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Electronic Structures and Various Physical Properties of Ferromagnetic-Shape-Memory Ni2MnGa Alloy Films

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Ni_2MnGa alloy is the only known ferromagnetic-shape-memory (FSM) alloy. In order to understand its various physical properties more thoroughly, the electronic structures of FSM Ni2MnGa alloy are calculated.

FSM Ni_2MnGa alloy gives us a unique opportunity to understand the relationship between the magnetism and lattice dynamics, because it undergoes a martensitic transformation near 220 K accompanied by a significant phonon softening in the TA_2 acoustic branch along the (110) direction. This kind of phonon softening is usually observed in most of some *B2*-phase alloys with martensitic transformation, such as NiTi, NiAl, and so on, and is closely related to the Fermi surface nesting (FSN). Our calculational results of the generalized susceptibility $X(\mathbf{q})$ and the geometry of Fermi surface with various magnetizations show that FSN is located at $\mathbf{q} = (\zeta, \zeta, 0)$ with $\zeta = 0.3$ in the paramagnetic phase and it moves towards the higher ζ values as the magnetization develops. The FSN effect is optimized at 83 % of full magnetization and the $\mathbf{q}$ vector of nesting at 83 % is exactly the same as that of phonon softening, $\zeta = 1/3$. The 83 % magnetization corresponds to the temperature at which the premartensitic transformation occurs. These results imply that FSN is still a driving force of phonon softening in the ferromagnetic phase and down to the temperature where the structural phase transition occurs. Therefore, the anomalies in the lattice dynamics and the structural phase transition in Ni_2MnGa alloy are closely related to the magnetic ordering through FSN.

Recently, we have found that disordered Ni_2MnGa alloy films exhibit a behavior similar to Pauli paramagnets without any ferromagnetic ordering down to 4.2 K. A possible explanation of the disappearance of the magnetic moment in the disordered film will be discussed with the aid of the first-principles electronic-structure calculations. The theoretical results showed that swapping of the Ni and Mn atoms in the Ni-Mn-Ni-Ga chain along the (111) direction, resulting in Mn-Ni-Ni-Ga chain, reduces the magnetic moment significantly. The loss of magnetism in the disordered film is ascribed to a significant redistribution in d-bands of both Ni and Mn. The redistribution is rather significant in the e_g character of Mn d electrons for a simple disorder [Mn-Ni-Ni-Ga chain along the (111)-direction], and is expected to become enhanced for the other characters of Mn and Ni d electrons if more disordering is introduced.