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Statistical mechanics of equilibrium crystal shapes: Interfacial phase diagrams and phase transitions

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Abstract

We review the present status of the statistical mechanical theory of equilibrium crystal shapes. Special emphasis is placed on the relation between singularities occurring in the shapes of three-dimensional (d—»3) crystals and the phase transitions of certain d—»2 models. We exploit the thermodynamic conjugacy of the Wulff plot and the equilibrium crystal shape to give interfacial phase diagrams in both density and field variables. From this perspective, sharp edges or points on the crystal shape correspond to first-order phase transitions, while smooth joining of curved and planar (â€œfacetedâ€) regions corresponds to second-order phase transitions. Equilibrium crystal shapes of a simple-cubic (Ising) lattice gas with nearest-neighbor (attractive) and next-nearest-neighbor (nnn) interactions are considered in detail. Typical equilibrium crystal shapes at nonzero temperature consist of facets and smoothly curved surfaces. When nnn interactions are

attractive, only second-order transitions occur. Both Kosterlitz-Thouless (â€œrougheningâ€) and Pokrovsky-Talapov (Gruber-Mullins) universality classes are represented. When nnn interactions are repulsive, first-order transitions and tricritical behavior also occur. The present experimental situation is summarized.

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