

Abstract Submitted
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Origin of martensitic transition in NiMnIn alloys¹ RENAT SABIRIANOV, NABIL AL-AQTASH, University of Nebraska at Omaha, LE ZHANG, ANDREI SOKOLOV, University of Nebraska Lincoln — We have performed density functional theory calculations of the effect of the martensitic transition on the electronic structure of Ni₂MnIn system. We find that both the cubic and tetragonally distorted (martensite) phases are ferromagnetic. The cubic phase has lower total energy than that of the tetragonal phase by $\Delta E=0.3\text{eV/f.u.}$ Larger relative concentration of Mn in Ni₂Mn_{1.5}In_{0.5} change the relative stability in favor of martensitic phase. Calculated local magnetic moment is $3.2\mu_B$ for Mn, while only $0.3\mu_B$ for Ni. The total minority densities of states exhibit a pronounced feature at Fermi level (related mainly to Ni3d states) that is sensitive to the local environment of Ni sites. The increase of the Mn content, where Mn substitutes for In sites and orders antiferromagnetically to the magnetization of the regular Mn sites, causes substantial modification in $N(E_F)$ affecting the transport properties upon the phase transition. The band structure analysis reveals that the tetragonal distortion changes the Fermi velocity at the Fermi level that may result in substantial change in resistance upon martensitic transition. We compare our results with the magnetic and transport measurements performed on the thin films of Ni₅₀Mn₃₅In₁₅ grown by laser-assisted molecular beam epitaxy deposition. Magnetic and transport measurements reveal the existence of martensite-austenite phase transition on tensile stressed films and co-existence of both phases at room temperature for compressively strained films. Thin films and experimental results were obtained in close collaboration with group of N. Ali, SIUC.

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Renat Sabirianov
University of Nebraska at Omaha

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