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Simulation of magnetoelastic response of iron nanowire loop

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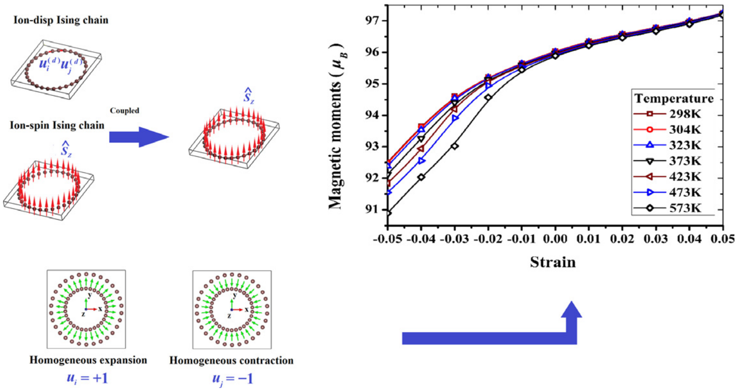
HIGHLIGHTS

- An particle-disp Ising model is proposed according to quantized particle energy.
- Helmholtz free energy of particle-disp model is coupled with spin Ising model.
- Numerical calculation is carried out with VASP package.
- Magnetoelastic response of nanowire under tension is different from that compression.
- Enhancement of magnetic moment takes place at atoms most adjacent to point defect.

GRAPHICAL ABSTRACT



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ABSTRACT

We analyzed the magnetoelastic responses of one-dimensional iron nanowire loop systems with quantum statistical mechanics, treating the particles in the systems as identical bosons with an arbitrary integer spin. Under the assumptions adopted, we demonstrated that the Hamiltonian of the system can be separated into two parts, corresponding to two Ising subsystems, describing the particle spin and the particle displacement, respectively. Because the energy of the particle motion at atomic scale is quantized, there should be more the strict constraint on the particle displacement Ising subsystem. Making use of the existing results for Ising system, the partition function of the system was derived into two parts, corresponding respectively to the two Ising subsystems. Then the Gibbs distribution was obtained by statistical mechanics, and the description for the magnetoelastic response was derived. The magnetoelastic responses were predicted with the developed approach, and the comparison with the results calculated with VASP demonstrates the validity of the developed approach.

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Nomenclatures

H	Hamiltonian of a system
U_0	Energy summation, except magnetic interaction
J_{ij}	Coupling constant, depending on spacing between Particles *i* and *j*
s_i	Spin identity of Particle *i*
B_i	Magnetic flux density of the applied field at the same site of Particle *i*
k_B	Boltzmann constant
T	Kelvin Temperature
Z_{N1}, Z_{N2}, Z_{N3}	Partition functions of combined system, particle-spin system and particle-disp system
U_{Ewald}	Ewald potential
$U_{e-e;} U_{s-s}$	Coulomb interacting energy between electrons; interacting energy between spin particles
u_i	Relative displacement identity for Particle *i*
c_{ij}	Elastic interaction parameter between Particles *i* and *j*
$a^{(ij)}$	Relative position of particles between Particles *i* and *j*
R_i	Magnetostrictive coupling parameter
H_0, H_1, H_2	Hamiltonians of combined system, particle-spin system and particle-disp system
K_0, K_1, K_2	Interact parameters of combined system, particle-spin system and particle-disp system
h_0, h_1, h_2	Reduced magnetic flux densities of combined system, particle-spin subsystem and particle-disp subsystem
λ_1, λ_2	Eigenvalues by transfer matrix of H_0
η_1, η_2	Eigenvalues of H_1 by transfer matrix
γ_1, γ_2	Eigenvalues of H_2 by transfer matrix
F	Helmholtz free energy
q_i	Virtual physical quantity identity
$\varepsilon_s, \varepsilon_u$	Energy levels of particle-spin system and particle-disp system
ψ_{igs}, ψ_{igu}	Wave functions for particle spin and particle displacement
g_{si}, g_{ui}	Degeneracy
n_{si}, n_{ui}	Filled particle numbers of each level
ϕ_t	Numbers of states
$\chi_{0N}, \chi_{1N}, \chi_{2N}$	Generalized magnetic susceptibilities of combined system, particle-spin subsystem and particle-disp sub-system
ε	Strain
G	Gibbs free energy
V_0	Equilibrium volume of supercell
M	Total magnetic moment of a system
a_0	Equilibrium lattice constant
μ_B	Bohr magneton
$p; a$	Pressure; Pitch of nanowire loop
$a^{'}, b^{'}, c^{'}$	Lattice constants of supercell

1. Introduction

The metal magnetic memory (MMM) property [1], ferromagnetic solid deformation fracture [2–5] and constitutive behavior of a magnetostrictive material are related to the relationship between magnetism and deformation. Macroscopically, the magnetic field intensity may be enhanced abnormally at a crack tip in a deformed ferromagnetic solid subjected to displacement fields, based on which a kind of non-destructive testing (NDT) method was developed and has become a practical technology. However, it is known that in the current MMM based NDT method, it is difficult to eliminate the disturbance from the background noise because of a lack of the knowledge of the mechanisms for magnetoelastic responses, especially in low-dimensional cases, which may account for why people unable to simulate the initiation of a crack based on the abnormality of the magnetic intensity. For this reason, to make clear the mechanisms of MMM at nanoscale and low-dimensional cases would help the development and application of NDT.

It has been realized to confine a single atom with the atom probe technique [6] and trapping technique [7] to enhance the stability of low-dimensional solids or to prepare low-dimensional nano-wires [8,9]. Thus, in the study of magnetoelastic response, we can design an experiment, in which a double-walled carbon nanotube can be stretched or compressed, where iron atoms are confined in a circular ring between the two walls, as shown in Fig. 1. In Fig. 1 the iron atoms confined to a circle constitute a nanowire loop, which could expand or contract homogeneously with the deformation of the nanotube. At the atomic scale, this problem cannot be taken as a plane strain problem as in continuum mechanics, and cannot be solved with the conventional theory of elasticity.