Stress Intensity Factors at the Nanoscale by Atomistic Simulations

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This presentation addresses the following question: *Can the available analytical or numerical solutions for stress intensity factors (SIFs), derived from classical continuum mechanics, accurately define SIFs in specimens with micro- or nanoscale dimensions?*

This question arises because, at such small length scales, interactions between atoms on opposing crack surfaces may become significant and influence the deformation field at the crack tip. The extent to which these atomistic interactions affect the validity of classical SIF solutions remains unclear in the literature.

In this work, we aim to provide insight into this issue by investigating the problem using molecular dynamics (MD) simulations. The SIFs will be determined from MD simulations employing an interatomic potential that is carefully validated against Density Functional Theory (DFT) calculations and available experimental data.

The SIFs will be evaluated using two complementary approaches:

1. A global method based on a discretized atomistic formulation of the J-integral, and
2. A local method based on a least-squares fitting of the crack-tip displacement/stress fields.

Finally, the SIFs obtained from the MD simulations will be compared with those predicted by classical continuum solutions.

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