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Spatio-temporal aspects of the domain propagation in a spin-crossover lattice with defect

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Abstract

the collective spatiotemporal dynamics of the metastable high-spin state (HS) upon relaxation towards the low-spin (LS) is investigated using an electro-elastic model which includes the change of the spin states and the lattice volume at the transition. The present work focusses on the case of a lattice in which is embedded a structural defect in the center, represented here by a hole with a fixed size. The simulations are made on a 2D rectangular-shaped and compared to those of an ideal system. To account for the volume change, we set the distances between the sites as spin-dependent which requires the use of Monte Carlo simulations on spin states and atomic positions to solve the present problem. It is found that the presence of the defect affects the dynamics of the spin-crossover transformations which starts stochastically from a corner of the lattice, then propagates in the first stage along the width (shortest distance to the surface), before to proceed via a second longitudinal regime whose velocity slows down significantly at the vicinity of the defect, which plays the role of a pining center. After a while, the interface leaves the defect, and accelerates when it approaches the lattice's border. We have also investigated the spatial dependence of the displacement field, from which we derived the distribution of the divergence and rotational of the displacement field, which directly connects to the trace of the strain tensor and to shear strains respectively. Valuable information on the relaxation process of the elastic field are derived and discussed in direct relation with the presence of the defect.

Abbreviations

- SCO, Spin crossover;
- MCS, Monte Carlo Steps;
- MC, Monte Carlo;
- HS, High-Spin;
- LS, Low-Spin

Keywords

- Spin Crossover;
- Phase transition;
- Interface propagation;
- Spatiotemporal effects, elasticity;
- Monte Carlo Simulations