Electrocrystallization of Supercooled Water in Confinement

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The paper discusses the features of supercooled water thin film of width d = 3.97 nm contained by the perfect graphene layers and crystallizing under external stationary electric field. It was found that the electric field applied perpendicular to graphene layers impedes structural ordering, while the electric field applied in lateral direction contributes to formation of the cubic ice (I_c) phase, which is thermodynamically less stable compared to the hexagonal ice (I_h) phase. It is shown that the growth of the I_c crystalline phase occurs without formation of intermediate crystalline phases. It was found that the crystallization rate depends strongly on the magnitude of the applied electric field. In particular, the processes of full electrocrystallization of the system do not appear over simulation time scale (~ 40 ns) if the electric field of the magnitude less than 0.07 V/Å is applied.

Keywords: electrocrystallization, supercooled water, molecular dynamics, structural ordering.

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