

## Electronic structure of $(\text{Tl}_{0.125}\text{Pb}_{0.875})\text{Te}$

I. Hase <sup>\*,1</sup>, T. Yanagisawa

*Nanoelectronics Research Institute AIST, Tsukuba 305-8568, Japan*

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### Abstract

We present an ab-initio supercell calculation of electronic band structures of  $(\text{Tl}_\delta\text{Pb}_{1-\delta})\text{Te}$  with  $\delta = 0$  and 0.125. PbTe is to be a very small gap semiconductor, and Tl doping induces a quasi-impurity band in this in-gap state. A local relaxation based on ionic model is discussed.

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Thallium is one of several elements known as ‘valence skipper’, which means that Tl forms the compounds in valence states  $\text{Tl}^{1+}$  and  $\text{Tl}^{3+}$  (corresponding to  $(6s)^2$  and  $(6s)^0$  outermost electron configuration, respectively), and naturally does not take  $\text{Tl}^{2+}$  state. If Tl atoms are forced to take  $\text{Tl}^{2+}$  valence state on average in a compound, they spontaneously dissipate to  $\text{Tl}^{1+}$  and  $\text{Tl}^{3+}$ . This situation corresponds to negative Hubbard  $U$  model, and if the outermost orbital of this ion is the s-orbital, the ground state becomes diamagnetic (no Curie term) [1]. Negative- $U$  impurity can induce superconducting pairing interaction [1–3]. In this point of view, superconductivity found in slightly Tl-doped PbTe [4,5] is newly enlightened by Matushita et al. by careful control of the Tl-content [6]. They found that PbTe becomes superconducting with maximum  $T_c \sim 1.5$  K by Tl-doping, on the other hand, all dopants except Tl bring about superconducting state below 0.01 K if at all, which is naturally anticipated by comparison with similar semiconducting materials, such as SnTe, GeTe and InTe. In these points of view, Tl-doped PbTe is a hopeful material that has negative- $U$  center, which is expected to have new fruitful physics, such as charge-Kondo effect,

superconductivity, and possible reentrance of normal state in extremely low temperature [7]. For understanding this fascinating feature, reliable energy-level scheme is indispensable. However, there is no report of band structure calculation for Tl-doped PbTe as we know.

In this paper we performed an ab initio band calculation for non-doped and Tl-doped PbTe. In order to investigate the polarization effect which is a possible origin for the negative- $U$  [6], we also examined the effects of lattice relaxation by Tl doping. We assumed that Tl takes  $\text{Tl}^{1+}$  (or  $\text{Tl}^{3+}$ ) valence state, and the six nearest-neighbor Te atoms move away from (or toward) Tl atom. The ionic radius of Tl is usually  $r(\text{Tl}^{1+}) = 1.59 \text{ \AA}$  and  $r(\text{Tl}^{3+}) = 0.895 \text{ \AA}$ , respectively [8]. The ionic radii of  $\text{Pb}^{2+}$  and  $\text{Te}^{2-}$  are  $r(\text{Pb}^{2+}) = 1.19 \text{ \AA}$  and  $r(\text{Te}^{2-}) = 2.11 \text{ \AA}$ , respectively. We assumed that the averaged Tl–Te distance is the same as the Pb–Te distance in Pb–Te, which is  $a_0 = 3.219 \text{ \AA}$ . Thus we may determine the Tl–Te distances by

$$d_1 = (r(\text{Tl}^{1+}) + r(\text{Te}^{2-})) * c_0 = 3.568 \text{ \AA}$$

$$d_3 = (r(\text{Tl}^{3+}) + r(\text{Te}^{2-})) * c_0 = 2.916 \text{ \AA}$$

Here  $c_0 = a_0 / (r(\text{Pb}^{2+}) + r(\text{Te}^{2-})) = 0.939$  is the scaling factor. However, due to the valence fluctuation and strong elastic force in the host lattice, such a large shift of Te atom may not be realized. We tentatively reduced the difference

\* Corresponding author. Tel.: +81 29 861 5147; fax: +81 29 861 5387.

E-mail address: [i.hase@aist.go.jp](mailto:i.hase@aist.go.jp) (I. Hase).

<sup>1</sup> AIST Central 2, Umezono 1-1-4, Tsukuba, Ibaraki 305-8568, Japan.

between  $d_1$  and  $d_3$  by factor  $2/3$ , and thus we set  $d_1 = 3.48 \text{ \AA}$  and  $d_3 = 3.03 \text{ \AA}$ . We take a  $2*2*2$  superlattice, i.e., fcc lattice with  $a = 4a_0$ , containing  $\text{TlPb}_7\text{Te}_8$  in a primitive cell. We replace one of the Pb atoms with Tl atom, corresponding to 12.5% Tl doping. By this replacement, the other seven Pb atoms occupy the 24d-site and 4b-site in space group  $\text{Fm}\bar{3}\text{m}$ . Eight Te atoms also occupy the 24e-site and 8c-site. The 24e-site has a free parameter  $x$

such as  $(x,0,0)$ , and we consider the relaxation of Te atom in 24e-site. Using above estimations, the position of Te atom is at  $x = 0.235$  for  $\text{Tl}^{3+}$ , and  $x = 0.27$  for  $\text{Tl}^{1+}$ . We investigated three cases,  $x = 0.235$ , 0.25 (no relaxation), and 0.27.

