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On the influence of crack front curvature on the fracture behavior of nanoscale cracks

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ABSTRACT

Atomic-scale fracture processes are traditionally investigated in quasi-2D models of straight, infinite cracks. This approach neglects crack front curvature effects, which might be particularly important for nanoscale crack nuclei in semi-brittle materials. Here we use 3D atomistic simulations to study penny-shaped cracks in body-centered cubic metals. Our results show extensive crack tip plasticity initiated by deformation twinning and followed by emission of screw dislocations which cross-slip along the crack front. Together with the interactions of dislocations and/or twins that are nucleated at differently oriented parts of the crack, these processes determine the fracture behavior of highly curved nanoscale cracks.

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1. Introduction

Traditionally, fracture mechanics mainly considers two plane states – plane stress and plane strain – thereby making the equations more amenable to an analytical solution [1]. Such essentially 2D theories have been very successful in describing fracture and fatigue on the macroscale where the crack front can often be approximated by a straight line. However, when the crack front is curved, the three-dimensional character of the crack problem must be taken into account. Nanoscale crack nuclei are a prime example for highly curved cracks, but crack front curvature effects play also an important role in the micromechanics of crack advance in locally heterogeneous brittle solids [2]. The treatment of curved cracks by linear elastic fracture mechanics is well established, both analytically [3–5] and by numerical methods [6–8]. The underlying models usually assume isotropic fracture behavior. Contrary to this assumption, many crystalline materials show a direction dependent fracture toughness [9,10], even for purely brittle fracture [11,12] and in case of grain boundary fracture [13,14]. It is well known that the orientation of dislocation slip systems with respect to the crack front is one of the determining factors whether an existing crack will blunt or propagate by brittle cleavage [15,16]. The influence of crack front curvature on crack tip plasticity has however not yet been systematically investigated.

Gaining insights in the factors controlling crack tip plasticity is of particular importance for understanding the fracture behavior of semi-brittle materials like many body centered cubic (bcc) metals, intermetallic phases and semiconductors [17–21]. These materials show a transition between brittleness at low temperatures or high strain rates and ductility at high temperatures or low strain rates. This brittle-to-ductile transition (BDT) is caused by the competition between bond breaking processes at the crack tip and the mechanisms that govern crack tip plasticity [19,21]. The temperature and strain rate dependence of the BDT have been shown to be mainly determined by the mobility of dislocations [19,22,23]. However,

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Nomenclature

2D	two-dimensional
3D	three-dimensional
a	crack radius
a_0	lattice parameter
b	Burgers vector
bcc	body-centered cubic
$c_{x,z}$	center of penny-shaped crack in x- and z-direction
E^*	effective Young's modulus
E_{pot}	potential energy
h	center of penny-shaped crack in y-direction
$L_{x,y,z}$	box size in x, y, z-dimension
ε_0	calculated fracture strain for a finite simulation box
ε_{crit}	determined fracture strain by atomistic simulations
ε_G	theoretical fracture strain according to the Griffith
ε_{yy}	applied strain in y-direction
$\dot{\varepsilon}_{yy}$	strain rate in y-direction
$\gamma_{surface}$	surface energy
γ_{usf}	unstable stacking fault energy
γ_{ut}	unstable twinning energy
ν	Poisson's ratio

the fracture toughness is known to critically depend on the quality of the crack front, in particular on the availability of dislocation sources at the crack front [19,22,24]. By changing the orientation of the crack front relative to the glide systems, crack front curvature can lead to the activation of new dislocation sources. This effect was demonstrated in recent atomistic simulations of the interaction of a propagating crack with obstacles [25,26]: the local crack front reorientation caused by the interaction with obstacles enabled the emission of blunting dislocations from the crack tip which was not possible for the original crack front orientation. These simulations allowed to explain the differences in the observed dislocation sources in static and dynamic fracture experiments in silicon [24,27,28].

Brittle fracture as well as dislocation nucleation ultimately involves the breaking of atomic bonds. Atomistic simulations methods have therefore played an important role in the study of fracture toughness and crack propagation, see e.g. [26] for a recent review. Most of the studies on dislocation nucleation at crack tips make use of periodic boundary conditions (PBC) along the crack front direction and simulate only straight crack front segments of minimal lengths [29–38]. Such essentially 2D setups neglect crack propagation by kinks [39] as well as dislocation emission on oblique glide planes. The study of dislocation nucleation from crack tip defects like ledges [40,41] requires to simulate long crack fronts and thus involves large numbers of atoms, which are often modeled using semi-empirical interaction models. The local environment at a crack tip, however, strongly deviates from the equilibrium bonding situation, and many otherwise reliable potentials fail to reproduce the fracture of specific materials [37].

Fully 3D simulations of cracks with curved crack front were only recently reported. Ersland et al. [42] investigated the fracture behavior of penny-shaped cracks on {100}, {110}, and {111} planes in bcc-Fe and found that these cracks were generally more prone to develop extensive crack tip plasticity than through-thickness cracks. For ⟨110⟩ and ⟨112⟩ oriented crack front segments, the formation of deformation twins and dislocations were observed in penny-shaped as well as through-thickness cracks. These observations agree well with other simulations on Fe using quasi-2D setups [33–35]. In contrast, cracks on {100} and {110} planes with infinitely long, straight crack fronts oriented along a ⟨001⟩ direction were shown to propagate by brittle cleavage [42], in agreement with other quasi-2D simulations [30,36–38]. Ersland et al. attributed the suppression of unstable cleavage crack propagation to limited local crack propagation, which changes the shape of penny-shaped cracks in such a way that slip systems become more easily activated [42]. The developing plastic zone around the penny-shaped cracks was however not analyzed in detail.

This paper follows a similar approach as Ersland et al. [42], but with emphasis on the development of the plastic zone and in particular on the interaction of dislocations or twins emitted from different segments of the crack front with each other or with the crack front. To this end, crack front reorientation effects were suppressed by studying blunted cracks. The potential by Ackland et al. [43] used in Ref. [42] furthermore shows the formation of planar faults at cracks on the natural {010} cleavage plane of bcc-Fe. The formation of such faults is however not observed in recent density functional theory (DFT) calculations [44], and assumed to result from inadequacies of the potential [37]. While considering a range of materials and orientations helps to reduce artifacts associated with the choice of potential, it cannot entirely avoid them, which is why the consideration of a range of interatomic potentials (as was done in this work) is also important. This allowed us to show that – independent of changes of the crack shape – penny-shaped cracks indeed display predominantly ductile deformation

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