Discrete Mechanical Model for 2D Melting*

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Our previous molecular dynamic simulation studies of simple 2D systems [1] suggested that both geometrical defects (localized, large-amplitude deviations from hexagonal ordering) and topological defects (dislocations and disclinations) play a role in 2D melting. To capture the main features of the 2D melting transition and investigate the respective roles of these two classes of defects, we have studied a discrete mechanical model consisting of an array of nodes connected by springs, for which the relative number of geometrical defects (modeled as springs with an equilibrium length of $\sqrt{2}$) and topological defects (nodes having a coordination number different from 6) may be precisely controlled. We have performed Monte Carlo simulations of this model in the isobaric-isothermal ensemble, and present the phase diagram as well as various thermodynamic, statistical and structural quantities as a function of the relative populations of geometrical and topological defects. These results are compared with those from simulations of 2D particle systems.

[1] *Adv. Chem. Phys.* **83**, 543 (1993).

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