Screw dislocation dynamics in the transient relaxation of confined Yukawa liquids after quenching

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In confined liquids, flat boundaries can suppress the transverse thermal motion of particles and induce layer formation nearby the boundary, with thickness about the structural correlation length of the bulk liquid. Through quenching the system below the melting point, the layering front can further invade the bulk liquid[1]. However, after the layers fully occupy the entire system in the transient relaxation after quenching, layers are not perfectly aligned. Thermal agitation can still generate layer undulation and facilitate the formation of local layering disorders in the system. Nevertheless, their generic dynamical behaviors remain unknown.

Screw dislocations (SDs) are fundamental filament-like defects with undefined phases winded around by helical layered fronts. They are important phase singularities commonly found in layered systems. For example, the spontaneously generated chaotic SDs in the *xyt* space of self-excited dust acoustic waves have been demonstrated experimentally, where *xy* plane is the plane normal to the wave propagation direction. The modulation instability leading to waveform undulation, rupture, and reconnection was found to be the key for SD generation[2]. Recent studies have also discovered SDs in macroscopic layered structures like biomineralized nacre and block-copolymer[3,4]. However, the generic behaviors of SDs and their dynamical evolutions in the *xyz* space remain elusive.

In this work, from the aspect of SDs dynamics, we numerically investigate the evolution of local disorders of confinement-induced layering in the transient relaxation of Yukawa liquids after quenching below the layer formation temperature, through Langevin-type molecular dynamic simulation. Two flat boundaries normal to the z-axis act as topological constraints, making particles form 49 layers. It is found that, after layers fully extend over the entire system, pairs of SDs with opposite helicities can be spontaneously generated, in the form of chaotic filaments. With increasing time after quenching. The small-scale fluctuations of SDFs gradually decrease, leaving large SD loops or long SD strings still exhibiting slow temporal fluctuations. The basic generic SD dynamical processes for SDF fluctuation, interaction, breaking-reconnection, etc., and their topological origins are classified and discussed. The constructed picture sheds light on understanding SD dynamics in other layered systems such as nonlinear traveling wave systems. This work is supported by the National Science and Technology Council of Taiwan, under contract No. MOST-111-2112-M-008-017.

References

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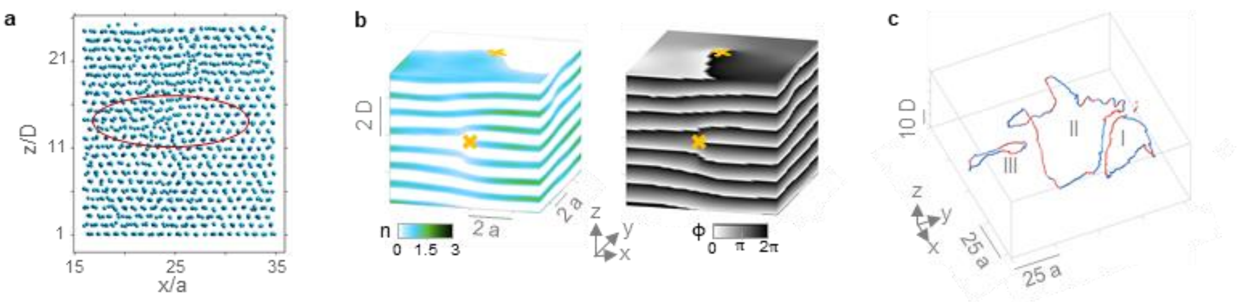

Figure 1. **a**, Typical side-view snapshot of the particle configuration with imperfect layering (circled region), in the lower half of the thin vertical slab (3 *a* in thickness, where *a* is the mean distance of two adjacent intra-layer particles) normal to the boundary, at a certain time after fully layering. Here, *D* for the vertical axis is the mean interlayer distance. **b**, Color-coded plots of the coarse-grained particle density *n* (left) and the corresponding phase ϕ (right) on the *xy, xz,* and *yz* planes. The crosses denote defect locations with undefined phases, located at the vertices of the pitchfork structure. The defect position in the front *xz* plane corresponds to the center of the circled region in (a). **c**, Typical SDF configuration in the entire simulation box at the same time, showing the formation of SD loops (labeled by I to III).