Molecular dynamical modeling of nanofracture of two-dimensional MoS_2 and h-BN

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Abstract

Monolayer molybdenum disulfide (MoS_2) and hexagonal boron nitride (h-BN) are among the recently generated two-dimensional materials with fantastic electrical and optical properties which have brought them many potential applications in nanodevices and nanomaterials. Although they both have graphene-like lattice structure, their atomic structures are more complicated than graphene. A reliable design and manufacturing of the devices using these materials necessitate a thorough understanding of their fracture properties. In this study, we use molecular dynamics modeling to investigate the fracture properties of h-BN and MoS_2 under mixed mode loading. We study the impact of chirality, crack tip configuration and loading phase angle on the critical stress intensity factor and crack propagation paths. The results show that MoS_2 and h-BN have similar fracture behavior while MoS_2 has a stronger bending stiffness. For both these materials, cracks tend to propagate along a zigzag path. Both of these materials undergo out-of-plane deformation under all mixed mode loadings due to the buckling under compressive stress induced by mode II loading. The out-of-plane deformation is more sever in h-BN as its thickness is smaller compared with MoS_2. Depending on the initial crack configuration and the loading phase angle, buckling cracks can nucleate before or after the propagation of the initial cracks.

References

[1] Xiaonan Wang, Alireza Tabarraei, Nanotechnology, **26** (2015) 175703.
[2] Alireza Tabarraei, Computational Material Science, **108A** (2015) 66-71.

Figures

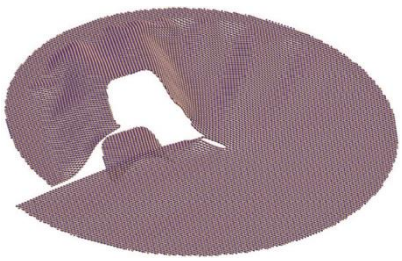

Fig 1. A buckling crack under pure mode II loading in boron nitride sheet.

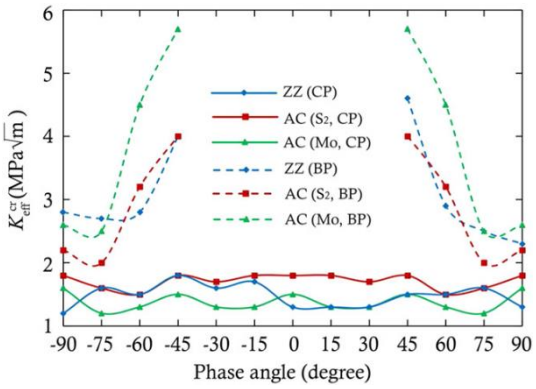

Fig 2. Critical stress intensity factors for armchair and zigzag cracks in MoS_2 sheet.