The molecular dynamics study of argon solid–liquid transition inside graphene nanobubble

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In this work, the results of atomistic simulations of the liquid–crystal phase transition of argon, trapped in graphene nanobubbles [1] are presented. The main emphasis is made on the methodology of phase transition modelling, i.e., we propose a technique which aims to avoid metastable states of argon. The scientific contribution of this work consists in the disclosure of how confinement affects phase transition parameters and structural evolution of argon.

Calculated results show that provided the same pressures, confined argon melts at temperatures 10–30 K higher, than in case of "free" argon. Also, the sliced structure of the argon stays after melting in case of confinement.

The calculations were performed using the LAMMPS molecular dynamics package. The potentials used in the work were: the Tersoff potential for the carbon interaction within graphene sheet, the Lennard-Jones potential for argon–argon and argon–carbon interactions. The argon pressure was calculated with two different approaches to minimize the error of computation of the temperature shift.

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[1] Khestanova E, Guinea F, Fumagalli L, Geim A K and Grigorieva I V 2016 *Nat. Commun.* **7** 1–10