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TOPICAL COLLECTION: ELECTRONIC MATERIALS FOR RENEWABLE ENERGY APPLICATIONS

Evaluation of the Conduction Band Discontinuity of MgSe/ZnCdSe Heterojunctions on InP Substrates Using *n–i–n* Diodes

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Conduction band discontinuity (ΔE_c) of MgSe/ZnCdSe heterojunctions were evaluated using *n–i–n* diodes consisting of an undoped *i*-MgSe layer sandwiched by *n*-doped ZnCdSe layers. The *n–i–n* diodes were fabricated on InP substrates by molecular beam epitaxy. Injection current density versus applied voltage (*J–V*) characteristics of the *n–i–n* diodes were measured at 77 K and room temperature. In addition, the theoretical *J–V* characteristics of the *n–i–n* diode were calculated while varying ΔE_c. By fitting the theoretical data to the experimental data, ΔE_c was estimated to be 1.2 eV from the result at 77 K. This value is similar to the ΔE_c estimated from the literature.

Key words: Band discontinuity, heterojunction, *n–i–n* diode, II–VI compound, InP substrate, molecular beam epitaxy

INTRODUCTION

II–VI compound semiconductors, such as ZnCdSe and MgZnCdSe, on an InP substrate are very attractive for a wide range of visible optical devices.[1,2] Using these materials, we are developing yellow and green light-emitting devices.[3–6] In the design and optimization of the device structures, it is very important to obtain precise values of the material parameters such as the bandgap energies and band discontinuities of the hetero-structures. In particular, band discontinuity data are indispensable for designing the interband and intersubband transition wavelengths of quantum wells (QWs) and the carrier confinement structures of various devices. Some methods of evaluating the band discontinuities of various heterostructures have been reported. For example, valence band discontinuities have been investigated by x-ray photoelectron spectroscopy (XPS) for many materials. Moreover, band discontinuities have been estimated from the optical transition data of QWs obtained by photoluminescence (PL), photoreflectance measurements, and so forth.

In this paper, we propose a method of evaluating band discontinuities using *n–i–n* diodes. Using this method, the conduction band discontinuities (ΔE_c) between the *n*- and *i*-barrier layers of devices are estimated by fitting theoretically obtained electrical characteristics to experimental data. In this study, the method was applied to evaluate ΔE_c for MgSe/ZnCdSe hetero-structures on InP substrates. As a result, ΔE_c was estimated to be 1.2 eV, similar to the value estimated from the literature.[7]

EXPERIMENTS

MgSe/ZnCdSe *n–i–n* diodes were fabricated to evaluate ΔE_c for MgSe/ZnCdSe heterojunctions. A schematic diagram of the device structure is shown in Fig. 1. The device consisted of a thin undoped *i*-MgSe barrier layer sandwiched by 300-nm-thick *n*-doped ZnCdSe layers. Each layer of the device was *n*-doped except the barrier layer. The device structure was grown on a S-doped (100) *n*-InP substrate by employing a double-chamber molecular beam epitaxy (MBE) system consisting of II–VI and III–V growth chambers. In the growth, the InP substrate surface was first thermally cleaned under P beam flux irradiation at 500°C in the III–V chamber. Then, 60-nm-thick Si-doped *n*-InP and 90-nm Si-doped *n*-InGaAs buffer layers were successively grown at 450°C and 470°C, respectively. Then, the

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wafer was transferred to the II–VI chamber through an ultrahigh-vacuum transfer chamber. Before the growth of the II–VI layers, Zn beam flux was irradiated on the n-InGaAs buffer surface at 240°C. Subsequently, a 5-nm-thick *n*-ZnCdSe low-temperature (LT) buffer layer was grown at 240°C. After that, *n*-ZnCdSe, undoped MgSe, and *n*-ZnCdSe layers were sequentially grown at 280°C. Here, the InGaAs and ZnCdSe layers were grown under the lattice-matching condition with the InP substrate, i.e., the elemental compositions were $In_{0.54}Ga_{0.46}As$ and $Zn_{0.48}Cd_{0.52}Se$, respectively. The MgSe layer was considered to be pseudomorphically grown because it was very thin (several nm) and the lattice mismatching with the InP substrates was very small (0.7%). *n*-doping of the ZnCdSe layers was performed by Cl-doping using a $ZnCl_2$ source. The thickness of the MgSe layer and the electron densities of the *n*-ZnCdSe layers are described later. After the growth, Au/Sn and 50-μm-wide Al stripe ohmic electrodes were formed on the back of the substrate and the top *n*-ZnCdSe layer, respectively, by thermal and electron beam evaporation and conventional photolithography techniques. The length of the device chip was approximately 130 μm.

