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Atomistic Study of Phonon Generation and Evolution During Dynamic Crack Propagation

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Project Description

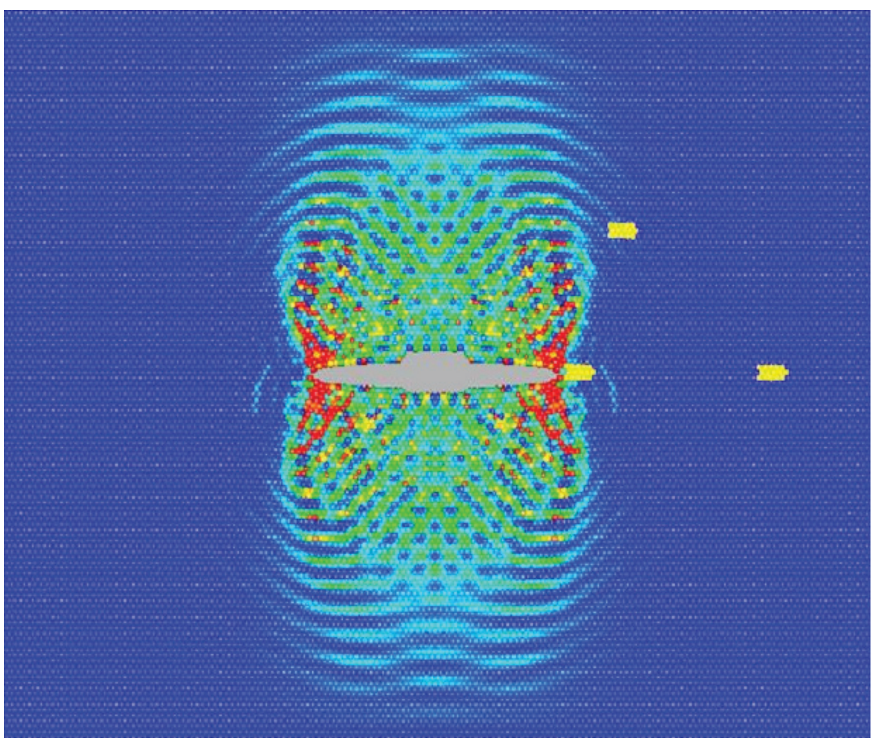
This project involves conducting molecular dynamics (MD) simulation of micro-crack propagation in materials. It will use MD simulation to study phonon generation mechanisms during initiation and propagation of a micro-crack; the MD simulation will be performed in 2-D and 3-D geometries.

Initially 2-D and 3-D crystal structures will be built using parallel computers. SageMD code will be parallelized and used in MD simulations. Details of the MD simulations will be defined.

With MD simulation, the sample will be loaded with boundary conditions specified under which initially the crack extension proceeds in the direction perpendicular to the crack plane. The temperature behavior of the quantities under study will be investigated, using a different temperature ensemble during the MD simulation.

Four tasks will be performed at the discretion of the Sandia principal investigator:

- Generating crystal structures;
- Conducting MD simulation in 2-D of crack propagation in crystal structures;
- Conducting MD simulation in 3-D of crack propagation in crystal structures;
- Analyzing and summarizing results.



Results of MD simulation of crack propagation.

Technical Purpose and Benefits

The understanding of material fracture mechanisms is an important phase in developing new materials with tailored responses. The crack propagation dynamics is an important mechanism responsible for prescriptive material responses. Despite the long history of the research into this effect, it is as yet not well understood.

This project proposes an atomistic study of the phonon generation and interactions that occur during dynamic crack propagation. The crack tip acts as a focal point at which stored strain energy is released upon the breaking of bonds. In the continuum point of view, this energy is converted to heat and elastic waves, whereas the atomic framework models the converted energy strictly as phonons. The evolution of these emitted phonons in atomistics plays an important role in governing the limiting speed and the onset of dynamic crack tip instabilities, although the exact processes are unknown. Also unknown is how this energy conversion differs when crack propagation is accompanied by the creation of material defects, such as dislocations.

We hope to gain from this collaboration a better understanding of fracture mechanisms—an essential gradient in developing predictive simulation capabilities.

Discussions in Vienna—From left to right: Dr. Robert Thomas, Dr. Tony Chen, and Dr. Alexander Selezenev.

Collaboration between Sandia National Laboratories (SNL), Livermore, CA, USA, and the Russian Federal Nuclear Center – All Russian Research Institute of Experimental Physics (RFNC-VNIIEF), Sarov, Russia

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