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Praca doktorska

Badanie własności sprężystych strukturalnie zmodyfikowanych kryształów Yukawy za pomocą symulacji komputerowych

Promotor

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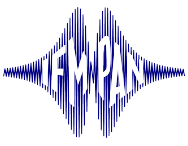

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Abstract

In the dissertation, the influence of size polydispersity and modifications of structure on the elastic properties of crystals in which the particles interact via the Yukawa potential have been investigated. A new approach for searching for mechanisms leading to the auxetic properties has been proposed. This approach is based on the modification of the structure at the atomic-molecular level. The objects of the research were two-dimensional and three-dimensional polydisperse Yukawa crystals, and Yukawa crystals with nanolayers and nanochannels. The studies by Monte Carlo simulations in the isobaric-isothermal ensemble have been performed, and the elastic properties were determined using the Parrinello-Rahman method.

The dissertation analyzes the influence of size polydispersion of particles on the auxetic properties of Yukawa crystals using the proposed parameter – the auxeticity degree. The studies showed that structural modifications of the Yukawa crystals lead to a number of possibilities that allow for controlling the elastic properties of these systems. In particular, it has shown that modifications of the structure of Yukawa crystals in the form of nanolayers and nanochannels allow not only for enhancing the auxetic properties in certain crystallographic directions, but also for their weakening, or even "removal", in the some crystallographic plane.