The Effect of Dislocation and Interface-Roughness Scattering on Electron Mobility in the MgZnO/ZnO Heterostructure

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Received 24 May 2022; Revised 18 June 2022; Accepted 30 June 2022; Published 2 August 2022

Academic Editor: Samia A. Gad

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In this work, the electron mobility in the MgZnO/ZnO heterostructure at room temperature is theoretically studied by considering interface roughness (IFR), dislocation (DIS), and polar optical phonon (POP) scattering. Analytical formulae are introduced to calculate the critical thickness and dislocation density in the barrier layer of MgZnO/ZnO heterostructures. The calculated critical thickness for the MgZnO/ZnO heterostructure is much smaller than that for the AlGaN/GaN heterostructure system. At room temperatures, POP scattering is found to be the most important scattering mechanism. On the other hand, the change of electron mobility limited by IFR as a function of the barrier thickness in the MgZnO layer is found to be quite different to that limited by DIS. High-density ($>10^{14}$ cm$^{-2}$) 2DEG can be obtained in the MgZnO/ZnO interface by increasing the thickness and Mg composition in the MgZnO layer.

1. Introduction

The II-VI semiconductor ZnO, a wide band-gap metal oxide material, has been proposed as new wide band-gap semiconductors for short-wavelength optoelectronic applications. ZnO and MgZnO can form heterostructures with polarization at the interface [1–4], which causes very high two-dimensional electron gas (2DEG). High 2DEG is very crucial for the realization of MgZnO/ZnO high electron mobility transistor (HEMT) applications [5]. The MgZnO/ZnO heterosystem is an effective candidate to confine carriers in the ZnO layer [6]. Recently, high electron mobility exceeding $1 \times 10^6$ cm$^2$/Vs in MgZnO/ZnO heterostructures was reported [7].

The electron mobility in heterostructures is limited by a combination of various scattering mechanisms related to ionized impurities (II), dislocations (DIS), interface roughness (IFR), acoustic phonons (AP), alloy disorder (ADO), and polar optical phonon (POP) scatterings. Begum et al. [8] investigated the role of AP and POP scatterings in the electron mobility at the MgZnO/ZnO heterojunction. Recently, Zan and Ban theoretically analyzed the electron mobility limited by interface optical (IF) and confined optical (CO) phonon modes in a symmetric MgZnO/ZnO quantum well structure [9]. Thongnum et al. reported the role of IFR in electron transport in MgZnO/ZnO [2], finding the scattering potential in the in-plane direction which can affect the electron mobility. GaN can have a dislocation density up to $10^8 \sim 10^{10}$cm$^{-2}$, which may dominate the electron mobility in AlGaN/GaN heterostructure systems [10, 11].

But in MgZnO/ZnO heterostructure systems, IFR and DIS scattering limitation to electron mobility is not fully investigated. In this work, we first deduced expressions to analytically calculate the critical thickness and dislocation density of in-barrier layer with a different Mg composition $x$ so that the electron mobility limitation due to DIS and IFR scatterings is analytically investigated.

2. Calculation Methods

In the effective mass approximation, the energy levels and the corresponding wave functions for electrons in the heterostructure are obtained by solving the Schrödinger and Poisson equations self-consistently. For more details of the
procedure used in the self-consistent numerical solutions, we can see [12, 13] and references therein.

In the case of unintentionally doping, the 2DEG in heterostructures is assumed to originate from the surface donor distribution [14]. The positive surface donor sheet density is determined by the following [15]:

\[ q\rho_{\text{ns}} = \frac{P_{\text{pc}}}{q} \left(1 - \frac{t}{\eta}\right), \]

where \( P_{\text{pc}} \) is the lattice mismatch, which is determined by

\[ f = \frac{(a_{\text{MgZnO}} - a_{\text{ZnO}})}{a_{\text{ZnO}}}, \]

where \( a_{\text{ZnO}} \) and \( a_{\text{MgZnO}} \) are the lattice constants of ZnO and MgZnO, respectively. The critical thickness \( t_{\text{cr}} \) is calculated according to the expression [17]:

