Gold-gold dimer buckling and electronic structure of epitaxial LaAuSb films

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Recently, a new subset of hexagonal Heuslers with composition *Ln*AuSb (*Ln* = La-Nd, Sm) was predicted to exist and shown to be stable in bulk polycrystalline samples[1]. These compounds contain 19 electrons per formula unit, typically thought to be unstable through traditional electron counting rules, however these compounds have been predicted to be stabilized through by highly localizing the 19th electron in Au-Au dimer bonds. Of these new phases, LaAuSb was also predicted through bandstructure calculations to be a Topological Dirac Semimetal (TDS). Here, we will (1) investigate this unique crystal structure and (2) study the electronic properties and structure of single phase epitaxial LaAuSb thin films.

In the original study, LaAuSb was grown in a bulk crystal, however it was both polycrystalline and full of impurity phases and thus it did not lend itself well to study. Here we use molecular beam epitaxy (MBE) to grow single crystalline thin films on c-plane sapphire to investigate the proposed "dimerized" structure. Growth was monitored in-situ by reflection high energy electron diffraction (RHEED) in which the resultant film patterns were streaky and well-resolved Kikuchi lines were observed (Fig. 1a,b), indicating the well-ordered and relatively flat surface of the film. Strong RHEED oscillations were observed throughout growth as well as Kiessig fringes (Fig. 1d,e) which is also consistent with a layer-by-layer growth mode resulting in a smooth surface and substrate/film interface. Magnetotransport measurements were conducted and show the expected metallic behavior with a residual resistivity ratio (RRR) of 2.25 (Fig. 1f). Angle-resolved photoemission spectroscopy (ARPES) measurements were conducted at BL-29ID at the Advanced Photon Source, using a vacuum suitcase to protect the film surface. The valence band density of states is compared to DFT calculations assuming both the dimerized and non-dimerized versions of the LaAuSb crystal. The crystal structure, magnetotransport, and electronic structure will be discussed.

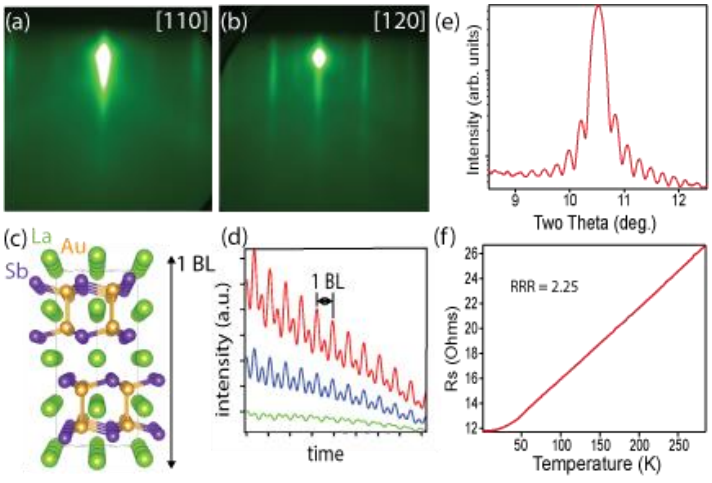

Figure 1. (a), (b) RHEED patterns of LaAuSb, (c) single unit cell of LaAuSb, (d) RHEED oscillations, (e) Kiessig fringes, (f), temperature dependent resistivity

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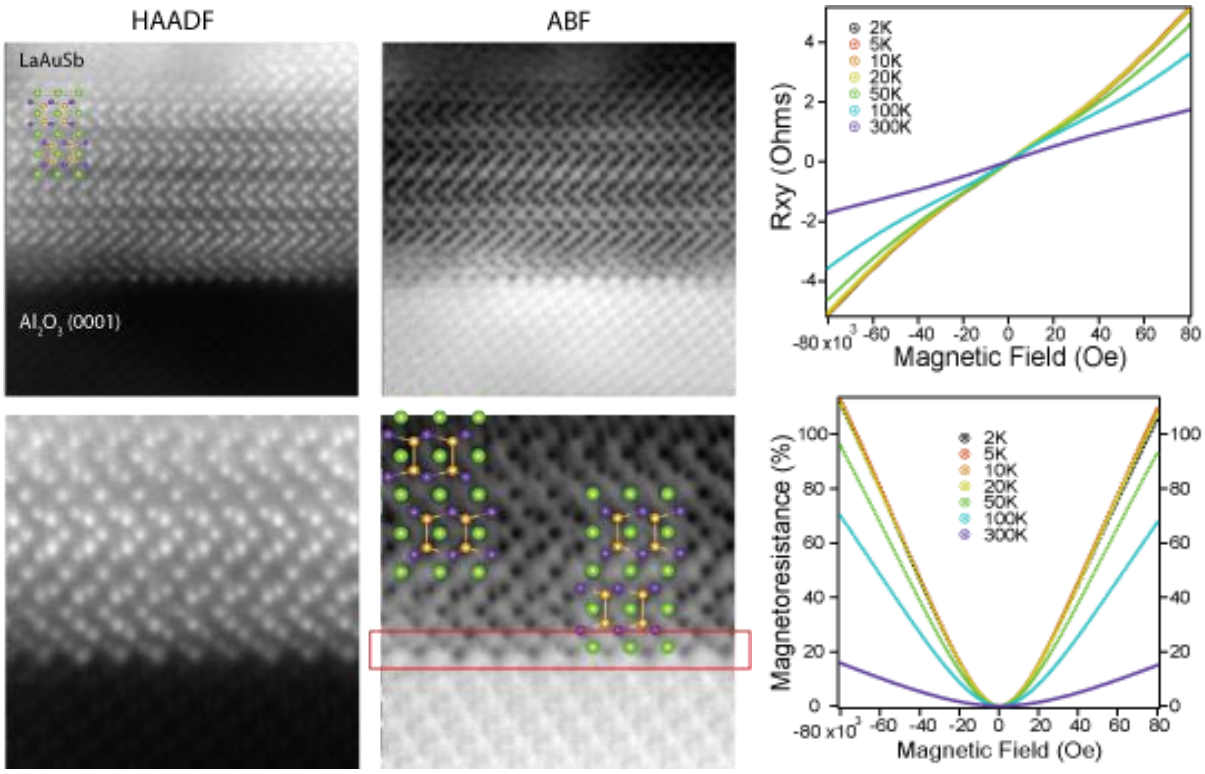

Figure 2. (a)-(d) Cross sectional STEM images of the interface between the LaAuSb film and Al_2O_3 substrate. Overlay is the predicted crystal structure from Siebel *et al.* In (d) the interfacial region is highlighted to emphasize the different chemistry observed at the interface. (e),(f) display magnetotransport data for a range a temperatures from 300K-2K. Film thickness is found to be roughly 40nm, giving a zero-field resistivity of ~54 μΩ*cm at 2K.