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Determination of symmetry reduced structures using a soft phonon analysis for magnetic shape memory alloys

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Abstract

Ni_2MnGa is a typical example of a Heusler alloy that undergoes a martensitic transformation. In the high temperature austenitic phase it has a cubic $L2_1$ structure, whereas below 200 K the symmetry is reduced by an orthorhombic distortion. Despite lattice deformations of more than 6% and large strains connected to this change, it is completely reversible. Therefore, Ni_2MnGa serves as a shape memory compound. The fact that Ni_2MnGa additionally orders ferromagnetically below 360 K makes the material particularly attractive for applications in actuators and sensors. Nevertheless, its structural details in the martensitic phase are still a subject of much debate. Several shuffling structures have been observed experimentally. The temperature and magnetic field dependent transformations between these structures need to be understood for improvement of the magnetic switching (e.g. operation with higher reliability and smaller magnetic fields).

Our tool for identifying the stable structures and the low energy transition paths is the calculation of free energy surfaces as functions of key reaction coordinates (e.g. the ratio c/a) in density functional theory. (The generalized gradient approximation to the exchange–correlation functional and the projector augmented wave approach implemented in VASP (Vienna *Ab initio* Simulation Package) were used in these investigations.) The different variants of the low symmetry orthorhombic structures lead to characteristic minima on this surface. However, the *ab initio* determination of the experimentally observed shuffling structures is challenging, due to the large phase space of possible atomic positions and the small shuffling formation energies of only a few meV per unit cell. Hence, we used the quasiharmonic approximation in order to compute and analyze phonon spectra. Starting with the symmetric structure of the austenite, the TA_2 (TA standing for transverse acoustic) phonon dispersion shows a phonon softening along the [110] direction. We were able to extract detailed information about the type of this lattice instability from the eigenvectors of the unstable phonon modes. By setting up the corresponding modulated harmonics in supercell calculations, we systematically and efficiently identified stable shuffling structures. The resulting structural phases (austenite, martensite, pre-martensite) allow us to assign and to interpret the experimental observations.

