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Abstract

Electron Localizations in Alloy Exhibiting Nanotwinning †

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Ni_2MnGa is a ferromagnetic shape memory alloy in which a large spontaneous deformation up to 12% has been observed after application of an external magnetic field [1]. The key to such material functionality is the ferroelastic microstructure of martensite with deep hierarchical twinning up to nanoscale [2]. However, the microscopic origin of the martensitic transformation between the high temperature austenitic and low temperature martensitic phases is not fully understood to date as well as exact origin of nanotwining in martensitic phases. In present work we have used first-principles calculations based on density functional theory (DFT) to simulate magneto-optical (MO) Kerr spectra for different phases of Ni_2MnGa alloy: austenite, nonmodulated martensite without nanotwinning and nanotwined martensite represented by 4O structure [3]. The MO spectra provide a valuable insight into the mutual dependence of the the structure of the material and electronic structure and magnetic ordering.

The work of Himmetoglu et al. [4] suggests that the Hubbard treatment of the on-site Coulomb interaction of d-electrons localized on Mn sites (DFT+U) is required to describe correctly the electronic structure of Ni_2MnGa alloy. A comparison of the calculated and measured spectra allowed us to estimate the proper value of Coulomb interaction parameter U, which we found significantly smaller than the value proposed in previous works [4,5]. Using smaller U, we obtain a better quantitative agreement with experiment at least in case of elastic constants and lattice parameters in Ni_2MnGa. Comparison of the newly calculated densities of states covering the electron localization then provides a better insight into the origins of martensitic transformation and nanotwinning.

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