\[ t_{\text{cr}} = \frac{b}{8\pi(1 + v)} \left(1 - \frac{t}{\eta}\right) \left(\frac{1}{f} + \frac{1}{b}\right), \]

where \( \eta \) is the Poisson ratio. B is the magnitude of the Burgers vector. The strain-related dislocation density \( \rho \) can be expressed as [18]

\[ \rho = \kappa \epsilon^2 \frac{a^2}{b^2}, \]

where \( \kappa \) is the material constant. \( \epsilon \) is the strain, which can be estimated by [19]

\[ \epsilon = \frac{r_{\text{Zn}} - r_{\text{Mg}}}{r_{\text{Zn}} + r_{\text{O}}} \times, \]

where \( r_{\text{Zn}} = 0.6\text{Å}, r_{\text{Mg}} = 0.57\text{Å}, \) and \( r_{\text{O}} = 1.38\text{Å} \) are Pauli covalent radii of Zn and O atoms, and \( x \) is the Mg composition.

Considering that the material system of MgZnO/ZnO is analogous to that of AlGaN/GaN, it is helpful to prepare the DIS scattering calculation based on the data from AlGaN/GaN. The real AlGaN/GaN HEMTs contain a high density of dislocations in the epitaxial layers of GaN, which forms because of the absence of a suitable lattice-matched substrate for growth. State-of-the-art AlGaN/GaN HEMTs have a defect density of the order of \( 10^7-10^{10}/\text{cm}^2 \). At the same time, when the thickness of the Al\(_{x}\)Ga\(_{1-x}\)N alloy layer exceeds the critical limit, the interface between the AlGaN barrier and the GaN channel suffers from crystal defects, resulting in misfit dislocation [20]. The effect of dislocation on electron transport can be analyzed by introduction of dislocation scattering. The corresponding scattering rate is obtained as [21].
IQ_he 2-DEG mobility inhibited by interface roughness scattering can be given by

$$\mu_{ifr} = \frac{e\tau_{ifr}}{m^*}.$$  

IQ_he polar optical phonon scattering between subband $i$ to subband $j$ is calculated as follows [23]:

$$\tau(k) = \frac{m^*c^2 \omega_{op}}{4.07 n^* h^2} \left( N_{ph} + \frac{1}{2} \right) \left( \frac{1}{\epsilon_{r,so}} - \frac{1}{\epsilon_{r,s}} \right) \int_0^{2\pi} J(q)d\theta,$$

$$J(q) = \int \left\{ \frac{1}{q} e^{-|\bar{k} - \bar{k}'|} |\phi_i(z)\phi_j^*(z')|\phi_f(z)\phi_f^*(z')dz dz' q \right\},$$

where $\bar{k}$ and $\bar{k}'$ are initial and final wave vectors, respectively. $\epsilon_{r,so}$ is the high frequency dielectric constant, and $\epsilon_{r,s}$ is the static dielectric constant of the system. The electron mobility inhibited by polar phonon scattering is calculated using the expression

$$\mu_{pop} = \frac{e}{k_BT} \sum_{n=1}^{N} \int_0^\infty \epsilon_r \left( f_0(\epsilon) - f_0(\epsilon_1 - f_0(\epsilon)) \right) d\epsilon,$$

where $f_0(\epsilon) = \left[ \exp \left( \frac{\epsilon - \epsilon_F}{k_BT} \right) + 1 \right]^{-1}$ is the Fermi–Dirac equilibrium distribution function, $\epsilon$ is the electron kinetic energy, and $N$ is the number of the subbands.

