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by a local increase of the atomic volume by 6-8 %. Generation and evolution of LSCs leads to the formation of structural defects of a higher level: dislocations, stacking faults, etc. It is noted that the indentation force and the number of atoms involved in the LSCs are well correlated. This behaviour is due to the fact that the generation of structural defects is a mechanism of elastic relaxation. It was found that the crystallographic orientation of the loaded specimen surface substantially affects nanoindentation response of copper.

PLASTIC DEFORMATION NUCLEATION IN BCC CRYSTALLITES UNDER NANOINDENTATION

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Micromechanical devices used in electronics incorporate small-sized components, which call for special-purpose methods for examination of their physical and mechanical parameters. It is common knowledge that the behavior exhibited by the solid on the macro- and meso-scale structural levels cannot be extrapolated to the nanostructural scale level. Nanoindentation incorporates a wide range of technical facilities for investigating the physical and mechanical properties of solids in the near-surface layers. Therefore, this is an effective tool for examination of material strength properties on the nanostructural level. Due to the rapid development of computer engineering, computer simulation enjoys wide use alongside experimental approaches by addressing problems pertaining to material properties investigations on the micro-scale level. Of particular interest are calculations performed in the frame of molecular dynamics. This method affords detailed information on the dynamics of structural changes and on the stress fields in the atomic system of studied material. Metals having BCC lattice are insufficiently studied by numerical techniques. Therefore, the goal of the given study is investigation of metal response to nanoindentation. The study was made using metals having ideal BCC lattice and metals having intergranular boundary.

The problem was addressed in the frame of molecular dynamics approach. The study was made for a BCC iron crystallite, which is widely used as a model system to study processes involved in the origination and development of plastic deformation in BCC metals. A symmetric crystal boundary was constructed in the simulated crystallite, which permitted correct use of periodic boundary conditions. The description of interatomic interaction was made using many-particle potential calculated on the base of Finnis-Sinclair approximation. For clarity and simpler indentation data interpretation, an extended cylindrical

indenter was used in the investigation and loading was realized by its lateral surface.

The calculations suggest that the intergranular boundaries would hamper structural defect propagation by indentation. It is found that the accommodation of the crystallite having grain boundary occurs due to the generation of defects in both the indenter/sample contact area and the vicinity of the intergranular boundary. The emergence of structural defects on the free surface causes its form changing, in particular, step formation. It was found that the crystallographic orientation of the loaded specimen surface substantially affects nanoindentation response of iron sample.

STRUCTURAL TRANSFORMATION FEATURES IN TITANIUM CRYSTALLITE UNDER MECHANICAL LOADING

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Plastic deformation of structural metals and alloys operating under severe mechanical loading to a large extent determines their operating efficiency and life. It is known that structural transformations in materials which are induced by external loading are a complex process associated with the nucleation and evolution of structural defects on different scales. Plasticity processes begin on the microscale (atomic scale) and determine defect structure development on higher scales. Structural defects formed in a material partially compensate the elastic fields induced by external loading and thus decrease the accumulated elastic energy in the material. Despite the considerable progress in the study of the structural response of various mechanically loaded materials, the generation of plastic deformation on the atomic scale has been insufficiently explored, still being the focus of extensive theoretical and experimental research. In this paper, molecular dynamics simulation is performed to study the atomic mechanisms of generation and development of structural transformations in a titanium crystallite under uniaxial tension. Titanium was chosen because of its wide application in science, industry, and medicine. Moreover, the generation of plastic deformation on the atomic scale in materials with hcp structure is less studied than in materials with fcc or bcc lattice.

The performed calculations have shown that the achievement of a threshold strain value in a titanium crystallite causes elastic energy redistribution. This process is related to the generation and an avalanche-like development of local structural changes in the material. Defect generation significantly impedes potential energy growth with a subsequent abrupt drop of the energy value and thus partially compensates the elastic stresses induced by crystallite deformation. Further loading of the simulated crystallite leads to the generation of classical structural defects, such as stacking faults formed as a result of local structural changes.