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## МЕЖДУНАРОДНАЯ КОНФЕРЕНЦИЯ Перспективные материалы с иерархической структурой для новых технологий и надежных конструкций 21 - 25 сентября 2015 г. Томск, Россия

ТЕЗИСЫ ДОКЛАДОВ

пластических деформаций в различных осях симметрии анизотропного материала в условиях знакопеременной деформации при их ударном нагружении. Получено, что увеличение скорости ударного нагружения преграды приводит к увеличению зон разрушенного транстропного материала преграды, особенно в случае, если минимальные упругие, пластические и прочностные свойства в плоскости прокатки сориентированы перпендикулярно направлению прокатки.

## PECULIARITIES OF PLASTIC DEFORMATION NUCLEATION IN COPPER UNDER NANOINDENTATION

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The last decades the study of plastic deformation is subjected to close attention. However, issues related to the peculiarities of the plastic deformation nucleation in metals at the lowest, atomic, level still remain poorly understood. The possibility of local structural changes, or LSCs, (precursors of plastic deformation) is supported by studies showing that mechanically loaded fcc metals experience specific local structural distortions which correspond to a local structural transition of the fcc-hcp type. It is demonstrated that these distortions are preceded by the generation of excess volume. Nanoindentation is one of the most visual and effective methods for the study of physical and mechanical properties of materials in contact interaction. It enables to influence the origin and evolution of the source of plastic deformation by changing indentation parameters. The aim of the present study is molecular dynamics simulation to elucidate the role of local excess volume in nucleation of plasticity in metals under nanoindentation.

The objects of the simulation are copper single crystals of the parallelepiped shape. The size of their edges is 160 Å, the initial temperature is  $300^{\circ}$ K. The simulated specimens contain about 400 thousand atoms. Loaded crystallite faces simulated as free surfaces. Crystallographic indexes of loaded surfaces in different calculations were next ones: (011), (001) and (111). Periodic boundary conditions were used in the direction parallel to the indenter axis. The rest of the faces perpendicular to the direction of the indentation are simulated as free surfaces. The indenter is moved with a speed of 25 m/s. Interatomic interaction was described in the frame of the embedded atom method.

The results of the simulations showed that local LSCs are formed during nanoindentation of the copper crystallites. Their nucleation is always preceded

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 manyparticle potential calculated on the base of Finnis-Sinclair approximation. For clarity and simpler indentation data interpretation, an extended cylindrical