphere on the *collective behavior* of dislocation networks using the Abelian sandpile model [36,37] and to establish a hydrogen-informed expanding cavity (HEC) model. Large-scale molecular dynamics (MD) simulations are performed to calibrate and verify the proposed continuum model. The manuscript is organized as follows: atomistic simulation details and analytical framework are given in Section 2; numerical results are discussed in Section 3; discussions are made in Section 4.

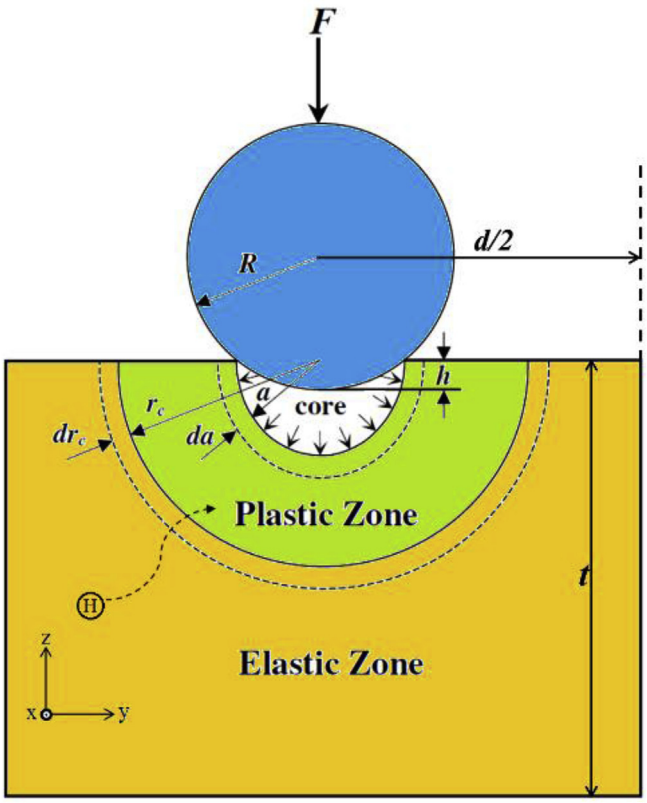

Fig. 1. Schematic illustration of a nanoindentation system under H environment.