



# Atomistic-based predictions of crack tip behavior in silicon carbide across a range of temperatures and strain rates

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## Abstract

The utility of silicon carbide (SiC) as an engineering material is often limited by its brittleness. This work attempts to better illuminate the key mechanisms associated with this property by studying crack tip behavior. A multipronged investigative approach is taken, utilizing direct molecular dynamics simulations with empirical potentials, analytic modeling and electronic structure calculations. This approach enables us (i) to make atomistic-based predictions of the key mechanisms that occur at a SiC crack tip across a wide range of temperatures and strain rates; and (ii) to better understand the strengths and deficiencies of these analysis tools for predicting fracture in covalently bonded materials.

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## 1. Introduction

Silicon carbide (SiC) has drawn significant attention because of its impressive thermal, mechanical and electrical properties. It has a high melting temperature, thermal conductivity, stiffness, hardness, electron mobility and a large band gap. SiC resists corrosion and creep, while having a low thermal expansion coefficient and low density. This collection of properties makes SiC an attractive material for new technologies that require high performance in extreme environments [1–5]. However, the utilization of SiC's impressive properties is often hindered by its susceptibility to fracture. This challenge has motivated a long quest to better illuminate the mechanisms that control crack growth in SiC, with the aim of improving mechanical failure prediction and possibly even illuminating new means for improving its fracture resistance.

SiC is brittle at room temperature. Fracture experiments on single crystals report a fracture toughness ( $K_{IC}$ ) of 3.2–3.3  $\text{MPa}\sqrt{\text{m}}$  [6,7], a value that is larger than the  $K_{IC}$  associated with the surface energy, 2.0  $\text{MPa}\sqrt{\text{m}}$ .<sup>1</sup> While this indicates that surface energy plays an important role in the room temperature  $K_{IC}$  of SiC, it also suggests that other energy dissipation mechanisms may be important. Transmission electron microscopy (TEM) observations suggest that small amounts of plasticity may occur near the crack tip, as an increased density of dislocations have been observed near fracture surfaces [8]. This limited room-temperature plasticity is thought to involve full dislocations residing on the shuffle set of the close-packed planes [9].

With increasing temperature, plasticity is thought to play a larger role in the fracture and deformation process. At intermediate temperatures (423 °K), a significant population of partial dislocations has been observed on the glide set of

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<sup>1</sup> Our electronic structure calculations predict a surface energy of  $\gamma_s = 4.2 \text{ J m}^{-2}$  on the close-packed fracture plane, as described in the Appendix.

close-packed planes [10]. While these partial dislocations are thought to be more mobile at elevated temperatures, the macroscopic response of SiC in this temperature range is still brittle. This is attributed to the trailing partial dislocations being largely immobile; thus, a scenario exists where plastic slip fills the material with stacking faults [11] inhibiting further plasticity. At higher temperatures, the macroscopic response undergoes a brittle-to-ductile transition (BDT) due to increased mobility of the trailing partial dislocations on the glide set of the close-packed planes. While the BDT temperature depends on strain rate, it is generally reported to occur at a temperature between 1400 and 2000 °K, depending on the specifics of the material and the test [9,12]. The increased mobility of dislocations above the BDT temperature also affects the fracture toughness. For instance, Henshall et al. [6] reported an increase in  $K_{IC}$  of slightly more than a factor of  $\sqrt{2}$  when the temperature is increased from 1000 to 1400 °K in single-crystalline 6H-SiC.

The objective of this paper is to report on our investigation into the mechanisms that control crack tip behavior in SiC. Using molecular dynamics (MD) simulations with empirical potentials, we have directly examined the crack tip processes across a range of temperatures and strain rates. The MD simulations revealed a collection of crack tip mechanisms, including cleavage on the {111} plane and dislocation nucleation and glide on the {111} and {100} planes. Acknowledging the brief timescale inherent to MD simulations and inaccuracies in the empirical potentials, a significant disconnect can exist between the MD results and real-world SiC behavior. To address this point, the MD results were examined with simple analytic models and high-fidelity electronic structure calculations. This multifaceted modeling approach served not only to illuminate the atomic processes that occur at a crack tip in SiC, but to also establish the utility of a hierarchical modeling approach whereby material parameters, calculated with electronic structure calculations, are fed into popular analytic models to predict the crack tip response in SiC.

