Applying molecular dynamics simulation to take the fracture fingerprint of polycrystalline SiC nanosheets

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Abstract

Graphene-like nanosheets are the key elements of advanced materials and systems. The mechanical behavior of the structurally perfect 2D nanostructures is well documented, but that of polycrystalline ones is less understood. Herein, we applied molecular dynamics simulation (MDS) to take the fracture fingerprint of polycrystalline SiC nanosheets (PSiCNS), where monocrystalline SiC nanosheets (MSiCNS) was the reference nanosheet. The mechanical responses of defect-free and defective MSiCNS and PSiCNS having regular cracks and circular-shaped notches were captured as a function of temperature (100–1200 K), such that elevated temperatures were unconditionally deteriorative to the properties. Moreover, larger cracks and notches more severely decreased the strength of PSiCNS, e.g. Young's modulus dropped to ca. 41% by the crack enlargement. The temperature rise similarly deteriorated the failure stress and Young's modulus of PSiCNS. However, the stress intensity factor increased by the enlargement of the crack length but decreased against temperature. We believe that the findings of the present study can shed some light on designing mechanically stable nanostructures for on-demand working conditions.