Measurement of band-alignments in semiconducting half-Heusler heterojunctions grown by MBE

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Half-Heusler (h-H) compounds are an exciting class of intermetallics due to their diverse electrical and magnetic properties, including semiconducting [1], half metallic [2], thermoelectric, and topologically insulating [3]. With a crystal structure and lattice parameters similar to III-V compound semiconductors, the possibility of h-H/III-V semiconductor heterostructures with unique properties is achievable. Integration of epitaxial h-H compounds with existing III-V technologies requires a deeper understanding of their interface. Most experimental studies of h-H compounds have been limited to bulk polycrystalline samples, which cannot be used for measurements of interface properties. CoTiSb has been extensively studied in the bulk and recently in molecular beam epitaxy (MBE) grown films where record high carrier mobilities were demonstrated [4] and the valence band offsets measured with lattice matched III-Vs [5]. However, the conduction band offsets expected from density functional theory vary immensely depending on the band gap obtained. Heyd, Scuseria, Ernzerhof functionals predict a bandgap of 1.45 eV [5], while the generalized gradient approximation gives 1.0 eV [1]. Electron transport across and confined to these interfaces can give great insight into these values.

In this presentation, the heterointerfaces formed between the semiconducting h-H compound CoTiSb and the III-V compounds, InAlAs and InGaAs, are investigated through vertical transport measurements. In addition, the heterointerface formed between CoTiSb and another semiconducting h-H, NiTiSn is investigated. Lattice-matched $In_{0.52}Al_{0.48}As$ and $In_{0.53}Ga_{0.47}As$ layers were epitaxially grown on InP (001) substrates in a dedicated III-V MBE system. The epitaxial CoTiSb and NiTiSn layers were grown in a separate dedicated MBE system. A variety of heterojunctions between CoTiSb and the III-Vs were designed and grown. Heterointerfaces between CoTiSb (intrinsically n-type) and n-InGaAs, p-InGaAs, n-InAlAs, and p-InAlAs were investigated. Temperature-dependent vertical transport I-V and C-V measurements of the n-n and n-p structures were performed for etched mesas of a variety of sizes. In addition, the valence-band discontinuity and interdiffusion in an abrupt CoTiSb/NiTiSn heterojunction were determined using XPS. Vertical and in-plane transport were performed to probe the band alignment. Finally, by alloying Fe with CoTiSb, p-type CoTiSb is achievable. CoTiSb based p-n homojunctions were formed and the electrical properties measured.

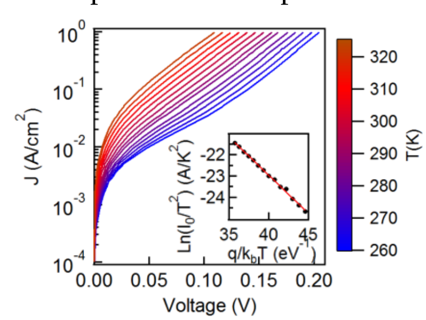

Figure 1. Temperature dependence of the I-V curves of a CoTiSb/p-InGaAs junction.

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Supplementary information:

