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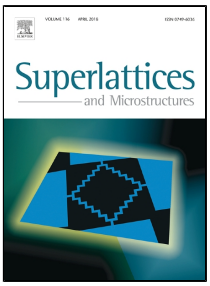

Experimental and First-principles study of defect structure of topological insulator Bi_2Se_3 single crystal

M. Zhang, T.T. Song, L.G. Liu, Q.Y. Liu, T.X. Zeng, H. Yang

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Experimental and First-principles study of defect structure of topological insulator Bi_2Se_3 single crystal

M. Zhang[a,*], T. T. Song[a], L. G. Liu[a], Q.Y. Liu [b], T. X. Zeng[a], , H.Yang[a]

[a] *College of Physics and Space science, China West Normal University, Nanchong, 637002, Sichuan, China*

[b] *Key Laboratory of Advanced Technology of Materials (Ministry of Education), Superconductor and New Energy R&D Center (SRDC), Mail stop 165#, Southwest Jiaotong University, Chengdu 610031, China*

Abstract: High quality single crystal of Bi_2Se_3 was grown using a modified Bridgman technique. Their phase structures, electrical transport properties and defects were studied. The results of X-ray diffraction and High-resolution transmission electron microscopy showed that the as-obtained bulk Bi_2Se_3 crystal has layered structure with (0 0 L) planes being aligned along one direction. Both the measurement of component and the electrical transport showed that the sample has Se vacancies. First-principles calculations showed that the vacancy point defects on the Se1 atom and antisite defect Bi_{Se1} (substitute one Se1 atom by Bi atom) are realistic.

Keywords: Topological insulator; Electrical transport; native defects; Bi_2Se_3.

* Corresponding author.
E-mail address: zmzmi1987@163.com. (M. Zhang)

1. Introduction

Bismuth chalcogenides materials Bi_2Se_3 single crystal in the series of V2VI3 semiconductors are known as thermoelectric materials in earlier study[1,2]. Recently, those materials with topological phases, named as topological insulators (TIs), have attracted intensive attentions both in theories and experiments[3,4]. Of the three-dimensional (3D) topological insulators, Bi_2Se_3 has the simplest band structure - and a relatively large bulk gap and a Dirac cone on the surface[5,6]. The special surface state of Bi_2Se_3 is protected by the time-reversal symmetry from any time-reversal perturbation, such as crystal defects and nonmagnetic impurities[7]. Many novel physical properties of 3D TIs confirmed by experimental and theoretical prediction, such as Driac cone[8], Majorana fermion[9], and magnetic monopole[10], leading to great potential for future application on spintronics and fault-tolerant quantum computing[11,12].

For thermoelectric applications, Bi_2Se_3 is not necessary to obtain particularly high crystal purity for single crystals. And topological insulators require single crystals for their specific topological properties. Therefore intrinsic defects in Bi_2Se_3 affect the performance of the material[13]. In order to explore the