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Keywords

ferromagnetic materials, stoichiometry, photoelectron spectroscopy, annealing

Disciplines

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Comments

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Modulation on $Ni_2MnGa(001)$ surface

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Abstract. We report periodic modulation on (001) surface of Ni2MnGa ferromagnetic shape memory alloy. For the stoichiometric surface, analysis of the low energy electron diffraction (LEED) spot profiles shows that the modulation is incommensurate. The modulation appears at 200K, concomitant with the first order structural transition to the martensitic phase.

Keywords: Low-energy electron diffraction, Commensurate-incommensurate transformations
PACS: 61.05.jh, 68.35.Rh, 71.45.Lr, 75.50.Cc

INTRODUCTION

There is a surge of interest in the basic physics of Ni-Mn-Ga ferromagnetic shape memory alloy because of its potential as a functional material with large magnetic field induced strain as a magnetic sensor with large negative magnetoresistance. Ni_2MnGa, which is ferromagnetic with Curie temperature of 375K, has a cubic $L2_1$ structure in the austenitic phase. Around 200K, it undergoes a first order structural transformation to the lower symmetry martensitic phase. Since the magnetic field induced strain is related to the modulated structure, its behavior at the surface is of fundamental importance. Furthermore, surface study of Ni_2MnGa is important because it could act as a smart substrate and modify the properties of the adlayers grown on it.

EXPERIMENTAL

Ni_2MnGa single crystal was grown by the Bridgman method. The bulk composition was confirmed by wavelength dispersive x-ray spectroscopy. LEED was performed at a base pressure of about 4×10^{-11} mbar using ErLEED optics from Specs GmbH, Germany. Stoichiometric $Ni_2MnGa(001)$ surface was prepared by sputtering with 1.5 keV Ar+ ions and annealing at 700K for 1 hr.[1] The cleanliness and the surface composition were determined using x-ray photoelectron spectroscopy (XPS). To obtain a single variant state in the martensitic phase, the crystal was clamped along [0,1] direction in a sample holder designed for studying complex metal surfaces. The martensitic transition temperatures for the bulk crystal have been determined using differential scanning calorimetry. Heat flow data show a clear signature of a first order martensitic transition with the martensitic start temperature (M_s) of 206.5K, martensitic finish temperature M_f= 205K, austenitic start temperature A_s= 215.7K and austenitic finish temperature A_f= 216.7K. The width of the hysteresis ($A_s - M_s$= 9K) is small. The latent heat is 0.2 KJ/mole.

RESULTS AND DISCUSSIONS

Ni_2MnGa is in the austenitic phase at room temperature since M_s is 206.5K. Sharp LEED spots representing the square reciprocal lattice is observed in (Fig. 1(a, b)), indicating that the surface is fairly well ordered. Comparison of LEED patterns recorded with different beam energies (E_p) shows that faceting and surface reconstruction are absent. The square unit cell shown by the dashed lines in Fig. 1(a) correspond to the (001) projection of the body centered tetragonal primitive unit cell of the bulk structure. A spectacular modification of the LEED pattern occurs in the matensitic phase with the appearance of an array of satellite spots that are observed over the range $85<E_p<120$ eV in the [1,0] direction in (Fig. 1(c–f)).

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The intensity profiles in Fig. 2 show that all the satellite spots move toward the (00) spot as E_p increases. To understand the origin of the satellite spots in the martensitic phase, we first examine their separations.

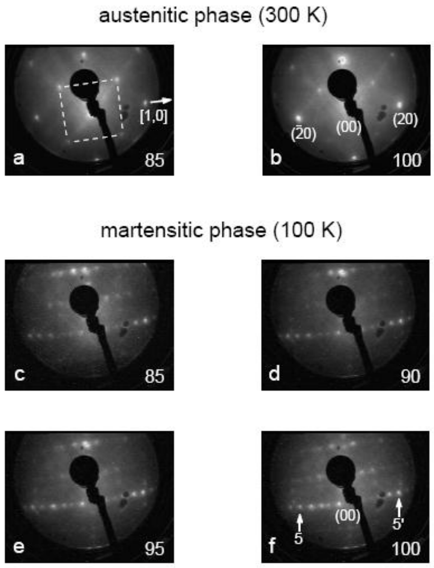

FIGURE 1. Low energy electron diffraction (LEED) patterns of Ni_2MnGa (001) in (a-b) the austenitic phase at room temperature and in (c-f) the martensitic phase at 100K. The electron beam energies (E_p) in eV are shown in the bottom right corners.

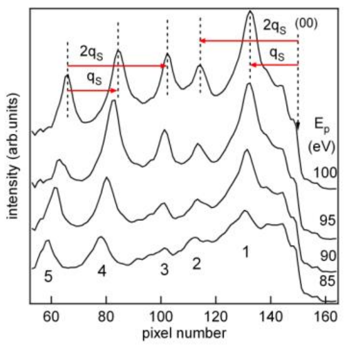

FIGURE 2. A series of intensity profiles in the martensitic phase at 100K along [$\bar{1}$10] for different E_p. where b^*_{MS} (=g_p) is the primitive RL vector.

To quantify the spot separations, we have considered 37 profiles for averaging, including those shown in Fig. 2. The separations are obtained as a fraction of the primitive RL vector b^*_{MS}, which is half of the non-primitive RL vector obtained by joining spot 5 and (00). It is clear that the fundamental reflections like spot 5 and (00) are surrounded by satellites corresponding to a surface modulation wave vector q_S with maximum n= 2, as shown in Fig. 2. Averaging over 50 spot separations excluding the 2-3 separation, we obtain q_S= (0.4246±0.0012)$b^*_{MS,}$ which is very close to the 5M incommensurate q_B value of 0.4248 for bulk Ni_2MnGa reported by Righi *et al.*[2] This similarity of q_S to q_B demonstrates that the modulation at the surface is indeed incommensurate.

Having demonstrated the existence of an incommensurate modulation for stoichiometric Ni_2MnGa surface, here we discuss its origin. The theoretical work by Bungaro *et al.*[3] established a dynamical instability of the TA2 phonon related to a long range anomalous contribution to the phonon frequency due to electronic screening, which was shown to arise due to Fermi surface nesting with a nesting wave vector of 0.43.[3] CDW is known to be driven by Fermi surface nesting and interestingly, the nesting wave vector (0.42-0.43) obtained from theory[3] is very similar to q_S (= 0.4246) obtained by us. Experimental support for CDW till date has come from anomalies in phonon dispersion curves from inelastic neutron studies and transverse modulation with q=0.43 was related to electron phonon interactions.[4]From present studies, evidence of CDW is obtained from the temperature dependence of the LEED pattern. Patterns recorded at small temperature steps of 2-3K during cooling show that the surface modulation appears at 200K, concomitant with the first order structural transition to the martensitic phase. Thus, 200K is the surface martensitic start temperature (M_{sS}). In the martensitic phase, as the temperature is decreased from 200K to 100K, the satellite peaks do not shift but become more intense with respect to the fundamental spot. This shows that the surface CDW is more stabilized at lower temperatures, which indicates electron-phonon coupling to be its possible origin.

To conclude, we demonstrate evidence of an incommensurate modulation on Ni_2MnGa(001) that possibly arises from surface charge density wave related to Fermi surface nesting.

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