Dielectric Function and Critical Point of GeSbTe Pseudo-binary Compound Thin Films

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We measure the dielectric functions of GeSbTe pseudo-binary thin films by using spectroscopic ellipsometry. We anneal the thin films at various temperatures. According to x-ray diffraction, the as-grown thin films are amorphous and the annealed films have metastable and stable crystalline phases. By using standard critical point model, we obtain the accurate values of the energy gap of the amorphous phase as well as the critical point energies of the crystalline thin films. The critical point energies are compared to the band gap energies determined by the method of linear extrapolation of the optical absorption. As the Sb to Ge atomic ratio increases, the optical (band) gap energy of amorphous (crystalline) phase decreases. Standard critical point fitting show several higher band gaps. The electronic band structures and the dielectric functions of the thin films are calculated by using density functional theory and are compared to the measured ones. The band structure calculations show in stable phase that GeTe, Ge$_2$Sb$_2$Te$_5$, and Ge$_1$Sb$_2$Te$_4$ have indirect gap whereas Ge$_1$Sb$_4$Te$_7$ and Sb$_2$Te$_3$ have direct gap. The measured indirect band gap energies match well with the electronic band structure calculations.

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