The scheme we used in our calculations is the standard full-potential augmented plane wave (FLAPW) method. The present energy-band calculation was performed using

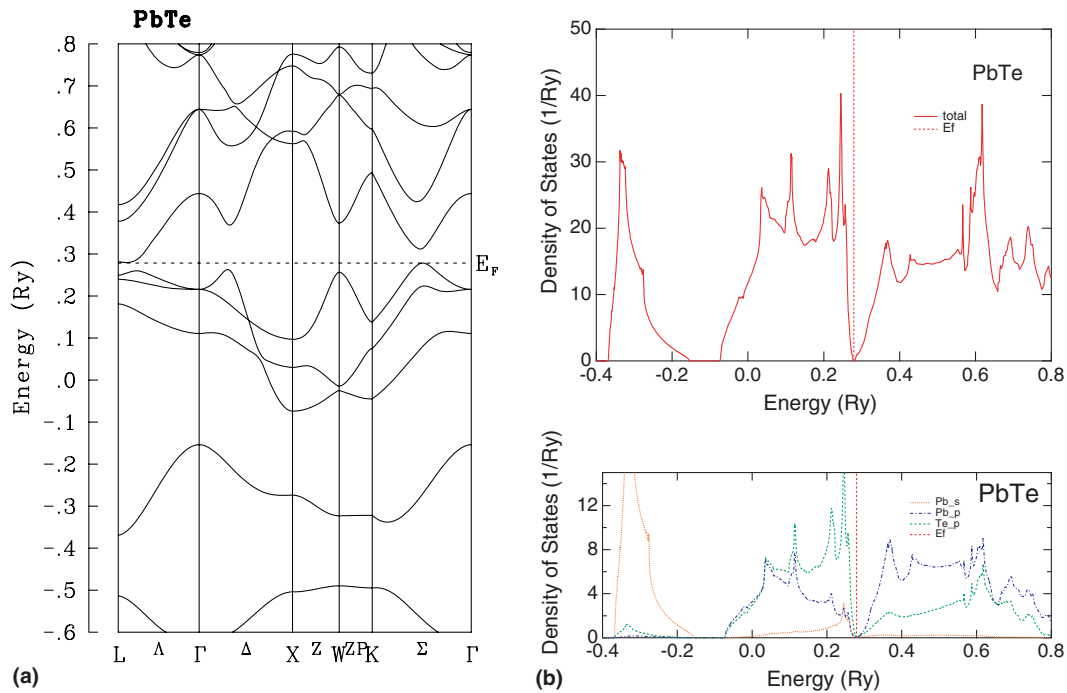


Fig. 1. (a) Band structure and (b) density of states (DOS) curve for PbTe.

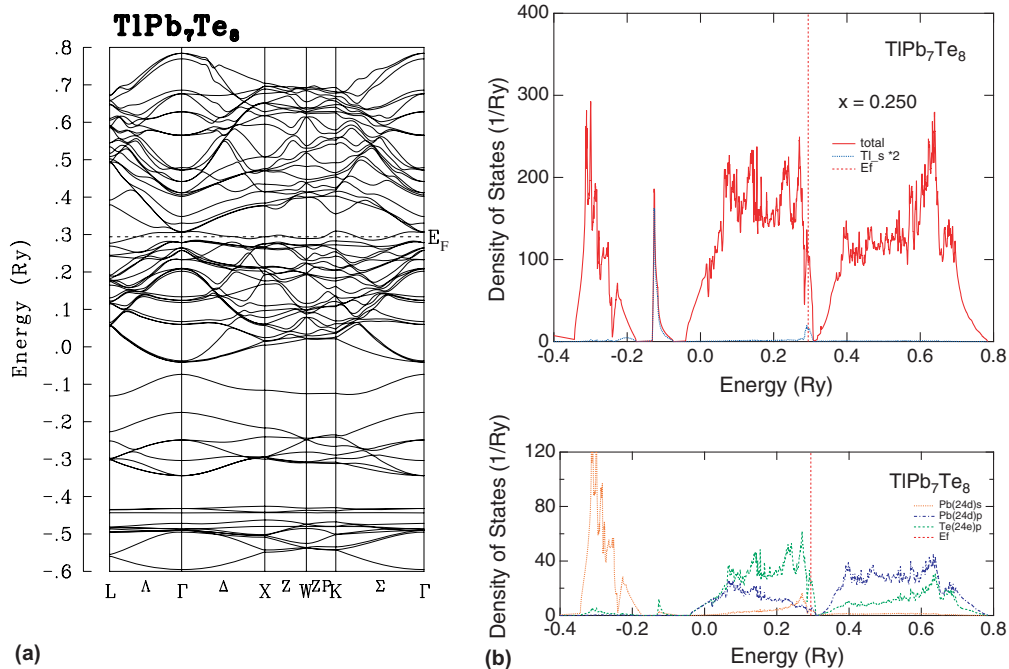


Fig. 2. (a) Band structure and (b) density of states (DOS) curve for  $\text{TlPb}_7\text{Te}_8$  ( $x = 0.25$ ).

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