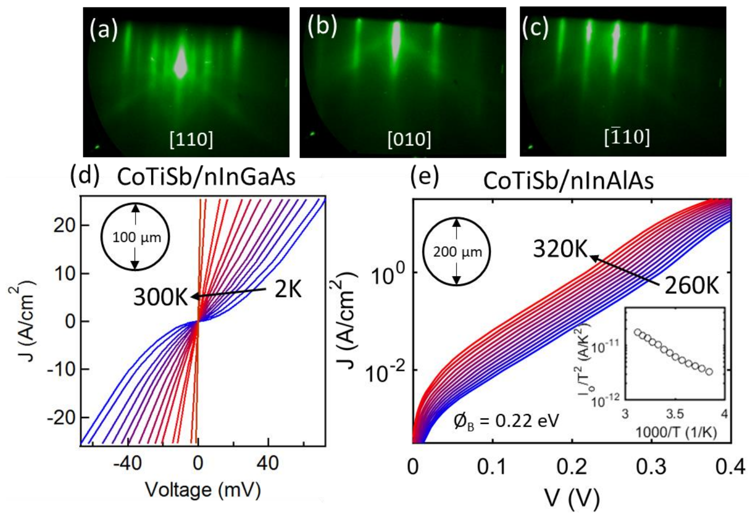

Figure S1. (a-c) Reflection high-energy electron diffraction patterns for 25 nm CoTiSb grown on InAlAs buffer layer. Temperature-dependence of the I-V curves for a 25 nm CoTiSb layer on (d) n-InGaAs (near Ohmic) and (e) n-InAlAs (rectifying) buffer layers grown on n-InP (001). The inset shows a Richardson plot of extracted from (e) that gives an effective barrier height of 0.22 eV.

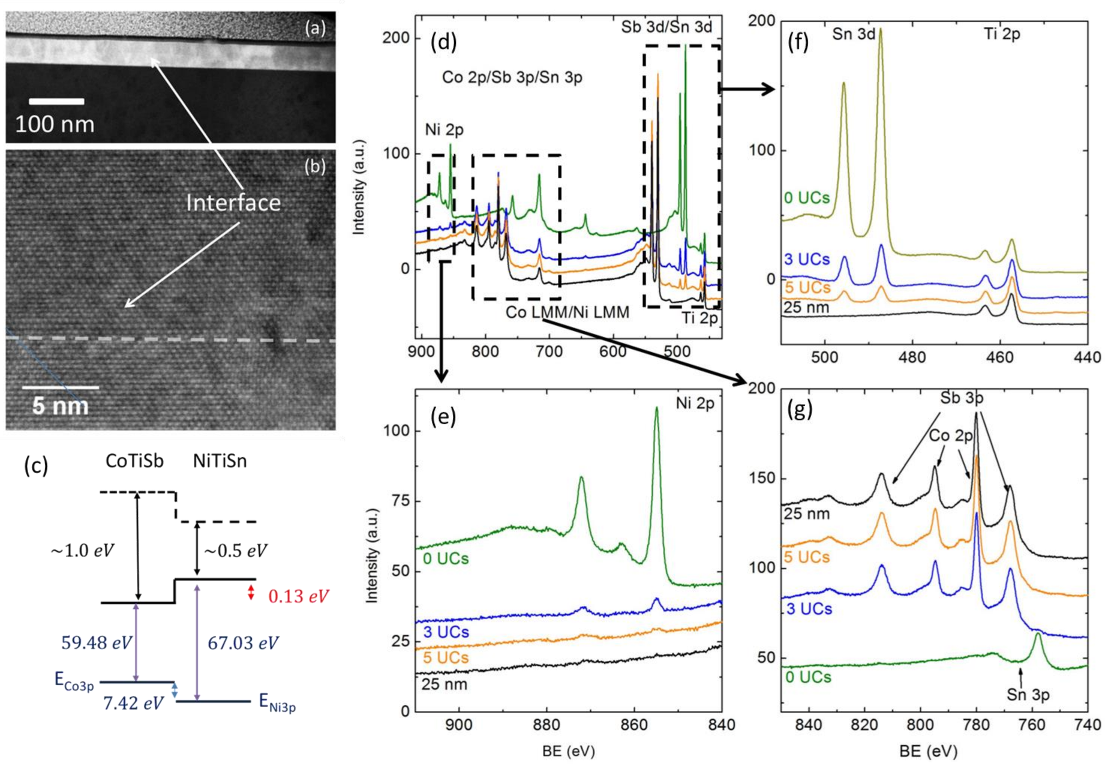

Figure S2. (a) Cross-sectional HAADF-STEM of a 25nm CoTiSb/ 25nm NiTiSn heterojunction grown on MgO taken along MgO [100] zone axis. (b) 20x magnification STEM of the CoTiSb/NiTiSn interface shown in (a). (c) CoTiSb/NiTiSn band alignment with the valence band offsets determined from X-ray photoemission spectroscopy (XPS) and the conduction band offsets estimated from band gaps calculated from DFT using the generalized gradient approximation. (d-g) XPS scans of CoTiSb/NiTiSn structures with varying CoTiSb thickness on top of NiTiSn.