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Simulation of a Solid-Solid Transition in Confined Colloidal Hard Spheres WEIKAI QI[1], Soft Condensed Matter, Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands, YI PENG, YILONG HAN, Department of Physics, Hong Kong University of Science and Technology, Hong Kong, China, RICHARD BOWLES, Dept. Chemistry, University of Saskatchewan, Canada, MARJOLEIN DIJKSTRA, Soft Condensed Matter, Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands — Recent experiments on a system of colloidal particles confined between two flat plates showed a two-stage nucleation process involving the transition of a solid, consisting of n+1 crystalline layers with a square symmetry (n+1 s-phase), to another solid consisting of n triangular layers (n t-phase), via an intermediate metastable liquid droplet [1]. Using event-driven molecular dynamics and Monte Carlo simulations, we study the 5s $\rightarrow$ 4t solid-solid transition in colloidal hard spheres confined between two planar hard walls. The 5s solid initially melts, forming a liquid droplet, within which the 4t solid nucleates. Calculations of the free-energy landscape confirm that the optimal kinetic pathway is a two-stage nucleation process with a critical nucleus consisting of liquid-like and t-solid-like particles. In addition, we find that the t-solid-like cluster nucleates near the planar hard walls, and contains both face-centered-cubic and hexagonal-close-packed ordered particles.

[1] Y. Peng, F. Wang, Z. Wang, A. M. Alsayed, Z. Zhang, A. G. Yodh and Y. Han, Nature Materials, In press (2014).

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