Epitaxial Growth and Electronic Structure of Semiconducting Half-Heusler FeVSb

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Although FeVSb is experimentally known as a high figure of merit thermoelectric material [1], challenges associated with fabricating high quality single crystalline samples have hampered a fundamental understanding of its electronic structure [2]. For example, while recent first-principles calculations show that the DFT band gap is highly sensitive to the choice of exchange and correlation functional (LDA predicts 0.36 eV and HSE predicts 1.45 eV [3,4]), its experimental bandgap is not known. Here, we demonstrate the epitaxial growth of FeVSb on MgO (001) by solid source molecular beam epitaxy. The single crystalline phase and epitaxial alignment were confirmed by reflection high-energy electron diffraction (RHEED) and X-ray diffraction (Fig. 1). By tuning the growth temperature and relative Sb flux, we find that FeVSb can be grown in a self-limiting, Sb adsorption-controlled window. Further tuning of the Fe:V flux ratio (by QCM and RBS measurements) then allows us to grow stoichiometric FeVSb. Our angle-resolved photoemission spectroscopy (ARPES) reveals that the band gap of FeVSb is at least 0.6 eV (Fig. 2), much larger than the 0.36 eV band gap predicted by LDA calculations, and the measured valence band width is smaller than the LDA width by nearly a factor of two. We present further calculations and experimental results to decipher this discrepancy.

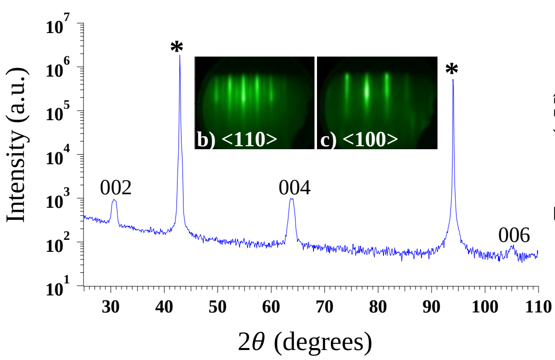

Figure 1 a) 2θ-ω scan of the 100 nm FeVSb on MgO (001). Substrate reflections are marked by asterisk. b) – c) RHEED pattern of the film grown at 490°C along the [110] and [100] azimuths respectively.

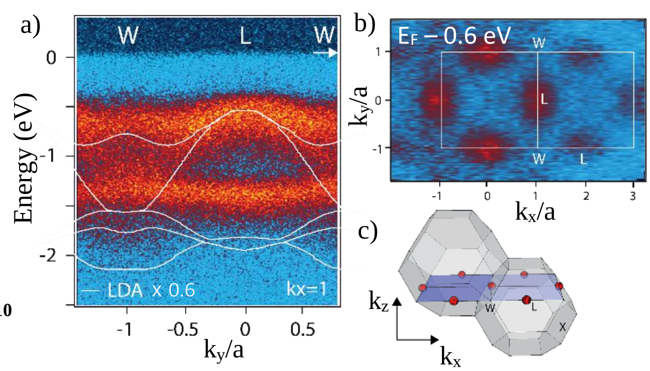

Figure 2 a) In-plane dispersion measured by ARPES (color scale) and comparison to calculation using the local density approximation. The measured valence band width of only 60% along W-L direction. b) Constant energy (E_F – 0.6eV) slice at constant k_z = π/a. c) Schematic bulk Brillouin zone and slice through constant k_z = π/a, corresponding to Fig. 2b.

[1] C. Fu, H. Xie, Y. Liu, T. Zhu, J. Xie, and X. Zhao, Intermetallics. **32**, 39 (2013).
[2] L. Jodin, J. Tobola, P. Pecheur, H. Scherrer, and S. Kaprzyk, Phys. Rev. B. **70**, 184207 (2004).
[3] F. Shi, M. Si, J. Xie, K. Mi, C. Xiao, and Q. Luo, J. Appl. Phys. **122**, 215701 (2017).
[4] B. Nanda, and I. Dasgupta, J. Phys.: Condens. Matt. **15**, 7307 (2003).

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