SIMULATION OF THE TI COATING MATERIALS DEPOSITION PROCESS

Sergienko M.V., *student*, Borisyuk V.M., *senior teacher*

Surface coating is one of the most effective ways of the material improving. It has a wide range application because of possibility of significant increasing of materials characteristics such as wear resistance, strength and toughness, the ability to resist short-term high-energy impact, temperature stability, etc.

The properties of the coated material are strongly depended on the deposition parameters such as adatom energy, compound of the sputtered substance and others. One of the possible ways to verify the characteristics of the modified material without performing the deposition is a numerical simulation. Molecular dynamics (MD) is a computer simulation of physical movements of atoms and molecules. A MD simulation requires the definition of a pairwise potential, such as Lennard-Jones or a description of the terms by which the particles in the simulation will interact. A pairwise potential implies that the interaction of two particles depends on their relative position and does not depend on the position of others. For simulation of the deposition process the embedded atom model (EAM) is used to realistically predict the effects of the many factors affecting the surface growth. It assumes that the crystal energy is the sum of a pairwise potential and an energy required to embed an atom into a local medium with a given electron density [1].

The deposition process of the Ti and Zr mixture onto Fe (100) facet was simulated through MD algorithm. The deposition rate and mixture compound were chosen according to existed experimental data. The adhesion forces and radial distribution function of the structure obtained by MD simulation were calculated. The results of the simulation are verified by the experiments.

1. X.W. Zhou, et al., *Acta. Mat.* **49**, 4005 (2001).