Nano-Scale Size Effects on Stress Intensity Factors and Crack Interactions Using a Reactive Molecular Dynamics Approach

Hossein Darban

Institute of Fundamental Technological Research, Polish Academy of Sciences
Pawińskiego 5B, 02-106 Warsaw, Poland
E-mail: hdarban@ippt.pan.pl

ABSTRACT

The stress intensity factor (SIF) is a critical parameter in fracture mechanics that characterizes the stress field near the crack tip. While closed-form SIF solutions for various configurations are available in fracture mechanics handbooks or can be readily computed using numerical methods, they often overlook size effects, which might be significant at micro- and nano-scales. Analytical studies, such as those based on nonlocal elasticity theories, have demonstrated that the SIF can be size-dependent. The findings in [1] reveal that cracks in nanobeams exhibit SIFs that deviate from the predictions of classical continuum mechanics-based fracture theories.

This work examines the impact of nano-specimen dimensions on SIFs and crack interactions using a reactive molecular dynamics (MD) approach. Brittle fracture in amorphous silica under mode I and mode II loading is modeled with the state-of-the-art ReaxFF reactive force field. SIF values are computed using two distinct global and local methods: (1) a discretized atomistic J-integral approach [2], where the J-integral is calculated as a summation over three-dimensional discrete regions; and (2) crack tip stress field analysis, previously validated for silica fracture toughness in [3]. The results are compared with classical SIF solutions to uncover size effects and their implications. Furthermore, examples of size-dependent crack interactions at the nano-scale are presented, with a focus on crack tip shielding and amplification mechanisms. These phenomena are analyzed using load-displacement curves obtained from MD simulations of parallel edge cracks under tension.

REFERENCES

[1] H. Darban, F. Fabbrocino, and R. Luciano, “Size-dependent linear elastic fracture of nanobeams”, *Int. J. Eng. Sci.*, Vol. **157**, article no. 103381, (2020).

[2] S.C. Chowdhury, E.A. Wise, R. Ganesh, and J.W. Gillespie, “Effects of surface crack on the mechanical properties of Silica: A molecular dynamics simulation study”, *Eng. Fract. Mech.*, Vol. **207**, pp. 99-108, (2019).

[3] A. Singh, and G. Singh, “A localized stress field approach for calculating the critical stress intensity factor for an isotropic solid at atomistic scale”, *Mech. Mater.*, Vol. **181**, article no. 104632, (2023).