Effects of Elastic Interactions in a Model Spin-Crossover Material

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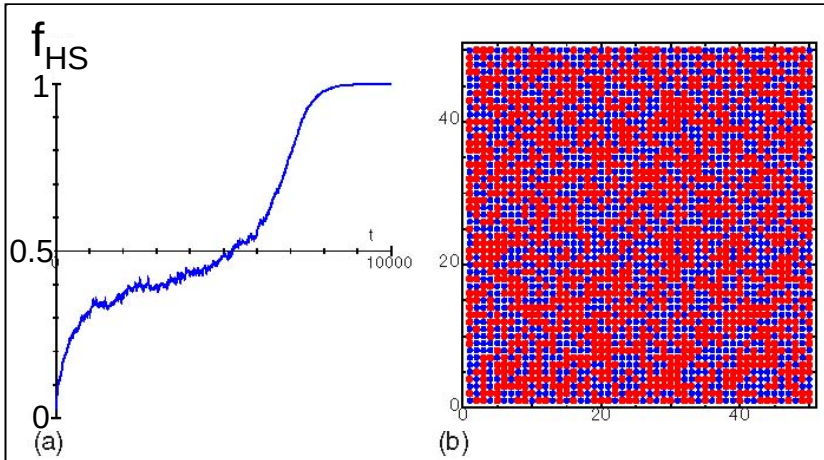
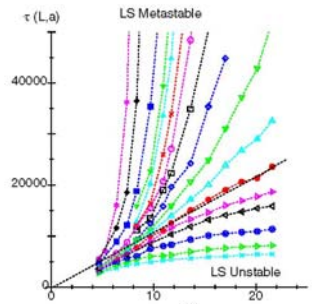
Spin-crossover (SC) materials are molecular crystals with a low-spin (LS) ground state and a highly degenerate high-spin (HS) excited state. The HS state can be induced at low temperatures by light irradiation. SC materials have many potential applications, including switches, displays, and recording media.

As the HS state has a larger volume than the low-spin state, elastic distortions may induce long-range intermolecular interactions that may cause phase transitions in SC materials to belong to the mean-field universality class. An experimentally observable consequence would be an absence of large clusters and thus of critical opalescence. Here we show kinetic Monte Carlo simulations of a model for such a SC material with elastic interactions, performed in collaboration with the group of Prof. Seiji Miyashita, Department of Physics, Faculty of Science, The University of Tokyo, Japan.

S. Miyashita, P.A. Rikvold, T. Mori, Y. Konishi, M. Nishino, and H. Tokoro, Phys. Rev. B **80**, 064414 (2009).



(a) The fraction of HS molecules vs time for a light intensity beyond the spinodal limit. (b) Snapshot of the configuration at t=6000 shows no compact clusters, in contrast to models with short-range interactions.



Lifetimes of the LS state vs (system size)$^{2/3}$, for light intensities below (top), at (straight line), and above (bottom) the spinodal limit.