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Computer Simulation of the Interaction of Metal Nanoparticles with a Substrate

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One of the modern technologies for obtaining new materials and coatings is the deposition of nanoparticles on a substrate. This process is relevant for many industries and the social sphere. Constantly increasing requirements for the quality and nomenclature of this type of product lead to the need for detailed theoretical and experimental studies of the spraying process in various conditions. One of the methods of such research is computer and supercomputer modeling. In this paper, a comprehensive the methodology of such modeling, covering all stages of the computational experiment. The basis of the technique is a direct atomic-molecular modeling of the deposition process on a microscopic scale. Parallel technologies are used for the computer implementation of the technique, which allow obtaining results with a given level of resolution and accuracy. In the upcoming report, various aspects of the developed modeling technology are discussed using the example of deposition of nickel nanoparticles on a substrate.

Summary

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