Journal of the Mechanics and Physics of Solids 90 (2016) 18–28

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

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

Crack tip blunting and cleavage under dynamic conditions

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ARTICLE INFO

Article history:
Received 4 August 2015
Received in revised form
11 December 2015
Accepted 22 February 2016
Available online 27 February 2016

ABSTRACT

In structural materials with both brittle and ductile phases, cracks often initiate within the brittle phase and propagate dynamically towards the ductile phase. The macroscale, quasistatic toughness of the material thus depends on the outcome of this microscale, dynamic process. Indeed, dynamics has been hypothesized to suppress dislocation emission, which may explain the occurrence of brittle transgranular fracture in mild steels at low temperatures (Lin et al., 1987). Here, crack tip blunting and cleavage under dynamic conditions are explored using continuum mechanics and molecular dynamics simulations. The focus is on two questions: (1) whether dynamics can affect the energy barriers for dislocation emission and cleavage, and (2) what happens in the dynamic "overloaded" situation, in which both processes are energetically possible. In either case, dynamics may shift the balance between brittle cleavage and ductile blunting, thereby affecting the intrinsic ductility of the material. To explore these effects in simulation, a novel interatomic potential is used for which the intrinsic ductility is tunable, and a novel simulation technique is employed, termed as a "dynamic cleavage test", in which cracks can be run dynamically at a prescribed energy release rate into a material. Both theory and simulation reveal, however, that the intrinsic ductility of a material is unaffected by dynamics. The energy barrier to dislocation emission appears to be identical in quasi-static and dynamic conditions, and, in the overloaded situation, ductile crack tip behavior ultimately prevails since a single emission event can blunt and arrest the crack, preventing further cleavage. Thus, dynamics cannot embrittle a ductile material, and the origin of brittle failure in certain alloys (e.g., mild steels) appears unrelated to dynamic effects at the crack tip.

1. Introduction

Tough structural metals are often composed of a ductile matrix phase and brittle inclusions or precipitates. Cracks initiate in the brittle phase and should be arrested when they encounter the ductile phase. Since such cracks run dynamically in the brittle phase after initiating from pre-existing flaws, the dynamic response of the system may govern the macroscopic "quasi-static" toughness (Hack et al., 1989; Cox et al., 2005). One important example is mild steel, where cracks develop within grain boundary carbides and propagate dynamically toward the primary α-ferrite grains. At sufficiently low temperatures, these cracks are often observed to cleave through the ferrite, resulting in an undesirable, low-toughness, transgranular mode of failure (Lin et al., 1987). Although referred to as "brittle", this mode of fracture is more accurately

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http://dx.doi.org/10.1016/j.jmps.2016.02.014
0022-5096/

termed "semi-brittle": the fracture toughness greatly exceeds the Griffith energy, and the fracture surfaces are not atomically flat (Lin et al., 1987). Moreover, the length scale of the fracture process zone greatly exceeds that expected for ideal, Griffith fracture.

One model for semi-brittle fracture in steels focuses on the dynamic aspect of crack growth from carbide to ferrite (Lin and Thomson, 1986; Lin et al., 1987). Freund and Hutchinson (1985) showed that for a visco-plastic material, the critical energy release rate for a static crack is orders of magnitude larger than that for a dynamic crack, since the large strain rates and correspondingly high yield stresses associated with dynamic crack growth considerably reduce the energy dissipated via plasticity. The semi-brittle fracture energy may still be significantly larger than the Griffith energy, however. Thus, a dynamic crack originating within a second-phase carbide could propagate dynamically through the surrounding ferrite grains. If the crack emits dislocations, causing it to blunt and arrest, the dynamic argument breaks down or requires an unknown mechanism for steady growth of a blunt crack. Thus, an additional assumption may be implicit in this dynamic model for semi-brittle fracture: notably, that crack-tip dislocation emission is unfavorable for a dynamic crack (Lin and Thomson, 1986). This idea borrows from the classical Rice–Thomson framework for the "intrinsic ductility" of materials (Rice and Thomson, 1974; Rice, 1992), wherein the toughness of a material is governed by the competition between two different crack tip deformation modes, Griffith cleavage and dislocation emission/crack blunting. In an intrinsically brittle material, the crack tip should cleave before blunting by dislocation emission; conversely, in an intrinsically ductile material, dislocation emission and attendant blunting should precede cleavage. Thus, expressed in terms of the Rice–Thomson framework, the dynamic fracture model seems to require that dynamics alters the crack-tip competition, transforming a nominally "Rice-ductile" material into a "Rice-brittle" material.