The total mobility then is given by Matthiessen’s rule as follows:

$$\frac{1}{\mu_{tot}} = \frac{1}{\mu_{dis}} + \frac{1}{\mu_{ifr}} + \frac{1}{\mu_{pop}}.$$  

**3. Results and Discussion**

The band diagram, eigenvalues, and subband wave functions are calculated using the material parameters adopted from [9] for MgO and ZnO, listed in Table 1. Mg$_x$Zn$_{1-x}$O material constants are determined by the interpolation calculation of MgO and ZnO material constants. The main parameters used for calculating DIS, POP, and IFR scattering rates are listed in Table 2. Because of the quantum confinement, electrons fly and are scattered mainly in the channel, so we only present the material parameters of ZnO in Table 2.

Figure 1 shows the conduction band edge profiles of a Mg$_0.3$Zn$_{0.7}$O/ZnO heterostructure which consists of an undoped Mg$_0.3$Zn$_{0.7}$O layer and a thick undoped ZnO buffer layer. The envelope wave functions and subband structures are calculated by self-consistently solving the one-dimensional Poisson–Schrödinger equations. We use a Schottky barrier
height of 0.7 eV for the metal-semiconductor interface [24]. Here, the Mg composition of the MgZnO layer is fixed as 0.3. The thickness of the MgZnO and ZnO layers is 30 nm and 400 nm, respectively. The energy difference between the ground subband and the first excited subband is approximately 0.17 eV; therefore, the electrons mainly occupy the ground subband.

The critical thickness as a function of Mg composition $x$ is calculated according to Equation (4). Poisson ratio of Mg$_{x}$Zn$_{1-x}$O $\nu$ is fixed as 0.351 according to the work [27]. Here, the magnitude of the Burgers vector $b = a_{\text{MgZnO}}/\sqrt{2}$ [28]. $a_{\text{MgZnO}}$ is the lattice constant of MgZnO, which is calculated from the corresponding values of MgO and ZnO for the given Mg mole fraction $x$ using linear relation. Figure 2 shows the calculated critical thickness as a function of Mg composition $x$. For a specific $x$, the critical thickness for the MgZnO/ZnO heterostructure is found much smaller than that for the AlGaN/GaN heterostructure.

Various design constraints exist to change the 2DEG density. For example, one may change the barrier thickness $w$. Figure 3 shows the MgZnO layer thickness dependence of carrier sheet density. We first choose $x$ to be 0.30 so that all layer thicknesses ranging from 10 nm to 30 nm are larger than the corresponding critical thickness. We find that the 2DEG density increases with increasing the barrier thickness, which is consistent with the experimental data of AlGaN/GaN heterostructure systems [15, 17] and theoretical data for MgZnO/ZnO heterostructure systems [29]. We can see that electron sheet density can reach a value of $4.3 \times 10^{13}$ cm$^{-2}$ at barrier thickness 10 nm, $9.5 \times 10^{13}$ cm$^{-2}$ at 14 nm, $3.5 \times 10^{13}$ cm$^{-2}$ at 30 nm, respectively. We then change $x$ to be 0.35. The corresponding results are shown by the dashed line in Figure 3. It is found that for a specific thickness, higher Mg mole fraction in the MgZnO barrier layer can result in higher 2DEG density. Hence, high-density 2DEG can be obtained in MgZnO/ZnO heterostructures by changing the barrier thickness and the Mg composition.

Dislocation (DIS) scattering plays an important role in electron transport and the resulted mobility. We know from Equation (7) that the DIS scattering rate is closely related with the dislocation density. Referring to the experimental data of dislocation density in [30], $\rho = 4.94 \times 10^{12}$ cm$^{-2}$, we determined the material constant $\kappa$ in Equation (5), $\kappa = 0.18$. Based on Equation (5), we draw in Figure 4 the calculated results of dislocation densities in the MgZnO barrier layer as a function of Mg composition $x$.

