doi:10.1017/S1431927617008066
Microsc. Microanal. 23 (Suppl 1), 2017

HAADF-STEM Study of MBE-Grown Dirac Semimetal Cd_3As_2

Salva S. Rezaie[1], Honggyu Kim[1], Timo Schumann[1], Manik Goyal[1] and Susanne Stemmer[1]

[1.] Materials Department, University of California, Santa Barbara, CA, USA

Topological semimetals have recently generated significant excitement as new quantum materials. They can exhibit states such as Weyl semimetal, topological superconductor, and topological insulators. Topological semimetals show high carrier mobilities, surface Fermi arcs, and unusual magnetoresistance behavior, which makes them great candidates for next generation electronic and spintronic devices [1]. Recently, cadmium arsenide (Cd_3As_2) has attracted significant attention due to its high mobility, enormous magnetoresistance, low effective mass, and nontrivial Berry phase [2]. Epitaxial films of Cd_3As_2 are needed for integration into devices. While the electronic properties of Cd_3As_2 have been studied, its microstructure and the influence it has on the properties have not yet been extensively studied.

The crystal structure of Cd_3As_2 consists of a large unit cell of 160 atoms (at room temperature) and furthermore depends on the growth conditions and temperature. It can be described as a Cd-deficient version of a Cd_4As_2 antifluorite structure that misses one-fourth of the Cd atoms. In this structure, Cd atoms shift from their ideal positions and displace toward Cd vacancies [3]. Cd atoms occupy the cube shaped array positions (similar to the F position in anti-fluorite CaF_2) and As atoms distributed at FCC positions of Cd_3As_2 film (Ca position in CaF_2 crystal) [3]. At high temperature, the Cd vacancies are disordered and the crystal has the high symmetry FCC structure of space group $Fm\bar{3}m$. Depending on growth conditions, at low temperature adopts either noncentrosymmetric $I4_1cd$ or centrosymmetric $I4_1acd$ crystal space group may be adopted [3]. Recent studies [4] suggested that lack of inversion symmetry in $I4_1cd$ structure causes a lifting of the spin degeneracy close to Dirac point and the formation of Weyl semimetal. Accordingly, the presence or lack of rotation symmetry has significant role in determining electronic properties of Cd_3As_2. However, at present it is unclear which crystal structure and symmetry epitaxial films will adopt. Hence, detail crystal structure study will help to better understand the electronic states of Cd_3As_2.

In this study [5], we investigate epitaxial Cd_3As_2 films on GaSb buffer layers grown by molecular beam epitaxy (MBE). We use quantitative STEM to determine their atomic structure. To improve signal to noise ratio and minimize scan distortion, 20 fast-scan images were cross-correlated and averaged. Figure 1(a) shows a high-angle annular dark-field (HAADF)-STEM image of Cd_3As_2/GaSb/GaAs heterostructure. Abrupt interfaces are obtained. Figure 1(b) shows a schematic of Cd_3As_2 in the $I4_1cd$ crystal space group along $[1\bar{1}0]$. The dashed circles indicate the position of the Cd vacancies in alternating directions. It is clear that the row along red arrow is occupied by Cd atoms, whereas the row indicated by blue arrow contains Cd vacancies. Alternating row of Cd vacancies can be identified in HAADF-STEM image of Cd_3As_2 along $[1\bar{1}0]$ in Figure 1(c). Figure 1(d) shows a drop in intensity of blue row with missing Cd atoms. The non-centrosymmetric $I4_1cd$ crystal structure also shows similar ordered Cd vacancies. Further analysis based on Cd atom position and its shift from ideal antifluorite position as well as low angle position averaged convergent beam electron diffraction (LA-PACBED) are used to determine crystal distortion and symmetry. The study provides insights into the epitaxial Cd_3As_2 crystal structure and symmetry and associated Dirac semimetal behavior [6].

References:

[1] Burkov, A. A., Nat. Mater. **15**, (2016), 1145.
[2] Liu, Z. K. et al.,Nat. Mater. **13**, (2014), 677.
[3] Ali, M. N. et al., Inorg. Chem. **53**, (2014), 4062.
[4] Wang, Z.et al., Phys. Rev. B **88**, (2013), 125427
[5] Schumann, T., Goyal, M., Kim, H. & Stemmer, S., APL Mater. **4**, (2016), 126110
[6] The authors acknowledge support by the U.S. Department of Energy (Grant No. DEFG02-2ER45994).

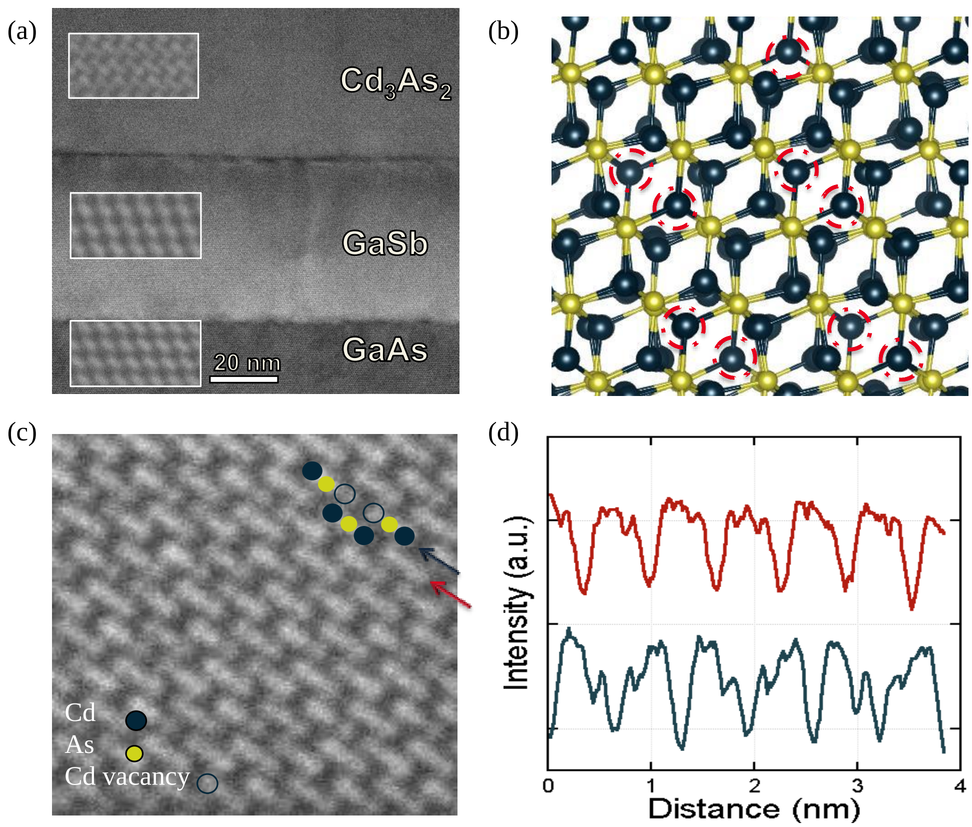

Figure 1. (a) HAADF-STEM image of Cd_3As_2/GaSb/GaAs heterostructure with high resolution image of each layer. (b) Schematic of the Cd_3As_2 structure in the $I4_1cd$ space group along $[1\bar{1}0]$ projection. (c) High resolution HAADF-STEM of Cd_3As_2 film with associated ordered Cd vacancies. (d) Intensity line along two red and blue rows

https://doi.org/10.1017/S1431927617008066 Published online by Cambridge University Press