Molecular dynamics study of the acoustic emission during nanoindentation of iron crystal.

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ABSTRACT

Analysis of acoustic emission (AE) is one of the most common methods for monitoring of mechanical systems and identification of vibrations. A distinctive feature of this approach is the ability to identify different structure changes by the generated acoustic signals without the active intervention and change the properties of the material, since AE relates to traditional methods of non-destructive testing. Chung and Kannatey-Asibu [1] notes, that initial and harmonic dislocation movement during plastic deformation of crystal (grains) can also be a source of emission AE. Lebyodkin et. al. in [2] observed the quasi-static behavior of the AE signal intensity on MgZr and AlMg alloys when it started from the very beginning of the tensile test. AE reached its maximum magnitude in deformation within the elastic-plastic transition range and finally reduced but its mean magnitude retained. Salje et. al. in [3] using molecular dynamics have shown, that on the atomic scale AE is determined by both potential and kinetic energy levels changes. The aim of present work is to study the influence of generated structure defects and change of internal energy of sample on AE signals during nanoindentation.

In the paper simulation of the indentation of iron crystal was carried out using the method of molecular dynamics. The iron model sample was 18x18x9 nm rectangular parallelepiped. The simulations were carried out for 0K and 300K temperatures. The zero temperature was used to evaluate the effect of heat motion on the system dynamics. An indenter was modelled in the form of a completely rigid 2 nm diameter cylinder. The indentation simulation was carried out in two stages when the first one was indenting the iron sample at the constant rate 0.1Å/ps. The second stage was that when the indenter penetrated 1 nm into the iron sample it began oscillating with an amplitude increment A(t)=0.05 Å/ps. The acoustic response to indenting was evaluated as forces acting on the atomic area sensor located on the sample's lateral face. We investigated the effect of vibrations on the AE under the impact of a single element with a certain amount of material. Fluctuations of the forces acting on the sensor, changing of the system energy and the formation of defects during loading were analyzed. The force signal showed the increase in its amplitude and power spectrum as well as the median frequency drop under loading by vibrating indentor. The rationale behind all these changes may be a dependence between the vibration amplitude and full system energy.

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