Epitaxial Growth and Electronic Structure of Half Heusler Co_{1-x}Ni_xTiSb

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Half Heusler compounds are an exciting class of intermetallics due to their multifarious electrical and magnetic properties, including semiconducting [1], half metallic [2], and thermoelectric [3]. Additionally, a number of the half Heusler compounds have been predicted to be topological insulators [4]. Their crystal structure and lattice parameters are closely related to III-V compound semiconductors, suggesting the possibility of half Heusler/III-V semiconductor heterostructures with unique properties. Applications of epitaxial half Heusler compound rely on a deeper experimental understanding of their electronic band structure. Most experimental studies of half Heusler compounds have been limited to bulk polycrystalline samples, which cannot be used for measurements of band dispersion and are not ideally suited for transport studies.

In this talk we demonstrate the epitaxial growth of the electron-doped half Heusler series Co_{1-x}Ni_xTiSb by molecular beam epitaxy (MBE). CoTiSb has been extensively studied in the bulk and recently in MBE grown films where record high carrier mobilities were demonstrated [5]. In this presentation, the influence of the addition of Ni doping/alloying to CoTiSb epitaxial films is investigated. Co_{1-x}Ni_xTiSb epitaxial films were grown on MBE-grown InAlAs (001) epitaxial layers grown on InP (001) substrates. The reflection high energy diffraction (RHEED) patterns were streaky indicating relatively flat surfaces and RHEED intensity oscillations were observed for all levels of nickel alloying investigated (Fig. 1). This is consistent with a layer-by-layer growth mode. The temperature dependent electrical transport measurements suggest that films of composition $x \le 0.1$ showed thermally activated transport (Fig. 1(e)). Using Sb-capping and decapping, ex-situ synchrotron based Angle-resolved photoemission spectroscopy (ARPES)

experiments for determining the electronic band structure were performed to investigate the effects of nickel. The appearance of the conduction band minimum at the bulk X point below the Fermi level occurs for x>0.1, suggesting a crossover from semiconductor to metallic behaviour. The effects of nickel alloying on the valence band, conduction band, and Fermi level positions will be discussed.



Figure 1. (a)-(c) RHEED patterns of $Co_{0.5}Ni_{0.5}TiSb$, (d) RHEED oscillations demonstrating layer-by-layer growth. (e) Temperature dependent resistivity.

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Supplementary information:



Figure 2. Normal emission measurement probing along Γ -X direction of the bulk Brillouin zone for (a) Co_{0.9}Ni_{0.1}TiSb and (b) Co_{0.5}Ni_{0.5}TiSb. Fermi surface slice (k_x vs k_y) 80meV below the Fermi level for (c) Co_{0.9}Ni_{0.1}TiSb and (d) Co_{0.5}Ni_{0.5}TiSb (001) surfaces measured with 110 and 104 eV photon energies respectively which corresponds to the bulk X point. In-plane dispersions showing cuts at k_x = 0 indicated by the arrows for (e) Co_{0.9}Ni_{0.1}TiSb and (f) Co_{0.5}Ni_{0.5}TiSb. (g) Bulk and surface Brillouin zones.