MD SIMULATION OF SELF-DIFFUSION IN (111) PLANE OF Ni DURING 2D DEFORMATION

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The diffusion coefficient and mechanism of self-diffusion in (111) plane of Ni in the conditions of deformation pressure-tension were studied by the method of molecular dynamics. It was investigated the influence of 2D hydrostatic and axial deformations on the mechanism of diffusion and diffusion coefficient. It was found, that the self-diffusion coefficient in the studied metal at the elastic deformation decreased at pressure and increased at tension. It was observed the considerable increase of the self-diffusion coefficient at a plastic deformation. In this connection, the diffusion took place mainly near the shear lines, appearing in the crystal because of a plastic deformation.

Key words: *self-diffusion, molecular dynamics, elastic deformation, plastic deformation, 2D metals*

1. Introduction

Some modern technological operations of the treatment of metallic materials by pressure (rolling, forging, pressing, etc.) use high-speed modes of deformation. When in operation, metallic materials usually suffer loading and deformation for a long time. The experiments show that the diffusion properties of the deformed metals and alloys depend on the value and velocity of deformation. The increase of the activation energy of diffusion is found at the elastic pressure of metals [1]. The considerable acceleration of the diffusion is observed at high velocities of the deformation of metals and alloys [1–4]. The diffusion coefficient can reach the values, typical for pre-melting temperatures. The majority of authors agree with the reason of such phenomena, it is plastic deformation [4–6]. But there is no single view on the mechanism of the phenomena. The experimental observation of the dynamics of the atomic structure, in particular micromechanism of the diffusion in the condition of deformation, in spite on the development of high-permission methods of the research, is a rather difficult task. That is why, the alternative approaches, especially the method of computer simulation, intensively developing in the present time, is of great importance.

In the present work, the diffusion coefficient and mechanism of self-diffusion in two-dimensional Ni in the conditions of deformation pressure-tension are studied by the method of molecular dynamics.

2. Model Description

The packing of atoms of the calculated block was corresponded to the plane [111] of FCC lattice. Interatomic interactions were described by pair central Morse potential. The

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