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EVOLUTION OF CONTINUUM-ATOMISTIC APPROACH FOR THE MODELING OF IRRADIATION OF METALS BY HEAVY IONS

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Research in the field of materials irradiation by high energy heavy ions (HEHI) has been actively made for several decades. The experiments in this area are labor-consuming and expensive. Therefore the improvement of existing mathematical models and the development of new ones based on the experimental data of interaction of HEHI with materials is of current interest. Currently, there are used two models for studying these processes: a thermal spike (TS) model [1] and a method of molecular dynamics (MD) [2]. Combining two these models (continuous-atomistic model (CAM)) will give the opportunity to investigate more thoroughly the processes of irradiation of materials by HEHI.

The work presents the evolution of using the CAM when irradiating metal targets with heavy ions of different energies. The applicability of CAM and the essential points of the model are discussed. A software package has been developed to solve the CAM equations and to test the block of MD of the software complex on the heterogeneous HybriLIT cluster [4]. The results of modeling the processes of interaction of uranium ions with different energies with a nickel target are obtained.

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Short biography note

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