Splitting effect of photocurrent for $CdIn_2Te_4$ single crystal

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Abstract : The single crystals of p-$CdIn_2Te_4$ were grown by the Bridgman method without the seed crystal. From photocurrent measurements, it was found that three peaks, A, B, and C, correspond to the intrinsic transition from the valence band states of Γ_7(A), Γ_6(B), and Γ_7(C) to the conduction band state of Γ_6, respectively. The crystal field splitting and the spin orbit splitting were found to be 0.2360 and 0.1119 eV, respectively, from the photocurrent spectroscopy. The temperature dependence of the $CdIn_2Te_4$ band gap energy was given by the equation of $E_g(T) = E_g(0) - (9.43 \times 10^{-3})T^2/(2676 + T)$. $E_g(0)$ was estimated to be 1.4750, 1.7110, and 1.8229 eV at the valence band states of A, B, and C, respectively. The band gap energy of p-$CdIn_2Te_4$ at room temperature was determined to be 1.2023 eV.

1. Introduction

Cadmium indium telluride ($CdIn_2Te_4$), which belongs to a chalcopyrite structure[1] with space group S^2_4–I4-, is an attractive material because it is practically applicable to electro-optical devices[1]. In this study, the single crystals of p-$CdIn_2Te_4$ were grown by the Bridgman method without the seed crystal. We also present the results of the temperature dependence of the p-$CdIn_2Te_4$ band gap energy obtained through PC spectroscopy. The valence band splitting for electronic transitions restricted by a selection rule is also discussed.

2. Results and discussion

A. Photocurrent spectra

Figure 1 shows the PC spectra of p-$CdIn_2Te_4$ single crystal at the temperatures ranging from 10 to 300 K. The electrons excited from the valence band to the conduction band by the absorbed photons flowed immediately out of the electrodes. Consequently, only the PC peaks corresponding to the band gap are detected. This band-to-band transition PC peak has been known as the intrinsic transition[2]. As shown in Fig. 1, the PC spectrum at 300 K shows two peaks: one at 1033.4 nm (1.1998 eV) and the other at 863.4 nm (1.4360 eV). The peak at 1.1998 eV is A peak. This peak is ascribed to the electronic transition from

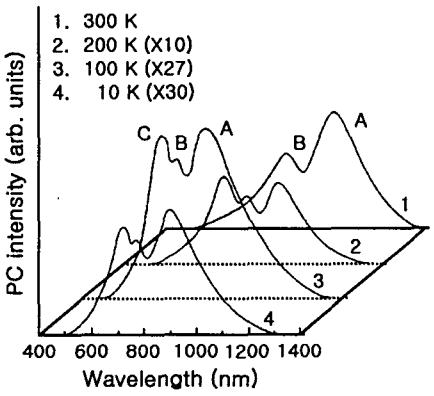

Figure 1 PC spectra of the p-$CdIn_2Te_4$ single crystal obtained at temperatures ranging from 10 to 300 K.

the Γ_7(A) of the valence band to the Γ_6 of the conduction band. Likewise, the peak at 1.4360 eV is B peak. This peak is associated with the electronic transition from the Γ_6(B) of the valence band to the Γ_6 of the conduction band. The PC spectra obtained from the temperatures ranging from 10 to 250 K show three peaks. The peaks at 10 K, especially, are located at 842.8 nm (1.4711 eV), 726.3 nm (1.7071 eV), and 681.6 nm (1.8190 eV). The two peaks at

1.4711 and 1.7071 eV correspond to peaks A and B, respectively. The peak at 1.8190 eV is labeled C peak. This peak is ascribed to the electronic transition from the Γ_7(C) of the valence band to the Γ_6 of the conduction band. However, only two peaks are observed in the PC spectrum at 300 K. This is related to the scattered electrons in the valence band.

B. Valence band splitting

Figure 2 shows the energy band structure of $CdIn_2Te_4$ at the Γ point based on the selection rule.This figure shows that the conduction band of s-like state has a Γ_6 symmetry, and that the valence band of p-like state is split into three double degenerate states such as Γ_7(A), Γ_6(B), and Γ_7(C). The Γ_7(A) is the uppermost valence band. The effective mass in the Γ_7(A) depends much on the direction of k. The Γ_6(B) is the middle band. The Γ_7(C) is the lowest valence band. Generally, the crystal field of the ternary compound has been observed by reflectance and photoconductivity measurement.[14-17] In this work, the valence band splitting of $CdIn_2Te_4$ owing to the crystal field was observed by using the PC measurement. The crystal field splitting, Δ_{cr}, is the energy difference between Γ_7(A) and Γ_6(B). The value obtained is 0.2360 eV from the energy difference between peak A, 842.8 nm (1.4711 eV), and peak B, 726.3 nm (1.7071 eV), at 10 K. This is almost an order of magnitude larger than those of II-VI analogues.[18] The spin orbit splitting, Δ_{so}, is the energy difference between Γ_6(B) and Γ_7(C). This value is determined to be 0.1119 eV from the energy difference between B peak, 1.7071 eV, and C peak, 1.8190 eV, at 10 K. The split gap energies between the three peaks at several temperatures are coincident to the values of 0.2360 and 0.1119 eV, respectively.

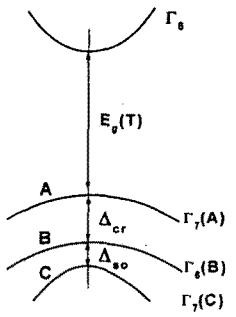

Figure 2 Fine structure for energy level of $CdIn_2Te_4$

3. Conclusions

The p-$CdIn_2Te_4$ single crystal was grown in a three-stage vertical electric furnace by using the Bridgman method without the seed crystal. This indicates that the electrons in the valence band are scattered because of the mutual interaction of electrons caused by carrier concentration. The peaks A, B, and C obtained are the intrinsic transitions from the valence band state of Γ_7(A), Γ_6(B), and Γ_7(C) to the conduction band state of Γ_6, respectively. The Δ_{cr} and Δ_{so} of p-$CdIn_2Te_4$ obtained are 0.2360 eV and 0.1119 eV, respectively. The temperature dependence of the band gap energy is well described by the equation of $E_g(T) \approx E_g(0) - (9.43 \times 10^{-3})T^2/(2676 + T)$. The $E_g(0)$ is estimated at 1.4750, 1.7110, and 1.8229 eV at the valence band states of Γ_7(A), Γ_6(B), and Γ_7(C) respectively. The band gap energy of p-$CdIn_2Te_4$ obtained at room temperature is 1.2023 eV.

References

[1]. O. Madelung, in Landolt-Börnstein : Numerical Data and Functional Relationships in Science and Technology, edited by O. Madelung (Springer-Verlag, Berlin, 1985), Vol. 17h, p.124.