First principles study of electronic and optical properties of liquid antimonide

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ABSTRACT

Antimonide such as InSb and Sb_2Te_3 is used as the best candidate material for the active layer in a super-resolution optical disc. The change in the optical properties of InSb and Sb_2Te_3 due to the phase transition was experimentally studied by Kuwahara et al. Their measurements show that optical absorption of InSb at a photon energy of 3.06 eV increases due to the melting, while that of Sb_2Te_3 decreases. In order to clarify the origin of the difference between InSb and Sb_2Te_3, we have performed ab-initio calculations about electronic states and optical responses of InSb and Sb_2Te_3 for both crystalline and liquid states.

In this study, the Vienna ab initio simulation package (VASP) was used. To obtain atomic structure of liquid state, ab initio molecular dynamics (MD) was performed. Electronic states and optical dielectric functions were calculated, considering the spin-orbit coupling (SOC) effect.

The calculated results indicate that for both InSb and Sb_2Te_3, the density of states around the Fermi level increases due to the melting, and the energy band gap opening near the Fermi level disappears. As a result, the optical properties change from semiconductor to metallic behavior. Liquid InSb shows more metallic properties, compare with liquid Sb_2Te_3. In the case of the crystalline state of InSb, a dominant optical absorption peak is located around 4 eV, and the optical absorption at 3.06 eV is relatively small. On the other hand, crystalline Sb_2Te_3 has a very large optical absorption peak at 2 eV, and its tail has relatively large value around 3.06 eV. The difference of optical transition strength at 3.06 eV between crystalline InSb and Sb_2Te_3 is suggested to be the origin of the difference of the change of the optical absorption due to the melting.

Key words: Ab initio calculation, optical dielectric function, density of states, phase transition, InSb, Sb_2Te_3