Abstract Submitted
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Origin of Martensitic Phase Transitions in Thin Films of Ni-Mn-In on MgO Substrate[1] RENAT SABIRIANOV, University of Nebraska at Omaha, ANDREI SOKOLOV, University of Nebraska Lincoln, NABIL AL-AQTASH, University of Nebraska at Omaha — We study the impact of the substrate on the martensite transformation of Ni-Mn-In thin films using density functional theory calculations. Our calculation of bulk $Ni_2Mn_{1.5}In_{0.5}$ alloy shows that the cubic phase is unstable against the tetragonal distortion phase and undergoes the martensitic transformation to form tetragonal martensite in ferrimagnetic state. $Ni_2Mn_{1.5}In_{0.5}$ thin films (in both cubic and tetragonal phases) on MgO (001) substrates are studied. The presence of MgO substrate changes the relative stability of ferrmomagnetic (FM) austenite and ferrimagnetic (FiM) martensite states. The energetically favorable structures of the MgO-$Ni_2Mn_{1.5}In_{0.5}$ systems depend on the lattice parameters. Our calculations show that the energy difference between FM austenite and FiM martensite states in 12 layers of $Ni_2Mn_{1.5}In_{0.5}$ film on MgO (001) substrate is (ΔE = 0.08eV) per NiMnIn f.u, compared to (ΔE = 0.24eV) in the bulk at the same lattice parameters. When the lattice parameters of 12 layers of $Ni_2Mn_{1.5}In_{0.5}$ film have values close to those of MgO substrate, this energy difference become (ΔE = -0.16eV) per NiMnIn f.u. These results clearly indicate the possibility of control of martensitic transition in thin films by substrate. We compare our results with the magnetic and transport measurements performed on the thin films of $Ni_{50}Mn_{35}In_{15}$ grown by laser-assisted molecular beam epitaxy deposition.

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