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Supercomputer modeling of interaction processes of different-material metal nanoclusters

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The problem of supercomputer modeling of the processes of creating metallic composite materials from nanomaterial nanoclusters is considered. The general relevance of the research is related to the development of technology for manufacturing nanoscale electronic components. The relevance of a specific study is related to the need to develop both mathematical and software tools for modeling all stages of manufacturing. In this paper, we analyze the final stage of the process, when individual metal clusters interact with each other and with the substrate. These processes are studied by classical molecular dynamics (MD) methods using parallel computing. The focus of the research is to develop an approach to calculating the interaction of different-material metal systems. The problem of interaction of copper and nickel nanoclusters in the manufacture of the corresponding composite is chosen as an example. Preliminary testing confirmed the effectiveness of the developed parallel computing procedure. The work was supported by the Russian Science Foundation, project No. 25-71-20016.

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