Phonon dispersion of off-stoichiometric Ni_2MnGa sigle crystal

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Inelastic neutron scattering experiments were used to study an off-stoichiometric Heusler-type $Ni_{2.16}Mn_{0.78}Ga_{1.06}$ single crystal. A triple-axis neutron spectrometer, AKANE, was used. The alloy has a martensitic transformation temperature around room temperature (293 K) coincident with a Curie temperature. It is ferromagnetic in the martensitic phase and paramagnetic in the mother phase and is expected as a magnetic-field-induced shape memory alloy. With decreasing temperature the alloy transforms from a cubic structure to a metastable orthorhombic structure and finally to a stable tetragonal structure.[1)] Diffraction patterns of the cubic structure and of the orthorhombic structure projected on the reciprocal cubic c^*-plane are shown in Figs. 1(a) and (b). At 400 K the alloy shows a cubic structure and at 279K it shows an orthorhombic one. In the orthorhombic structure at 279 K, we see several elastic diffuse scatterings along the ⟨110⟩ and ⟨100⟩ directions of the orthorhombic c^*-plane and many weak satellite peaks on these diffuse scatterings. These diffuse scatterings and the satellite peaks appear to show that the lattice is modulated to various extent along ⟨110⟩ and ⟨100⟩ directions.

TA_2-phonon dispersions with ⟨110⟩ and ⟨100⟩ propagations in the cubic phase were measured at several temperatures. As shown in Figs. 1(c) or (d), the softening of the phonon is observed at q=0.3 or at q=0.23, respectively. The softening of the phonon with ⟨110⟩ propagation is explicitly temperature dependent. However, the temperature dependence of the softening of the phonon with ⟨100⟩ propagation is not clear. Near the position in the q-space corresponding to the softening of the TA_2-phonon dispersion, the elastic satellite peaks in the metastable orthorhombic structure appear. Thus, the softening of the TA_2-phonon in the mother phase appears to be a precursory phenomenon to the metastable martensitic structure.

1) K. Inoue, Y. Yamaguchi, H. Hiraka, *et. al.*: J. Phys. Soc. Jpn. **78** (2009) 034602.

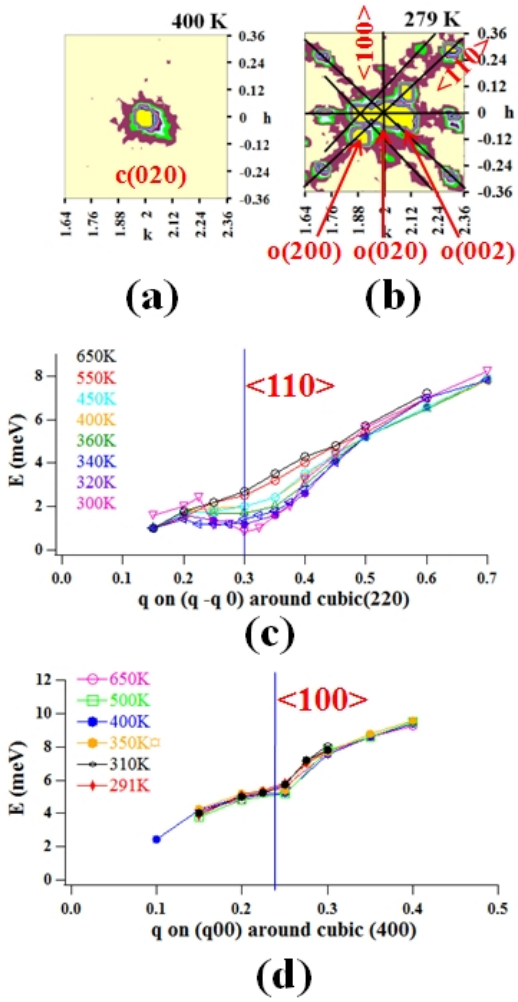

Fig. 1. (a), (b) Elastic q-mesh scans on the reciprocal lattice cubic c^*-plane at 400 and 279 K, (c), (d) TA_2-phonon dispersions with cubic ⟨110⟩ and ⟨100⟩ propagations.