ABSTRACT

Diploma work: 101 pp., 10 tab., 34 draw., 59 sources.

MOLECULAR DYNAMICS, FREE SURFACE, SIMULATION, SURFACE RELAXATION, MULTILAYER SYSTEM, TITANIUM MONOCRYSTAL, GRAPHEN.

The object of the research – structural changes in Ti surface layers under graphene film influence.

Work purpose –theoretical study of graphene films on structural changes and stress in the surface layers of Ti on the (0001), $(11\bar{2}0)$, $(1\bar{1}00)$ surfaces.

Method of research – the method of molecular dynamics.

The models of a Ti crystal before and after application of graphene films for (0001), $(11\bar{2}0)$, $(1\bar{1}00)$ surfaces are created. The multilayer relaxation of the Ti surface was simulation by the MD method. MEAM (Modified Embedded Atom Method) potential and LAMMPS software were used in modeling. Dependence of atoms distribution in depth, the radial distribution function in the planes, and the dependence of interplanar distances were determine and analyzed for the researches of structures in near-surface relaxed layers. The value of interplanar distances was compared with data from other sources. The stresses in the systems were calculated as a whole and separately for each subsurface plane. The simulations were at temperatures of 300 K and 400 K.

Conclusions about the nature of structural changes and stress were made depending on the packing density of surface layers and temperature.