Spin-lattice models for magnetoelastic effects in FM and AFM cubic materials

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We present an approach based on the Néel model to build a classical spin-lattice Hamiltonian for cubic crystals capable of describing magnetic properties induced by the spin-orbit coupling like magnetocrystalline anisotropy and anisotropic magnetostriction, as well as exchange magnetostriction. Taking advantage of the analytical solutions of the Néel model, we derive theoretical expressions for the parametrization of the exchange integrals and Néel dipole and quadrupole terms that link them to the magnetic properties of the material. This approach allows us to build accurate spin-lattice models with the desired magnetoelastic properties. We also explore a possible way to model the volume dependence of magnetic moment based on the Landau energy. This feature allows us to consider the effects of hydrostatic pressure on the saturation magnetization. We apply this method to develop a spin-lattice model for BCC Fe and FCC Ni, and we show that it accurately reproduces the experimental elastic tensor, magnetocrystalline anisotropy under pressure, anisotropic magnetostrictive coefficients, volume magnetostriction, and saturation magnetization under pressure at zero temperature. [1] In addition, we have constructed spin-lattice model for the antiferromagnetic cubic compounds. Here we develop a methodology to integrate magnetic properties into interatomic potentials for cubic antiferromagnets by adding a magnetic Hamiltonian which includes both the Heisenberg exchange and Néel model. [2] We apply this approach to NiO by constructing two potentials: one based on the Born model of ionic solids and another using a reference-free modified embedded atom method. Both potentials include magnetoelastic interactions and are validated against Density Functional Theory calculations, showing excellent agreement in mechanical and magnetic properties at zero temperature. These models enable large-scale simulations of magnetoelastic phenomena in antiferromagnets and open avenues for molecular dynamics studies involving coupled electric and magnetic fields in metal oxides.

References:

[1] P. Nieves and J. Tranchida and S. Arapan and D. Legut, Physical Review B 103 (2021) 094437

[2] I. Kornienko and P. Nieves and J. Šebesta and R. Iglesias and D. Legut, Journal of Computational Physics (under review - 2026)