Molecular dynamics study of the process of crystal formation in the deposited layers of molten metal

Andrey I. Dmitriev*, Anton Yu. Nikonov *† and Evgeny A. Kolubaev*

* Institute of Strength Physics and Materials Science SB RAS, Akademicheskii Av. 2/4, 634055, Tomsk, Russia
e-mail: root@ispms.ru, web page: http://www.ispms.ru

† National Research Tomsk State University, Lenin Av. 36, 634050, Tomsk Russia
e-mail: rector@tsu.ru, web page: http://www.tsu.ru/english/

Key Words: Molecular dynamics, Grain boundaries, Molten layers, Titanium, Aluminium crystallite

ABSTRACT

In recent years additive manufacturing (AM) is becoming one of the most discussed modern technologies [1, 2]. In contrast to conventional processing method the additive manufacturing is based on an increment by layer-by-layer manufacturing, which allows one to design not only the external form but inner structure of the product as well. Significant achievements of the AM in metals today are mainly connected to the unprecedented freedom of component shapes this technology allows. But full potential of these methods lies in the development of new materials designed to be used specifically with AM. In this regard, it is important to have a deep understanding of the processes occurring in the volume of material at all stages of production: from the preparation up to the final state. The most effective for this purpose is to use methods of computer simulation. From the point of view of understanding the patterns of formation of the structure of the material in conditions where temperature can change dramatically (for example, from several thousand degrees to ambient value), the advantages of the method of molecular dynamics can be effectively used. In the present work, this method was used to simulate the process of crystal formation in the molten layer of the deposited material, when the influence of interfaces like grain boundaries is explicitly taken into account. Studies have been performed for titanium and aluminum samples. The influence of the crystallographic orientation of the models being modeled and the technological parameters of the model reflecting the electron-beam 3D printing has been analyzed. The calculation results are compared with the available experimental data.

Investigations have been carried out with the financial support from the Fundamental Research Program of the State Academies of Sciences for 2013-2020, line of research III.23.2.4.

REFERENCES
