

열처리된 CuGaSe2 단결정 박막의 점결함연구  
 A study on point defect for thermal annealed CuGaSe2 single crystal thin film

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A stoichiometric mixture of evaporating materials for CuGaSe2 single crystal thin films was prepared from horizontal electric furnace. Using extrapolation method of X-ray diffraction patterns for the polycrystal CuGaSe2, it was found tetragonal structure whose lattice constant  $a_c$  and  $c_0$  were 5.615 Å and 11.025 Å, respectively. To obtain the single crystal thin films, CuGaSe2 mixed crystal was deposited on thoroughly etched semi-insulating GaAs(100) substrate by the hot wall epitaxy (HWE) system. The source and substrate temperatures were 610°C and 450°C, respectively. The crystalline structure of the single crystal thin films was investigated by the photoluminescence and double crystal X-ray diffraction (DCXD). The carrier density and mobility of CuGaSe2 single crystal thin films measured with Hall effect by van der Pauw method are  $5.01 \times 10^{17} \text{ cm}^{-3}$  and  $245 \text{ cm}^2/\text{V}\cdot\text{s}$  at 293K, respectively. The temperature dependence of the energy band gap of the CuGaSe2 obtained from the absorption spectra was well described by the Varshni's relation,  $E_g(T) = 1.7998 \text{ eV} - (8.7489 \times 10^{-4} \text{ eV/K})T^2/(T + 335 \text{ K})$ . After the as-grown CuGaSe2 single crystal thin films was annealed in Cu-, Se-, and Ga-atmospheres, the origin of point defects of CuGaSe2 single crystal thin films has been investigated by the photoluminescence(PL) at 10 K. The native defects of  $V_{\text{Cu}}$ ,  $V_{\text{Se}}$ ,  $\text{Cu}_{\text{nt}}$ , and  $\text{Se}_{\text{nt}}$  obtained by PL measurements were classified as a donors or acceptors type. And we concluded that the heat-treatment in the Cu-atmosphere converted CuGaSe2 single crystal thin films to an optical n-type. Also, we confirmed that Ga in CuGaSe2/GaAs did not form the native defects because Ga in CuGaSe2 single crystal thin films existed in the form of stable bonds.