

Crystal structure of a system with three-body interactions in strong confinement

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It is well known that confinement strongly changes many properties of liquids [1]. It leads to modulation of local density, changes in diffusion coefficient etc. In particular, crystalline structure of the system can be strongly different from the bulk one [2]. The simplest example of confinement is a slit pore, i.e., the system is being enclosed into two parallel walls. Such systems split into several layers parallel to the walls. Until recently the crystal structure of a system in a slit pore was described as “number of layers + structure of the layers” [3]. In our recent paper, it was shown that more accurate and elegant description of this structure is to represent it as a slice of fcc or hcp one [4]. In the present work, crystal structure of a Stillinger–Weber system [5] in a narrow slit pore is studied. It is discovered that depending on the density the system forms several different crystal phases. Importantly, the system splits into several layers, and the symmetry of different layers can be different, which is not observed in systems with pair interaction only. The work was supported by the Council of the President of the Russian Federation for State Support of Young Scientist (grant No. MD-6103.2021.1.2).

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