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Modulation on Ni$_2$MnGa(001) surface


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Abstract. We report periodic modulation on (001) surface of Ni$_2$MnGa 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

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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$_2$MnGa, 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$_2$MnGa is important because it could act as a smart substrate and modify the properties of the adlayers grown on it.

EXPERIMENTAL

Ni$_2$MnGa 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 4x10$^{-11}$ mbar using ErLEED optics from Speex GmbH, Germany. Stoichiometric Ni$_2$MnGa(001) surface was prepared by sputtering with 1.5 keV Ar$^+$ ions and annealing at 700K for 1 hr. 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$_2$MnGa 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 martensitic 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)).
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$_2$MnGa (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 [-10] for different $E_p$, where $b^*_{MS} (\approx g_5)$ 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 $q_S = (0.4246 \pm 0.0012)b^*_{MS}$, which is very close to the 5M incommensurate $q_S$ value of 0.4248 for bulk Ni$_2$MnGa reported by Righi et al. 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$_2$MnGa surface, here we discuss its origin. 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 $q_S = (0.4246 \pm 0.0012)b^*_{MS}$, which is very close to the 5M incommensurate $q_S$ value of 0.4248 for bulk Ni$_2$MnGa reported by Righi et al. This similarity of $q_S$ to $q_B$ demonstrates that the modulation at the surface is indeed incommensurate.

To understand the origin of the satellite spots in the martensitic phase, we first examine their separations. 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 $q_S = (0.4246 \pm 0.0012)b^*_{MS}$, which is very close to the 5M incommensurate $q_S$ value of 0.4248 for bulk Ni$_2$MnGa reported by Righi et al. 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$_2$MnGa surface, here we discuss its origin. The theoretical work by Bungaro et al. 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. CDW is known to be driven by Fermi surface nesting and interestingly, the nesting wave vector (0.42-0.43) obtained from theory 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. 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$_2$MnGa(001) that possibly arises from surface charge density wave related to Fermi surface nesting.

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**REFERENCES**