## 2. Simulation setup

The orientation of the crack, load and crystallography can have a significant effect on crack tip response [13]. The orientation studied here was selected following the subsequent line of reasoning. The geometric features of typical engineered structures are large relative to the size and density of microscopic defects in the material. Thus, one can safely assume that the highly stressed regions of a component encompass a population of microscopic material defects. Accordingly, it is then the growth of the most critical microscopic material defect that leads to the formation of a macroscopic crack, ultimately leading to structural failure. Simplifying the material defects to be microscopic cracks, we assume that the important microscopic cracks reside on the low surface energy close-packed planes and the greatest principle stress is normal to the crack plane.

Following this line of reasoning, we began this work by performing MD simulations of 3-D 3C-SiC single-crystal specimens with a (111) penny crack in their center. Tensile stress was applied normal to the crack plane. Upon reaching a critical load, dislocations nucleated from three locations, each having the crack front parallel to  $\langle 110 \rangle$  directions, where the crack tip was coincident with the inclined {111} planes. Thus, the mode I stress intensity factor ( $K_I$ ) for dislocation nucleation along these three directions is lower than that for cleavage along all other directions. From this result, we assume that these three directions are the most resistant to crack growth, noting that nucleated dislocations shield the crack tip from the applied load and increase the required far-field load for cleavage. Consequently, the overall growth of the penny crack is controlled by its growth in the  $\langle 112 \rangle$  directions of the (111) fracture plane. This follows from the idea that an initially circular crack first grows in the directions with the least crack growth resistance, but the relative driving force in these directions decreases as the crack shape changes. Hence, the growth of the crack in the most resistant directions governs the growth of the embedded crack as a whole [14]. For this reason, this study investigates a (111) through crack with a  $[1\bar{1}0]$  crack front, as this orientation is thought to be key in the development of macroscopic cracks from a population of random defects.

While this work focuses on 3C-SiC, our findings can provide insight into crack tip behavior in other common SiC polytypes such as 4H and 6H. For instance, the close-packed basal plane of the hexagonal polytypes has the same nearest-neighbor bonding as the close-packed {111} slip and fracture plane in the 3C structure. Further, Umeno and coworkers [15] have predicted with electronic structure calculations that the ideal shear strength of the basal planes of SiC varies by less than 10% across polytypes.

The simulations were conducted on a specimen measuring  $200 \text{ \AA} \times 200 \text{ \AA} \times 20 \text{ \AA}$  ( $X \times Y \times Z$ ) with a  $60 \text{ \AA}$  through crack created by shielding the atomic interaction between atoms above and below the shuffle set of a (111) plane (Fig. 1). The effect of the specimen size and the exact crack geometry was investigated, by removing a layer of silicon and carbon atoms on the (111) plane rather than shielding atomic interactions. In all cases, the change in the critical  $K_I$  was not significant.

Consistent with the previous discussion, the  $X$ ,  $Y$  and  $Z$  axes were oriented to the  $[11\bar{2}]$ ,  $[111]$  and  $[1\bar{1}0]$  directions of the crystal, creating a (111) crack plane and a  $[1\bar{1}0]$  crack front. Traction-free boundary conditions were applied in the  $X$  and  $Z$  directions, while tensile stress was applied in the  $[111]$  direction by enforcing an average displacement on the atoms along the  $Y$  boundaries of the simulation cell. These boundary conditions create dislocation image forces which encourage dislocation nucleation and glide out of the specimen; although we note that the boundary-induced image force on a nucleating dislocation at a crack tip is negligible due to the geometry of the

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