Since the electron transport in HEMT is closely related with the band offset of heterostructures, we first investigate the electron mobility as a function of the Mg composition $x$ in the Mg$_{x}$Zn$_{1-x}$O layer. Correlation length $\Lambda = 6.0$ nm and averaged height $\Delta = 0.22$ nm are used for the calculation of IFR scattering rates. The MgZnO and ZnO layer thicknesses are fixed as 40 nm and 60 nm, respectively. We only consider the mobility limitations by IFR, POP, and DIS scatterings, so the total electron mobility $\mu_{\text{tot}}$ is calculated by Equation (14). The dislocation densities used for the calculation of DIS scattering rates are chosen from Figure 4. The corresponding results are displayed in Figure 5. The solid line in Figure 5(a) is for the IFR mobility $\mu_{\text{ifr}}$, and the dashed line is for the total mobility. For comparison, the electron mobility limited by DIS scattering is displayed in the inset. This gradual decrease for the mobility with increasing Mg composition is consistent with those in [24]. On the other hand, we can see from Figure 5(a) that $\mu_{\text{tot}}$ is close to $\mu_{\text{ifr}}$, which means that IFR scattering is dominant over DIS and can describe the electron transport of MgZnO/ZnO heterostructures in the low Mg composition ($x < 0.4$). Because the dislocation scattering rate $w_{\text{DL}} \propto N_{\text{dis}} \cdot \eta^{3/2}$ [18], $\eta_{s}$ increases with $x$, so we see from the inset in Figure 5(a) that the DIS mobility increases at low Mg composition, and then it decreases with increasing $x$. POP scattering is the most important one for polar wide band-gap semiconductor materials in room temperature. For comparison, we present
We find that POP scattering is the dominant mechanism in limiting electron mobility at room temperature. We reduce $\Delta$ and increase $\Lambda$ that were used in Figure 5(a), setting $\Delta = 0.11$ nm, and $\Lambda = 6.0$ nm, 8.0 nm, 10.0 nm, respectively. The corresponding calculated IFR electron mobilities are shown in Figure 5(c). We find that IFR mobility strongly depends on the average height of roughness. Here, the value used for average height is very small (0.11 nm), compared with the typical value of roughness (0.286–3.38 nm) [31]. In Figure 5(d), we fix correlation length $\Lambda = 6$ nm and slightly vary the averaged height: 0.535 nm, 0.684 nm, and 0.832 nm. In these cases, the obtained IFR electron mobilities are still much smaller than DIS electron mobility, which further confirms IFR scattering as the domain mechanism for the electron mobility limitation in MgZnO/ZnO heterostructures.

Figure 6 shows the dependence of electron mobility on the Mg$_{0.35}$Zn$_{0.65}$O layer thickness. We find from Figure 6(a) that electron mobility is limited by IFR scattering drops with the increase of barrier thickness. This phenomenon is due to the fact that the electron sheet density $n_s$ increases with increasing MgZnO barrier thickness, as shown in Figure 3 and that the IFR scattering rate is proportional to $n_s^2$, as presented in Equation (8). Figure 6(b) shows that the electron mobility limited by DIS scattering increases with increasing MgZnO barrier thickness, which displays a reverse behavior in contrast to IFR electron mobility shown in Figure 5(b).
4. Summary and Conclusion

In this study, we theoretically investigated electron mobility limitations by the interface roughness, dislocation, and polar optical phonon scatterings in MgZnO/ZnO heterostructures at room temperature. Analytical formulae are introduced to calculate dislocation density in the barrier layer of heterostructures. The results confirmed that the strength of the electron-optical-phonon interaction in MgZnO/ZnO heterostructures is high enough to constitute a strong mobility limiter. The 2DEG mobility as a function of the MgZnO barrier thickness in the MgZnO layer which is limited by interface roughness is found to be quite different to that limited by dislocation scattering; the former increases and the latter decreases with increasing the barrier thickness. Higher Mg mole fraction and a thicker MgZnO barrier layer can generate higher 2DEG density in MgZnO/ZnO heterostructures. The mobility limited by IFR is an order of magnitude higher than that of DIS, suggesting that IFR scattering, compared to DIS scattering, is the major limitation to electron mobility at room temperature. The work presented here could help in the design of future devices, such as high electron mobility transistors (HEMT).

Data Availability

Data available on request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

This work was supported by the Science and Technology Program of Guangzhou, China (Grant no. 201804010444).

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