The supercooling and superheating limits of the uniaxial to biaxial phase transition in nematic liquid crystals : A Monte Carlo Simulation Study

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The metastable behaviour of liquid crystals near phase transitions has attracted considerable interest due to its connection with fluctuation effects and nucleation phenomena. This phenomenon usually occurs in isotropic to uniaxial phase transition and is well studied. However the metastable behaviour of nematic liquid crystals near uniaxial to biaxial transition has not been reported yet. The reason behind this is that the uniaxial-biaxial transitions for most of the nematogenic models are second order in nature and thus the question of metastable behaviour does not arise. In our recent work we simulated a phase diagram for a nematogenic model [M.K. Debnath, S. Pramanick, S. DasGupta, N. Ghoshal, Phase diagram of a biaxial nematogenic lattice model: A Monte Carlo simulation study, Physica A 674(2025) 130697] which has a first order uniaxial-biaxial coexistence line. In the present work, we investigate the supercooling and superheating limits of the uniaxial to biaxial phase transition in nematic liquid crystals simulating the same nematogenic model. Our study predicts that the uniaxial nematic phase can be supercooled below the equilibrium transition temperature before the occurrence of the biaxial nematic phase. This metastability arises due to the presence of a free-energy barrier separating the two phases. In the present investigation phases are analyzed and the temperature limits of supercooling and superheating are determined from the disappearance of the metastable minima in the free energy landscape. The study provides insight into the thermodynamic stability and metastable behaviour of nematic liquid crystals and helps in understanding the weakly first-order character of the uniaxial to biaxial transition.