STRESS WAVE RADIATION FROM BRITTLE CRACK EXTENSION BY MD AND FEM

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Keywords: molecular dynamic, finite element simulation, bcc iron crystal

We present results for molecular dynamic (MD) and finite element (FEM) 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 MD were chosen in such a way as to invoke a cleavage crack extension. Acoustic emission (AE) sources caused by the crack were analysed 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, behaviour 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]. The change of T-stress can also be recalled due to the geometry of a cracked sample under uni–axial tension, as follows from [5]. It was utilized in 3D atomistic MD simulations [6] together with special boundary conditions to invoke cleavage fracture. As mentioned in [6], AE sources from MD are well visible in the planes perpendicular to the crack front, but not in the crack plane due to a continuous bond breakage in the atomistic sample. It is a reason why surface Rayleigh waves cannot be recognised in the crack plane from MD.

In this paper we repeat 3D atomistic simulations from [6] where cleavage crack extensions have been invoked along the whole crack front. Acoustic emission sources in 3D, recalled by the brittle fracture, are analysed on both the atomistic and FEM level utilizing information from MD on residual forces in the crack plane during crack propagation.

At MD and FEM simulations we consider a pre–existing central crack of $2l_0 = 2a$ length, embedded in a rectangular sample. The crack surfaces lie on (001) planes, the crack front is oriented along the z–direction [110] and the potential crack extension is in the $x = [\bar{1}10]$ direction. The crack is loaded uni–axially in mode I, i.e. the sample borders are loaded in y $\langle 001 \rangle$directions. Due to the symmetry of the problem, we simulate only one half of the sample in the x–direction. To maintain the symmetry, the atoms lying on the left border plane are fixed in the x–direction. The other atoms are free to move in the x–, y– and z–directions, excepting surface atoms on $\{110\}$ surfaces that are fixed in the z–direction. This serves to decrease stress concentration and prevent the plastic process at the corners, where the crack front penetrates the free surfaces. We utilize an N–body potential for bcc iron of Finnis–Sinclair type [7]. Interatomic interactions across initial crack faces are prevented, in order to simulate a pre–existing crack occurring in continuum models and in linear fracture elastic mechanics.

The half crack length is $l_0 = 178 d_{110}$, where $d_{110} = a_0\sqrt{2}/2$ and $a_0 = 2.8665\,\text{Å}$ is the lattice parameter and the initial half crack opening is $c_0 = d_{001}/2 = a_0/4$. The thickness of the crystal corresponds to 30 layers (110) in the z–direction parallel to the crack front. Crystal consists of 300 planes $[\bar{1}10]$ in the x–direction and 300 planes (001) in the y–direction.

Newtonian equations of motion for individual atoms are solved by a central difference method, using time integration step $h = 1 \times 10^{-14}\,\text{s}$. We use a ramp loading, i.e. the sample is loaded up to a level

σ_A gradually (linearly) during 4000 time steps, as in [6]. When a prescribed stress level σ_A is reached, the applied stress is held constant.

Prior to external loading, the atomistic samples are relaxed to avoid the influence of surface relaxation on the microscopic processes at the crack front. At selected time steps, the local number of interactions, the local kinetic energies and the coordinates of individual atoms are monitored for purposes of graphic treatment of the MD results. When bond breakage occurs in the atomistic system, residual atomic forces in the middle of the crack plane are monitored each time step for purposes of FEM.

The wave motion modelling in the sample was carried out by using the finite element (FE) code COMSOL [8]. The FE sample of width $150a_0\sqrt{2}$, height $150a_0$ and thickness $15a_0\sqrt{2}/2$ (half of the MD sample) was considered as a linear anisotropic elastic medium with cubic symmetry. Plane strain conditions inside the sample together with zero displacements in the z–direction have been utilized in the anisotropic FE model of the same orientation as in MD. The FE sample is supposed to be without any initial stress/strain. For the time integration the full mass matrix and integration time step Δt was 1×10^{-13} s were used.

At higher applied loads, positive T–stress contributes to cleavage crack extension in MD. Under the ramp loading during 4000 time steps, 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 modelling. The strongest pulse emission comes from stress relaxation at the crack front, after the crack initiation.

Simplified modelling 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.

Acknowledgement

The work was supported by the grant GA CR No 101/09/1630 and by the Institute Research Plan AV0Z20760514.

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