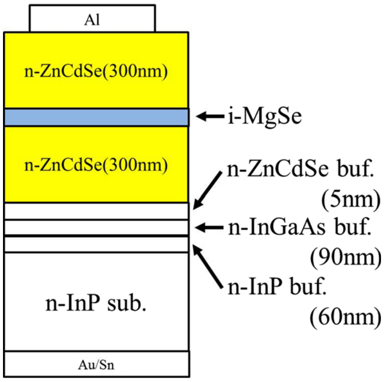

Fig. 1. Schematic diagram of MgSe/ZnCdSe *n–i–n* diode on InP substrate.

Injection current density versus applied voltage (*J–V*) characteristics of the *n–i–n* diodes were measured at 77 K. A typical *J–V* characteristic is shown in Fig. 2a. Here, the forward bias was determined as the current flow from the top *n*-ZnCdSe layer to the substrate. Nonlinear Schottky characteristics due to the heterobarrier effect at the MgSe/ZnCdSe junction were observed, as shown in Fig. 2a.

THEORETICAL FITTING

The theoretical *J–V* characteristics of MgSe/ZnCdSe *n–i–n* diodes with the same structure as the fabricated device were calculated while changing ΔE_c to fit the theoretical data to the experimental data. The schematic energy band structure used in the calculation is shown in Fig. 3. The *J–V* characteristics were calculated using the following equation[8,9]:

$$J = \frac{e m_n^* kT}{2\pi^2\hbar^3}\int_0^\infty \mathrm{Tr}(E)\cdot\ln\left\{\frac{1+\exp\left(\frac{E_f-E}{kT}\right)}{1+\exp\left(\frac{E_f-E-eV}{kT}\right)}\right\}\mathrm{d}E \quad (1)$$

In Eq. 1, J is the current density, E is the electron energy, E_f and m_n^* are the Fermi energy and the electron effective mass in the n-ZnCdSe layers, respectively, e is the elementary charge, k is the Boltzmann constant, T is the absolute temperature, and $\mathrm{Tr}(E)$ is the transmission probability of electrons with energy E. $\mathrm{Tr}(E)$ is given by the Wentzel–Kramers–Brillouin approximation as follows.[8,10]

$$\mathrm{Tr}(E) = \exp\left\{-\frac{4}{3}\frac{W_b\sqrt{2m_i^*}}{eV\hbar}(\Delta E_c - E)^{\frac{3}{2}}\right\} \quad (2)$$

In Eq. 2, V is the applied voltage, W_b is the thickness of the *i*-MgSe barrier layer, and m_i^* is the

