ТЕЗИСЫ ДОКЛАДОВ

МЕЖДУНАРОДНАЯ КОНФЕРЕНЦИЯ
«Перспективные материалы с иерархической структурой для новых технологий и надежных конструкций»

X МЕЖДУНАРОДНАЯ КОНФЕРЕНЦИЯ
«Химия нефти и газа»

Томск

Издательский Дом ТГУ

2018

DOI: 10.17223/9785946217408/119

PECULIARITIES OF PLASTIC DEFORMATION NUCLEATION IN NANOCRYSTALLINE VANADIUM UNDER SHEAR LOADING

Kryzhevich D., Zolnikov K., Korchuganov A.
Institute of Strength Physics and Materials Science SB RAS, Tomsk, Russia

Nanostructured materials are widely used in many practical applications due to their unique physical, mechanical and chemical properties. They are characterized by high strength, hardness and wear resistance, which are due to nanoscale and interface effects. In addition to the above mentioned properties, structural materials must have a high impact ductility to prevent damage during their operation. As a rule, the creation of nanostructured metal materials combining high strength and impact ductility is a non-trivial task. This is due to the fact that materials with high strength are characterized by low impact ductility and vice versa. It was shown earlier that the creation of nanostructured metallic materials with good ductility and high strength at room temperature and superplasticity at high temperatures is possible. The main physical reason for the low ductility of nanocrystalline metals was that plastic deformation mechanisms based on the generation and motion of dislocations do not act in nanoscale grains. To obtain nanostructured materials with high strength and ductility, it is necessary to form a nanostructure consisting of grains with nonequilibrium boundaries and large misorientation angles relative to each other. The nonequilibrium of the grain boundaries is determined, first of all, by numerous grain boundary defects, which are formed in the process of severe plastic deformation. In this case, nonequilibrium grain boundaries are formed only at large accumulated deformations.

The calculations were carried out for a nanocrystalline vanadium sample composed of grains of identical sizes with large misorientation angles relative to each other. The sample had the form of a parallelepiped, the grains were formed on the basis of the Voronoi polyhedrons. The sample dimensions were 300x200x200 Å. Periodic boundary conditions were set in two directions of the simulated sample. In the third direction, a shear load was applied to the opposite faces of the sample (Fig. 1). The thickness of the shifted regions (punches) was 15 Å. The punch atoms were assigned a constant velocity in the shear direction, in two other directions their coordinates were fixed. Each punch was displaced at a speed of 5m/s. The calculations were carried out for room temperature.

The simulation results showed that the plasticity nucleation in nanocrystalline vanadium under shear loading is associated with the movement of dislocations from the grain volume into grain boundary regions. This leads to an increase in the degree of nonequilibrium of grain boundaries and facilitates grain boundary sliding which is the main mechanism of plastic deformation of the simulated samples. Shear deformation leads to the appearance of strong compressive and tensile stresses in the grain boundaries. Due to the fact that some neighboring grains move in different directions, regions with an excess atomic volume appear on the boundary between them where pores can nucleate.