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Structural relaxation of confined 3-dimensional Yukawa liquids after quenching

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After sudden quenching below the freezing point, the liquid exhibits interesting spatiotemporal evolutions of micro-structure and motion in its transient relaxation toward supercooled or glassy states. The emergence of multiscale crystalline ordered domains with different lattice orientations, and gradually increasing averaged domain size, associated with dynamical slowing down are the good examples [1]. Nevertheless, other than bulk liquids, the transient relaxation dynamics of the tightly confined liquid in a mesoscopic gap after quenching remain unknown.

For liquids under confinement, flat boundaries suppress transverse thermal motion, line particles up, and induce layering formation nearby boundaries. The thickness of the layered region is about the structural correlation length of the bulk liquid, which can be extend inward by cooling the system [2,3].

Recent studies showed that the scale-free fluctuating layering front propagates inward from the boundary after sudden quenching [2], and the disorder-order transitions of layering and intralayer structural orders follow the generic behaviors governed by the percolating theory, in steady states under different temperature and normal distance to the boundary [3].

Namely, the confinement boundary breaks the system symmetry and introduces additional long-range order. The induced layering formation turns the layered region into a 2+1dimensional system with different intralayer and interlayer coupling, which makes the system prefer intralayer triangular lattice packing, the formation of 3D crystalline ordered domains with specific lattice orientations normal to boundaries, and relative interlayer slipping. Nevertheless, how the interplay of orders from particle mutual coupling and boundary confinement, and disorder from stochastic spatiotemporal fluctuations leads to the interesting spatiotemporally heterogeneous disorder-order transitions from the boundary toward the center of a tightly confined liquid remains an unexplored fundamental issue.

In this work, the above unexplored issue is unraveled numerically using a Yukawa liquid, which allows the formation of 16 layers in a tight gap as a platform. Langevin-type molecular dynamic simulation is conducted. It is found that, right after sudden quenching, the two opposite outmost layers form many small intralayer crystalline ordered domains (ICODs) with different intralayer lattice orientations θ_6 . Then a fluctuating layering front invade toward the center from each boundary with increasing time, associated with the gradually increases of layering and intralayer bound orientation orders with increasing time. When two layering fronts touch each other, un-layered liquid clusters surrounded by layered sites emerge, which shrink and disappear with increasing time. In the center region, the two different θ_6 from the two opposite layering regions compete. Eventually, one of them dominates and makes the entire region in the gap share the same θ_6, except one outmost layer remaining its different original θ_6.

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References

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