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Wave propagation from crack extension by molecular dynamic and FEM simulations

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We present results for molecular dynamic and finite element simulations in 3D bcc iron crystals, with embedded central through crack (001)[110] of Griffith type, loaded in mode I. The sample geometry and border conditions in molecular dynamics were chosen in such a way as to invoke a cleavage crack extension. Acoustic emission (AE) sources caused by the crack were analyzed on both the atomistic and continuum level with FEM.

Crack (001)[110] (crack plane/crack front) can extend in a brittle manner, as atomistic simulations under plane strain conditions (e.g.[1]), but also fracture experiments on iron crystals [2, 3] have shown. However, behavior at the crack front depends not only on the stress intensity K_I, but also on the so–called T-stress acting parallel to crack plane [4]. Change of the T-stress from negative to positive values may recall the ductile–brittle transition, as indicated in atomistic simulations under bi–axial loading, as well as continuum predictions [4].

Each displacement of the crack front is accompanied by bond breakage and a stress relaxation at the crack front, which causes acoustic emission of the stress waves in the 3D crystal. This stress wave radiation can be monitored via mapping of local kinetic energies of the individual atoms, as illustrated in Fig. 1 upper, for two layers (110) perpendicular to the crack front in the middle of the crystal at time 48.5 ps. Both quasi–longitudinal and quasi–transverse stress waves can be generated during bond breakage in 3D crystal. The partial AE events may be well recognized at the crack surface.

The stress wave pattern obtained by elastic FEM simulations [5], of the dynamic process caused by crack tip hop, may be seen in Fig. 1 lower. Plane strain conditions inside the sample, were utilized in the anisotropic FEM model with the same orientation as in MD. The FE sample is supposed to be without any initial stress/strain. Only the lower right quarter of the sample treated in MD is utilized in FEM, due to symmetry. The crack initialization was modeled by the prescribed velocities in the crack tip.

At higher applied loads, positive T–stress contributes to cleavage crack extension in MD. Under the ramp loading during 40 ps, the crack was initiated at the critical Griffith stress intensity. MD simulations show that cleavage crack initiation in the 3D bcc iron crystal forms an AE–source, where qL–waves dominate. However, qT–waves are also generated during a continuous bond breakage in the crystal, which is new knowledge from 3D modeling. The strongest pulse emission comes from stress relaxation at the crack front, after the crack initiation.

Simplified modeling of the pulse emission by FEM shows that, besides the qL and qT–waves, Rayleigh waves can also be generated at the (001) free crack faces, in agreement with expectations according to continuum analysis.

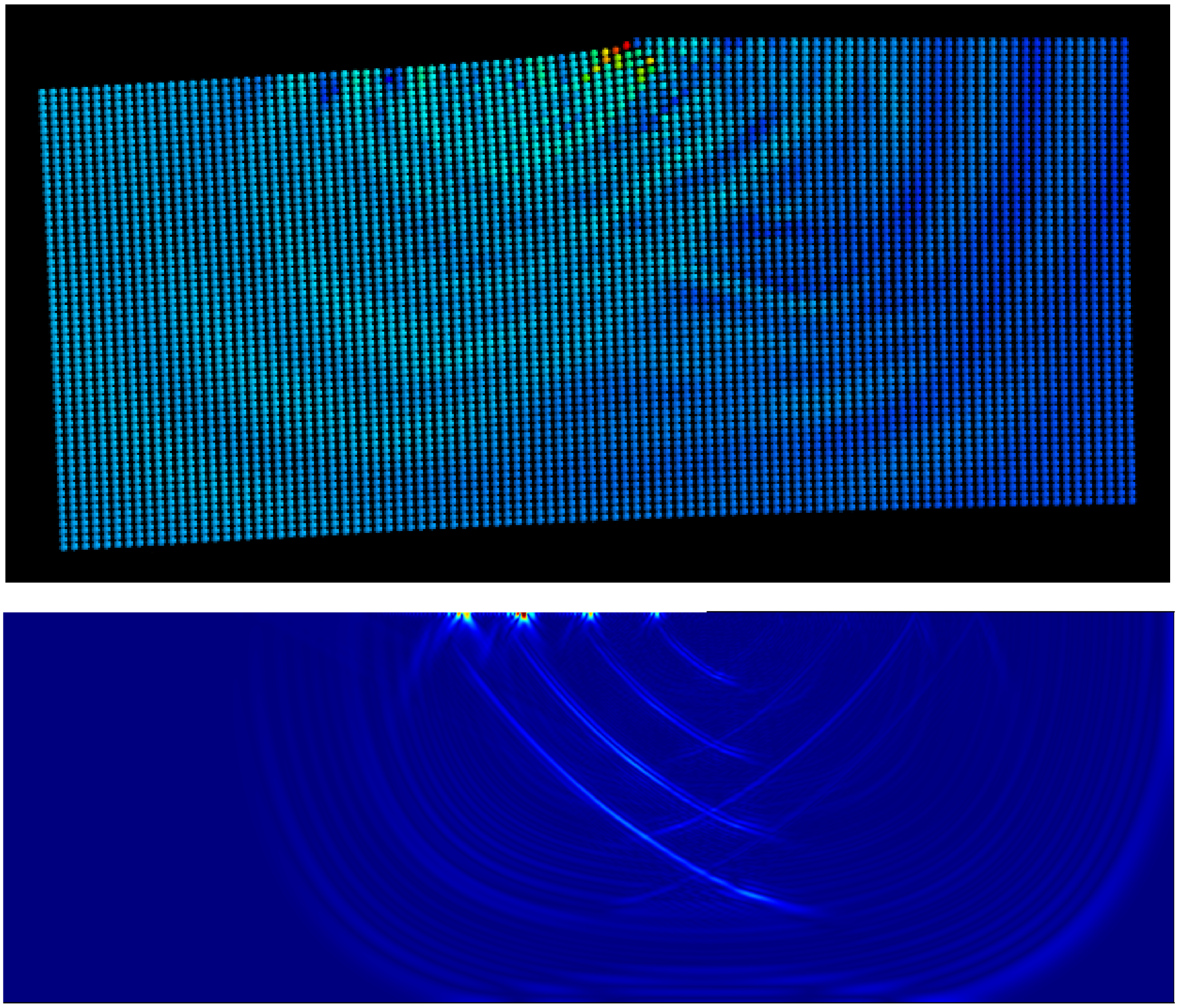

Fig. 1. Results of the MD (upper) and the FEM (lower) simulation.

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