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GaAs(001)上に成長した$CuGaSe_2$単結晶薄膜のフォトルミネセンス

Photoluminescence of single crystal thin film chalcopyrite $CuGaSe_2$ grown on GaAs(001)

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We are focusing on $CuGaSe_2$ (CGS), which will be ideal for the top absorber cell with a bandgap of 1.68eV (room temperature). Even though its bandgap is higher than that of the optimal bandgap (Shockley-Queisser limit) of an absorber layer which is 1.4eV, its effective electron mass of $0.14m_0$ and excitonic binding energy of 20meV make it a higher absorption coefficient material even compared to $CuInSe_2$ (CIS). For the CGS solar cells, realization of n-CGS is very important. Hence, we are concentrating in fabrication of n-CGS thin films using migration-enhanced epitaxy. We have grown CGS, doped with several dopants such as Sn, Mg and Si which may become donors in CGS. However, we are unsuccessful in fabricating n-CGS till now.

Here, we report on the photoluminescence (PL) characteristics of undoped and Si-doped CGS. Our growth was performed by using MBE equipment on semi-insulating GaAs (001) substrate. First, we reconfirmed the optimal growth condition with proper vapor pressure of Cu, Ga and Se. The substrate temperature, Ts and Si cell temperature were varied between 560 - 600°C and 1100°C, respectively. Optimal recipe of undoped CGS was established when we obtained hole concentration of $1.2\times10^{17}/cm^3$. Utilizing the recipe, we have doped with Si for the donor impurity, but we found that an increased hole concentration of $2.4\times10^{17}/cm^3$ was obtained instead of decreasing. This anomalous phenomenon upon doping can be explained as number of holes increasing at a higher ratio compared to electrons. It can be attributed to an increase of Cu-vacancy along with hole compensation by Si donors.

We have measured and analyzed the PL of undoped and Si doped CGS. Fig. 1 shows a typical result of undoped and Si doped samples. In addition to the strong edge emission (1.715eV), weak peaks appear at 1.68, 1.64 and 1.61eV (see arrows). These peaks are probably caused by ①Band-acceptor PL band, ② Donor- acceptor pairs (DAP) and ③LO phonon band of DAP emission. These DAP emissions are probably due to Si-donors and Cu-vacancy. In Fig. 2 it is shown that the PL peak energy increases with temperature. This phenomenon can be explained by considering the DAP recombination. As temperature increases, distant D-A pairs tend to be ionized, and thus closer D-A pairs contribute to the emission. Thereby, the PL peak is shifted to a higher energy side. In addition, deeper peaks are observed at 1.31, 1.40 and 1.43eV (Fig. 1) which needs further investigation.

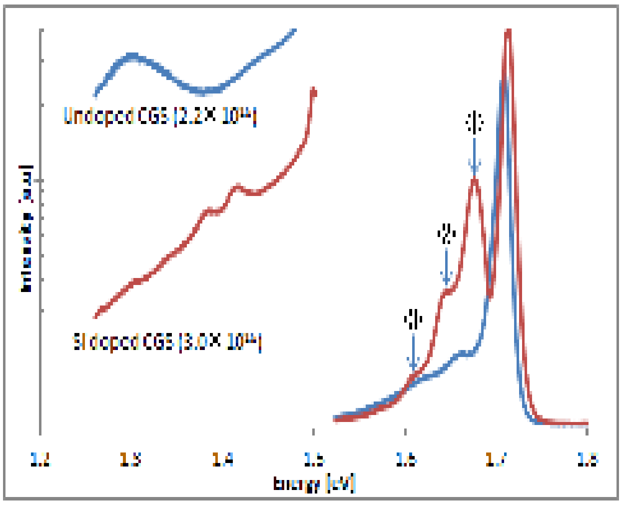

Fig. 1: Photon energy versus PL intensity characteristic of CGS, where Ts = 560°C and T_{Si} = 1100°C

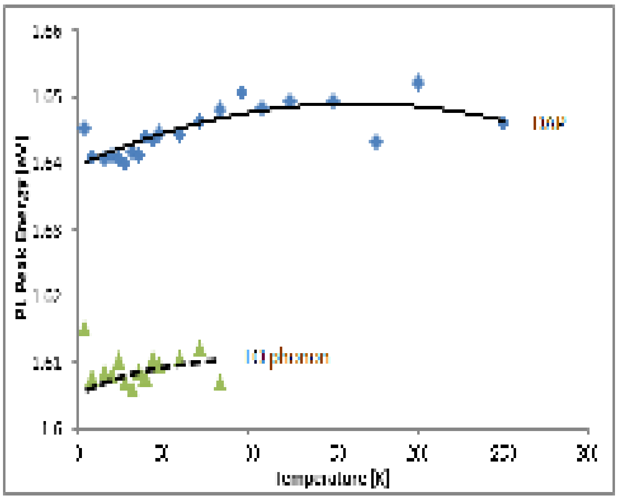

Fig. 2: Temperature versus PL peak energy of Si doped CGS