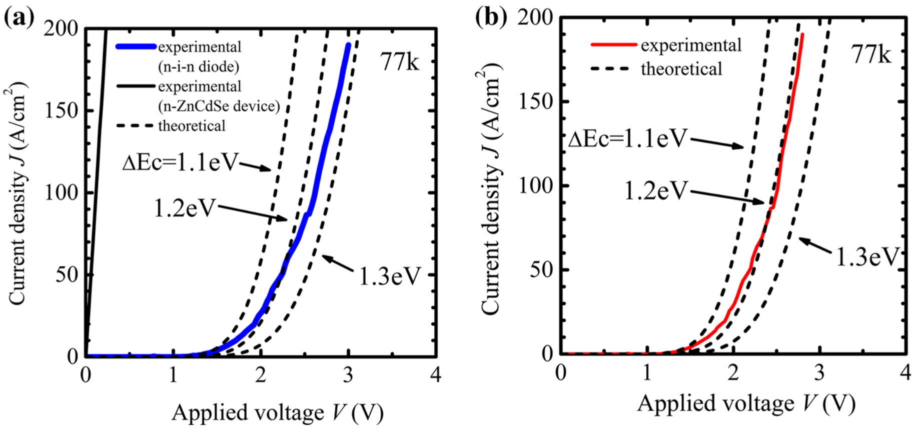

Fig. 2. (a) Experimental and theoretical *J–V* characteristics of the MgSe/ZnCdSe *n–i–n* diode at 77 K. The theoretical data were calculated for ΔE_c = 1.1 eV, 1.2 eV, and 1.3 eV. The *J–V* data of the n-ZnCdSe single layer device are also shown. (b) Modified *J–V* characteristic of the *n–i–n* diode at 77 K, plotted with the theoretical data.

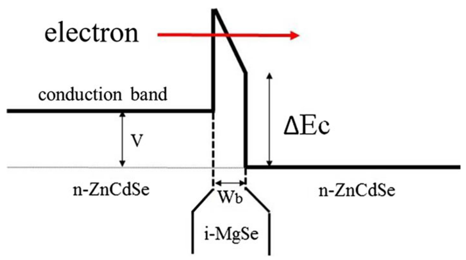

Fig. 3. Schematic energy band structure of the MgSe/ZnCdSe *n–i–n* diode used in the theoretical calculations.

electron effective mass in the barrier layer. Before the calculation, W_b was evaluated by cross-sectional transmission electron microscopy observation to be 3.8 nm. In addition, E_f was estimated from the electron density (n) of the n-ZnCdSe layers, which was obtained by Hall effect measurements of another n-ZnCdSe sample fabricated for measurements under the same growth and doping conditions as the n–i–n diode. n and E_f were 9.0×10^{18} cm^{-3} and 0.028 eV, respectively. In the J–V calculations, m_n^* and m_i^* were assumed to be $0.12m_0$ (m_0 is the free electron mass) and $0.23m_0$, respectively. T was 77 K.

The J–V characteristics calculated for ΔE_c = 1.1 eV, 1.2 eV, and 1.3 eV are shown in Fig. 2a for comparison with the experimental data. In this figure, the J–V characteristic in the case of ΔE_c = 1.2 eV was in good agreement with the experimental data when J was less than 70 A/cm^2. On the other hand, the theoretical data gradually deviated from the experimental data when J exceeded 70 A/cm^2. This deviation was considered to be due to the resistance components such as the resistance of each layer and the contact resistances with the electrodes of the actual device (i.e., factors excluding the n–i–n structure), which were not taken into account in the theoretical calculations. Then, an n-ZnCdSe single layer device was fabricated and characterized to estimate the resistance components of the n–i–n diode. The structure of the n-ZnCdSe device was the same as that of the n–i–n diode except that it did not include the i-MgSe barrier layer. Also, the growth conditions of the n-ZnCdSe device were the same as those of the n–i–n diode. A typical J–V characteristic of the n-ZnCdSe device at 77 K is shown in Fig. 2a. This characteristic is clearly ohmic, which proves that every part of the n–i–n diode, such as the other heterojunctions and the contacts with the electrodes, had ohmic characteristics except for the n–i–n structure, and that the Schottky characteristics of the n–i–n diodes were due to only the Schottky barrier effect at the n–i–n heterojunctions. The resistivity per unit area of the n-ZnCdSe device was estimated to be 1.1×10^{-3} Ω cm^2 from the J–V characteristic.

Then, the J–V characteristic of the n–i–n diode with no resistance component was obtained by subtracting the J–V data of the n-ZnCdSe device from those of the n–i–n diode to fit the theoretical data to the experimental data. The modified J–V characteristic of the n–i–n diode is shown in Fig. 2b with the theoretical data. It is clearly shown that the theoretical J–V characteristic when ΔE_c = 1.2 eV was in very good agreement with the modified experimental data. From this, ΔE_c for the MgSe/ZnCdSe heterojunction was estimated to be 1.2 eV.

