Exploring the high-pressure bcc alloy phase of topological Insulator $PbBi_4Te_7$: synchrotron x-ray diffraction measurement and DFT simulations

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Alloys are important because of their superior physical properties and are extensively used in industries. Substitutional alloys are formed by randomly substituting one element by another. The formation of substitutional alloys made from metals are ruled by Hume Rothery rules. These rules say that an alloy can be formed only if, the difference in atomic size of the solute and solvent is within 15%, the valency of solute and solvent is similar and the difference in electronegativity is small. Very few alloys have been synthesized from non-metallic elements. Well known examples are the pnictogen chalcogenides (Bi_2Te_3, Sb_2Te_3, Sb_2Se_3, Bi_2Se_3) which form a disordered bcc substitutional alloy at high pressure [1-6]. It is interesting to know that this is despite the fact that the atomic radii of Se is 26 % and 28 % smaller than Sb and Bi respectively. In order to understand if the presence of Pb will still lead to the formation of a substitutional alloy we have investigated the high-pressure behaviour of this layered topological insulator, $PbBi_4Te_7$[6] consists of a seven-layer block Te-Bi-Te-Pb-Te-Bi-Te, where the layers are linked by weak van der Waals forces.

Our x-ray diffraction studies show that $PbBi_4Te_7$ undergoes a phase transition at 6.15 GPa. However, beyond 10 GPa it transforms to a cubic bcc substitutional alloy despite the presence of Pb. Our ab-initio density functional theory-based calculations show that at high pressure, there is a charge transfer from Bi and Pb atom to Te atom which makes the radii of these atoms approximately equal thus favouring the formation of a substitutional alloy. The covalent bonds become weaker with pressure as the ionicity increases. It was also observed that insertion of Pb enhances the charge transfer and thus lowers the pressure at which the substitutional alloy is formed in comparison to the parent compound Bi_2Te_3.

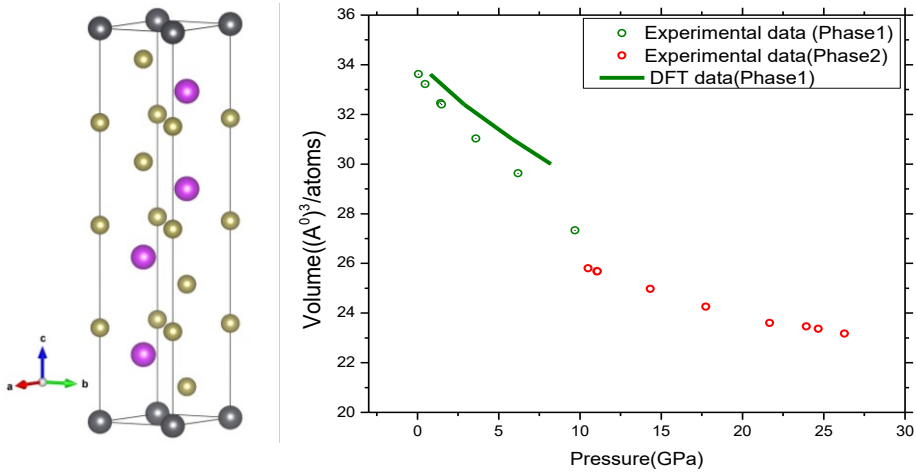

Figure 1. Layered structure of $PbBi_4Te_7$(left); P-V diagram for both low pressure and high-pressure phases.

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