7th African Conference on Non Destructive Testing (ACNDT) & the 5th International Conference on NDT and Materials Industry and Alloys (IC-WNDT-MI)

2016

SPATIO-TEMPORAL ASPECTS OF THE DOMAIN PROPAGATION IN A SPIN-CROSSOVER LATTICE WITH DEFECT

Rachid Traiche, Hassane OUBOUCHOU, Mourad ZERGOUG, Kamel Boukheddaden

Abstract : We study the spatiotemporal formation and spreading of the high-spin state (HS) during the cooperative relaxation of the photo-induced metastable high spin (HS) state at low temperature of anelastic lattice, in the presence of a defect injected in the center of the lattice. For that, we designed a 2D rectangular-shaped lattice with discrete spins coupled by springs. The distances between the sites are spin-dependent which prevents any analytical resolution of the present problem. The elastic coupling between the spin-crossover (SCO) sites results in a long-range effective interactions between the spin states from which originates the complexity and the richness of this problem. The numerical resolution of the problem is performed using Monte Carlo simulations on the spin states and theatomic positions. The simulations are restricted to a lattice with a hole (simulating the defect) with afixed size. The presence of the defect shows the dynamics of the spin-crossover transformations startsfrom one corner of the rectangular lattice and propagates along the width (shortest distance to thesurface).Then a second regime of longitudinal propagation takes place, whose velocity slows down significantly in the vicinity of the defect. Then the interface leaves the defect, where it was pinned atlow velocity and accelerates when it approaches the border of the lattice. We have also investigated the spatial dependence of the displacement field, from which we derived the spatial distribution of the divergence, which directly connects to the distribution of the internal strain and elastic energy. Valuable information is derived from the time-dependence of the total elastic energy in particular around the defect.

Keywords : Spin Crossover, phase transition, interface propagation, Defects, elasticity, Monte Carlo Simulations