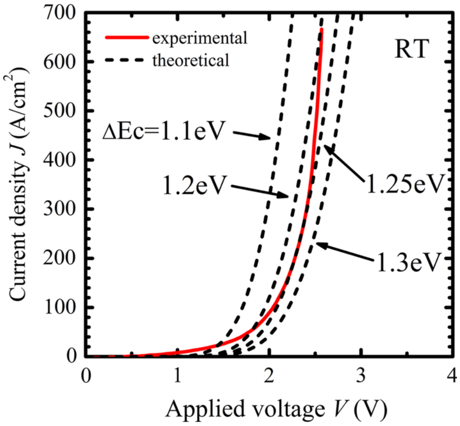

Fig. 4. Experimental and theoretical *J–V* characteristics of the MgSe/ZnCdSe *n–i–n* diode at RT. The experimental *J–V* characteristic is the data after subtracting the resistance component from the raw *J–V* characteristic of the *n–i–n* diode. The theoretical data were calculated for ΔE_c = 1.1, eV 1.2 eV, 1.25 eV, and 1.3 eV.

In addition, the processes similar to those at 77 K (i.e., J–V measurements and theoretical fitting) were also carried out at room temperature (RT). Experimental and theoretical J–V characteristics of the n–i–n diode at RT are shown in Fig. 4. Here, the experimental J–V characteristic is the data obtained by subtracting the resistance component from the raw J–V characteristic of the n–i–n diode, like Fig. 2b. The theoretical data were calculated for ΔE_c = 1.1, eV 1.2 eV, 1.25 eV, and 1.3 eV. This figure shows that the experimental data approximated to the theoretical values when ΔE_c = 1.2 eV near J = 600 A/cm^2. This result accorded with that at 77 K. However, there was some deviation between the experimental and theoretical data when $J <$ 500 A/cm^2. Rather, the experimental data approximated to the theoretical values when ΔE_c = 1.25 eV near J = 300 A/cm^2. Thus, a precise ΔE_c value was not obtained from the data at RT. The cause of the deviation is unknown for the moment. The analytic model (i.e., taking into account the quantum tunneling effect at the i-barrier layer) of the n–i–n diode described above is considered to be valid at not only 77 K but also RT, because the heterobarrier is predicted to be high enough (i.e., $\Delta E_c >$ 1 eV) compared to thermal energy of transmission electrons at RT. In fact, however, good agreement of the experimental and theoretical data like that at 77 K was not obtained in the whole current range at RT, as shown in Fig. 4. Some unexpected causes such as heat generation by current injection in the device, crystal defects, and device structure imperfections (e.g., layer thickness inhomogeneity) might have affected the *J*–*V* characteristic more at RT, resulting in causing the deviation and disagreement of the experimental and theoretical data. In any case, further improvements of the theoretical analysis of the *n*–*i*–*n* diode are necessary to match the theoretical values to the experimental data at RT.

The estimated ΔE_c value was compared with the literature data. ΔE_c for a $Zn_{0.53}Cd_{0.47}Se/Zn_{0.27}Cd_{0.23}Mg_{0.50}Se$ single QW was evaluated using electroreflectance by another group who reported ΔE_c of 590 meV.[7] From the data, ΔE_c for the MgSe/ZnCdSe heterojunction can be extrapolated to be 1.18 eV, which is in very good agreement with our value (i.e., 1.2 eV). This shows the validity of the value of ΔE_c estimated in this study and the high effectiveness of the method proposed in this paper for evaluating ΔE_c values.

SUMMARY

n–*i*–*n* diodes consisting of an undoped *i*-MgSe layer sandwiched by *n*-doped ZnCdSe layers were fabricated on InP substrates by MBE to evaluate ΔE_c for MgSe/ZnCdSe heterojunctions. *J*–*V* characteristics of the *n*–*i*–*n* diode were measured at 77 K and RT. In addition, theoretical *J*–*V* characteristics of the *n*–*i*–*n* diode were calculated while changing ΔE_c. By fitting the theoretical data to the experimental data, ΔE_c was estimated to be 1.2 eV at 77 K, in good agreement with the value of ΔE_c extrapolated from literature data.

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