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Abstract

Adsorption of Long Straight Rigid Rods on Two-Dimensional Lattices: Study of Orientational Surface Phase Transitions from Entropic Considerations †

Eugenio Vogel [1,2], Julian J. Riccardo [3], José L. Riccardo [3], Pedro Marcelo Pasinetti [3] and Antonio José Ramirez-Pastor [3]

[1] Department of Physics, Universidad de La Frontera, Temuco, Chile
[2] Centro para el Desarrollo de la Nanociencia y la Nanotecnología, CEDENNA, Santiago, Chile
[3] Departamento de Física, Instituto de Física Aplicada, Universidad Nacional de San Luis-CONICET, Ejército de los Andes 950, D5700BWS, San Luis, Argentina

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The orientational phase transitions occurring in a system of long straight rigid rods of length k (k-mers) on square lattices are studied by combining Monte Carlo simulations and theoretical analysis. The phenomenology of this model was examined in Refs. [1–5]. A nematic (N) phase, characterized by a big domain of parallel k-mers, is separated from a disordered-isotropic (D) state, by a continuous transition occurring at intermediate density. A second phase transition, from an N order to an ordered-isotropic (O) state, occurs near saturation density values. In the present work, the process is analyzed by following the number of accessible adsorption states along the vertical[horizontal] direction as a function of the surface coverage $W_v(q)$[$W_h(q)$], which allows us to define a vertical[horizontal] configurational entropy. These quantities show strong variations with coverage (eventually leading to ergodicity breakdown), allowing to identify the different phases (N, D and O) characterizing the critical behavior of the system. Comparisons between Monte Carlo simulations and analytical calculations were performed in order to evaluate the reaches and limitations of the theoretical model.

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