

Modeling the Effect of Grain Reorientation on Crack Propagation in SiC

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The study of crack propagation in ceramics is critically important due to their widespread use in high-temperature and structural applications, where mechanical failure can lead to severe consequences. Silicon carbide (SiC) is particularly noteworthy because of its exceptional hardness and thermal stability; however, its brittleness necessitates a thorough understanding of fracture mechanisms. Molecular dynamics simulations have become a valuable tool for investigating crack dynamics at the atomic scale, offering insights that are difficult to achieve through experimental methods alone.

In this work, crack propagation was modeled in a SiC bicrystal, where one grain was rotated relative to the other by a specified angle to induce grain reorientation. Stress-strain curves were computed for bicrystal structures with varying reorientation angles, and the resulting crack paths were analyzed. The simulations demonstrate how grain misorientation influences both the mechanical response and the trajectory of crack propagation, providing crucial information for developing more fracture-resistant SiC-based materials.

Type of presence

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