The competition between deformation modes of a dynamic crack tip is therefore an issue of both engineering relevance and scientific interest. One fundamental question is how the dynamic crack behaves when the energy release rate G, or stress intensity factor K, exceeds both the Griffith cleavage value and the dislocation emission value. Is it possible that cleavage is preferred over dislocation emission in such an "overloaded" dynamic condition, even though dislocation emission is preferred under quasistatic conditions? There is no theoretical basis for the supposition that a dynamic crack prefers to cleave rather than to blunt. Lin and Thomson (1986) analyzed the role of dynamics in the context of the classical Rice–Thomson analysis (Rice and Thomson, 1974) in mode III loading, and found that dynamic effects were negligible when the slip plane was inclined relative to the crack plane. Furthermore, as we show in Section 2, the more rigorous, energy-based analysis of Rice (1992) yields a similar conclusion in mode II: the criterion for dynamic dislocation emission is *identical* to that for quasi-static emission. Thus, even when its speed is nonzero, the energy barrier to dislocation emission from a crack tip is $G = \gamma_{us}$, where γ_{us} is the unstable stacking fault energy for slip (Rice, 1992). However, it is also possible that atomic-scale effects are important. It is well-known that continuum fracture mechanics is unable to explain many important fracture phenomena, including lattice trapping (Rice, 1978; Curtin, 1990; Thomson et al., 1971), crack tip instabilities (Fineberg et al., 1991; Fineberg and Marder, 1999; Buehler et al., 2003; Buehler and Gao, 2006), and crack velocities in steady-state (Marder and Gross, 1995), all of which depend intimately on the details of bonding between atoms (Marder, 2004). Atomistic simulations have therefore become increasingly popular for studying crack tip deformation mechanisms and their implications for ductility (Li et al., 2003), both in quasi-static (Wu and Curtin, 2015; Warner and Curtin, 2009; Pérez and Gumbsch, 2000; Hung and Carter, 2011) and dynamic (Holland and Marder, 1998; Hauch et al., 1999; Kermode et al., 2008; Marder, 2006) conditions. In the latter case, *model* interatomic potentials have found great utility in molecular dynamics simulations (Holian and Ravelo, 1995; Gumbsch et al., 1997; Zhou et al., 1998; Abraham et al., 1998, 2002; Buehler et al., 2003; Buehler and Gao, 2006). Although such potentials do not correspond to any specific real material, they help to elucidate the general principles governing crack tip behavior and fracture, such as "hyperelasticity" (Buehler et al., 2003; Buehler and Gao, 2006). Our work here is pursued within the same framework of providing insight into general question in dynamic fracture.

We use molecular dynamics simulations to investigate the influence of atomic details and properties on the dynamic behavior of cracks in ductile materials. Specifically, we assess whether dynamics can suppress dislocation emission in a nominally ductile material, as seems to be implicit in the aforementioned model for semi-brittle fracture. To study this problem in a controlled manner, we employ a family of novel interatomic potentials for which the intrinsic ductility is *tunable* (Rajan et al., 2016). Specifically, for all potentials, the lattice constant, elastic constants, and fracture surface energy are held constant, so that the critical energy release rate for cleavage, G_{Ic}, is fixed. However, the unstable stacking fault energy γ_{us} can be independently varied to tune the critical energy release rate for dislocation emission, G_{Ie}. This allows us to conduct a "dynamic cleavage test" in which a crack initiates within a brittle material and runs dynamically into a second material (typically ductile). We find that dynamics *cannot* embrittle a ductile material; that is, if a crack tip at rest emits dislocations, then the same crack tip in motion will also emit dislocations. Our study focuses on the competition between brittle cleavage and dislocation emission at zero temperature. Although dislocation emission is a nucleation process, the energy barrier increases rapidly with decreasing applied stress intensity (Rice and Beltz, 1994; Zhu et al., 2004; Warner and Curtin, 2009) so that the critical stress intensity at 0 K is a good measure of the behavior at finite temperatures and finite strain rates. Furthermore, in the dynamic situation where cracks are running at speeds comparable to the wave speed, the time for nucleation is negligible so that thermally-assisted nucleation is not expected to be significant.

The remainder of this paper is organized as follows. In Section 2, we present the continuum analysis of dislocation emission and cleavage under quasistatic and dynamic conditions. In Section 3, we conduct molecular dynamics simulations of the dynamic cleavage test described above. In Section 4, we discuss our results in the context of the competition between