

Solid-to-molecular-orientational-hexatic melting induced by local environment determined defect proliferations

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Two-dimensional (2D) melting is a fundamental research topic in condensed matter physics, which can also provide guidance on fabricating new functional materials. Nevertheless, our understanding of 2D melting is still far from being complete due to existence of possible complicate transition mechanisms and absence of effective analysis methods. Here, using Monte Carlo simulations, we investigate 2D melting of 60° rhombs which melt from two different surface-fully-coverable crystals, a complex hexagonal crystal (cHN) whose primitive cell contains three rhombs, and a simple rhombic crystal (RB) whose primitive cell contains one rhomb. The melting of both crystals shows a sequence of solid, hexatic in molecular orientation (H^{mol}), and isotropic phases which obey the Berezinskii-Kosterlitz-Thouless-Halperin-Nelson-Young (BKTHNY) theory. However, local polymorphic configuration (LPC) based analysis reveals different melting mechanisms: the cHN-H^{mol} transition is driven by the proliferation of point-like defects during which defect-associated LPCs are generated sequentially, whereas the RB-H^{mol} transition is driven by line defects where defect-associated LPCs are generated simultaneously. These differences result in the observed different solid-H^{mol} transition points which are $\phi_A = 0.812$ for the cHN-H^{mol} and $\phi_A = 0.828$ for the RB-H^{mol}. Our work will shed light on the initial-crystal-dependence of 2D melting behavior.

Keywords: two-dimensional melting, phase transition, molecular-orientational forming liquid crystal, local environment, melting mechanism

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1. Introduction

Understanding two-dimensional (2D) melting is a long-term subject in condensed matter and statistical physics.^[1,2] In late 1950s, Bernal introduced geometrical degrees of freedom to understand the entropy differences between solid and liquid phases, which has opened a door for an intuitive understanding of 2D melting.^[3-4] Afterwards, motivated by the absence of true long-range order in two dimensions,^[5] Berezinskii,^[6,7] as well as Kosterlitz, Thouless, Halperin, Nelson and Young, developed a novel theory (BKTHNY theory) for 2D melting based on the evolution of topological defects in systems,^[2,8-10] which states a two-step melting process: the unbinding of pairs of dislocations drives a continuous transition from solid to liquid crystal phase (n-atic), and subsequently, the dissociation of pairs of disclinations (i.e. single dislocations) drives the second continuous transition from liquid crystal phase to isotropic

fluid. The BKTHNY theory strongly inspires researchers to investigate 2D melting behavior.^[14-20] On the other hand, with the advances of detection and analysis techniques, other transition behaviors that the BKTHNY mechanism cannot cover have also been discovered,^[19,22,24-26,28-34] suggesting that our understanding of 2D melting is still not complete.

The melting mechanism suggested by the BKTHNY theory have been tested in different particle systems,^[2,8-10,24,28] and three types of 2D melting scenarios have been revealed up to date,^[17,19,22,26,28,35-37] which are a first-order transition directly from solid to isotropic fluid, a two-step melting with a continuous solid-to-liquid crystal transition and a first-order liquid crystal-isotropic fluid transition, and a two-step melting with continuous transitions for both solid-liquid crystal and liquid crystal-isotropic fluid. For example, both hard disks^[19,22,25] and regular polygons with an edge number $n \geq 7$ ^[28] show a two-step melting behavior including a continuous

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