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The influence of the excitation pulse shape on the stress wave propagation in a bcc iron crystal

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In this article we describe 3D simulations of an elastic wave propagation in a bcc iron crystal based on a molecular dynamic (MD) method. In present simulations we use an N-body potential of a Finnis-Sinclair type for a transition metals, [1] and parallel programming [2]. This research is a continuation of the topics mentioned in [3, 4, 5]. The behavior of stress waves caused by a surface impulsion in perfect crystals is described in [3, 4]. The mechanical response of the crack to the applied pressure stress waves in the framework of the non-linear atomistic model is studied in [5].

In present simulations the stress wave propagation is studied both in perfect crystal and in the presence of a crack. A central Griffith crack is embedded in a bcc iron crystal with the basic cubic orientation. The crystal is loaded by a stress pulse on its front face and the response is detected on its opposite face. The various shapes, amplitudes, and widths of the stress pulse are considered. The tasks of this type have a physical sense only if the information is not influenced by the stress wave reflections from the free surfaces of atomistic samples. For that reason the samples should be large enough and the simulations on these models can be realized only with a massive application of parallel programming techniques, [2].

All MD simulations were performed in bcc iron plates. The plate thickness was 400 atoms in the y axis direction. The infinity in the other two directions was reached by the application of the periodic boundary conditions on the rectangular sample with the edge of 400 atoms in the x axis direction and the edge of 500 atoms in the z axis direction. The thickness of the possible Griffith crack corresponds 2 atoms and height is 100 atoms. The all–area excitation has been used for loading in the y axis direction on the front side of the crystal. Surface relaxation has been performed in the sample before external loading. Initial temperature corresponded to 0 K and the further thermal atomic motion was not controlled in the system.

The applied external stress has two pulse shapes with various width and amplitude. The stress pulses began at 30^{th} time integration step. The pulse shapes, their widths and the values of applied stress in GPa are given in tab. 1. The performed simulations for particular shapes and widths of pulses, and for individual levels of loading are denoted by the mark (✓) in this table. The denoted simulations were done both for the samples without a crack and with the Griffith crack. All tests, where the local atomic interactions across the free crack faces were monitored, are marked in tab. 1 by the star (*).

To solve Newtonian equations of motion we used time integration step 10^{-14} s in all the simulations. The tests were done between the steps 0 and 3000. The total energy balance (the kinetic energy, the potential energy and the work of external forces), the total number of the atomic interactions, and the local number of the atomic interactions at free crack faces were monitored at each time step.

Tab. 1 The excitation pulse types.

Stress pulse shape	Pulse width [fs]	Applied stress		
		Level 1 0.675 GPa	Level 2 2.700 GPa	Level 3 10.800 GPa
	200	✓	✓	✓
	400		✓	✓*
	800		✓	
	1 600		✓*	
	400			✓
	800			✓
	1 600		✓	✓*

The calculations were done on 50 CPUs of the CESNET METACentrum clusters KONOS, MINOS, SKIRIT and SKURUT (the implementation of one simulation step intervened between 21 and 55 seconds depending on a machine performance).

The comparison of the perfect crystal and the crystal with the embedded crack is mentioned here. A pre-existing Griffith (through) crack has been considered, where the local atomic interactions across the free crack faces did not exist initially. The influence of the shape, width and amplitude (stress level) of the excitation pulse was studied. We observed behavior differences of the atoms in the crack neighborhood caused by activation of the local interatomic interactions across the initially free crack faces. The acquired results are very important for the new NDT nano scale methods.

Our future research will be oriented to investigations of a stress wave propagation after the critical interaction crack-pressure pulse and on a possible mapping of the internal cracks in materials via this non-linear phenomenon.

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