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Ga segregation impact on $Al_{0.35}Ga_{0.65}As$/GaAs SQW energy bandgap

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ABSTRACT

We have studied the impact of Ga segregation on energy bandgap of $Al_{0.35}Ga_{0.65}As$/GaAs single quantum well system as a function of growth temperature and growth rate using kinetic model and Empirical Tight Binding method. This work indicates how much redshift we expect when the growth temperature changes from 500°C to 710°C and how much blue shift we expect when growth rate increases from 0.1 ML/s to 1ML/s because of Ga segregation in $Al_{0.35}Ga_{0.65}As$/GaAs SQW system. This work suggests in order to compensate for the Ga segregation and keep the energy bandgap of $Al_{0.35}Ga_{0.65}As$/GaAs SQW system at 1.53 eV equivalent to 808 nm wavelength, we need to reduce 4 ML of the GaAs QW thickness from ideal case when there is no Ga segregation.

Keywords: Gallium Segregation, Growth Temperature, Growth Rate, Energy Bandgap, Kinetic Model, Empirical Tight Binding Method.

1. INTRODUCTION

High-performance optoelectronic devices such as lasers, light emitting diodes (LED), solar cells and infrared detectors can be fabricated based on the complex quantum structures of III-V

semiconductors. Quantum structures such as quantum wells (QW), quantum dots (QD), and super-lattices can be grown with high quality using molecular beam epitaxy (MBE). However, abrupt interface between different semiconductor compounds is a challenge due to interfacial atomic segregation [1,2].

For low growth temperatures (for example 600^{o} C in AlGaAs/GaAs system), atomic arrangement in the crystal is determined by surface or near-surface processes and atoms have less chance to rearrange after burial under upcoming layers. However, due to the surface mobility, atoms can displace on the growing surface. Higher growth temperature leads to the increase of the surface mobility that can result in smoother surface; however, it also causes the so-called "surface segregation" that is the exchange between the sub-layer atoms with the impinging atoms on the growing surface. Atomic surface segregation is driven by the differences in their binding and elastic energies [3]. Several experimental and theoretical studies indicate that both group III and V atoms with weaker bond strength and elastic energy segregate to the surface [2-7]. For instance, on the well-known AlGaAs/GaAs QW system, theoretical and experimental results show Ga segregation in AlGaAs layer that can cause a composition asymmetry at the normal interface for both AlGaAs/GaAs and GaAs/AlGaAs growths [8-14]. The composition asymmetry at the interfaces results in the change of the energy band alignment of the quantum structures, which alters the optoelectronic properties. Therefore, to design an optoelectronic device based on the III-V semiconductor structures, it is important to predict and compensate the concentration profile change due to the segregating of atoms. In this work, we use kinetic model (KM) and empirical tight-binding method (ETBM) to predict and compensate Ga segregation impact on $Al_{0.35}Ga_{0.65}As$/GaAs SQW energy bandgap.

2. THEORETICAL COMPUTATION

2.1 Atomic Concentration Profile

Various theoretical atomic segregation approaches have been proposed for predicting the atomic concentration profile such as kinetic Monte Carlo (KMC) and KM [3, 15-17]. Using KMC, the

growth processes can be simulated based on the short-range surface diffusion of adatoms which exponentially depends on the activation energy for the surface diffusion [15]. Consequently, the concentration of constituent atoms can be calculated for each monolayer (ML) [15]. On the other hand, the KM is a kinetic thermodynamic model, where the atomic concentration profile is calculated based on the probability of the exchange of atoms on the surface with the atoms in the underlying layer [3].

The KM can simulate a layer by layer growth mode of an $A_xB_{1-x}C$ of group III-V alloy on a BC substrate; in which A and B are the group-III elements and C belongs to the group-V elements. In KM, the exchange is considered between the atoms on the uppermost layer (surface) and in one layer below the surface (bulk). The exchange process occurs when atom-A takeover atom-B site by overcoming a barrier energy of $E_{A/B}{}^{b\rightarrow s}$ to move from the bulk to the surface. The inverse exchange also happens when atom-A on the surface overcomes the barrier energy of $E_{A/B}{}^{s\rightarrow b}$ and moves into the bulk. The exchange rate, therefore, is given by [3, 16]:

$$P_{A/B}^{b\rightarrow s} = v\, e^{\left(\frac{-E_{A/B}^{b\rightarrow s}}{k_B T}\right)} \quad (1)$$

and the inverse exchange rate from surface to bulk is given by:

$$P_{A/B}^{s\rightarrow b} = v\, e^{\left(\frac{-E_{A/B}^{s\rightarrow b}}{k_B T}\right)} \quad (2)$$

Where, v = 10^{13}Hz is the atomic vibration frequency, T is the growth temperature, and k_B is the Boltzmann constant. Therefore, segregation driving force (E_s) is determined as:

$$E_s = E_{A/B}^{s\rightarrow b} - E_{A/B}^{b\rightarrow s} \quad (3)$$

Assuming that the segregation is only due to the exchange processes, the balance of the incoming to and leaving atoms from the surface gives the evaluation of the number of atom-A on the surface. Therefore, we will have [3]:

$$\frac{dX_A^s(t)}{dt} = \Phi_A + P_{A/B}^{b\rightarrow s} X_A^b(t) X_B^s(t) - P_{A/B}^{s\rightarrow b} X_A^s(t) X_B^b(t) \quad (4)$$

Here, Φ_A is the impinging flux of atom-A, $X^s{}_A(t)$ and $X^b{}_A(t)$ are the concentration of atom-A at time t on the surface or in the bulk, respectively. On the other hand, due to the mass conservation for atoms and the fact that $X^b{}_A(t) + X^b{}_B(t) = 1$ at any time, the following conditions must be achieved [3, 16]:

$$X_A^s(t) + X_A^b(t) = X_A^s(0) + X_A^b(0) + \Phi_A t \quad (5)$$

$$X_A^s(t) + X_B^s(t) = X_A^s(0) + X_B^s(0) + (\Phi_A + \Phi_B)t \quad (6)$$

Using equations (4)-(6), we are able to predict the atomic concentration profile for different growth conditions.

Based on KM, barrier energy of atoms and growth conditions such as growth temperature and growth rate, can alter the segregation length which is the maximum Ga segregation length. For example, In segregation length in AlSb/InSb system has been reported to be 15 ML at growth temperature of 520°C with a growth rate of 0.5 ML/s [18].

In this work, we calculated Al concentration profile for 19 MLs of GaAs sandwiched between 39 MLs of $Al_{0.35}Ga_{0.65}As$ SQW at different growth conditions. This SQW system has 0.04% mismatch which makes it a good candidate for MBE 2D growth.

Figure 1 shows the calculated Al concentration profile for both non-segregated and segregated $Al_{0.35}Ga_{0.65}As$/GaAs at a growth temperature of 710°C and a growth rate of 0.1 ML/s.

It demonstrates that Ga segregation has no effect on GaAs profile, while it alters the AlGaAs profile. Based on this calculation, the segregation length in AlGaAs layer is expected to be 7 MLs at growth temperature of 710°C with a growth rate of 0.1 ML/s which is much smaller than In segregation length in similar systems.

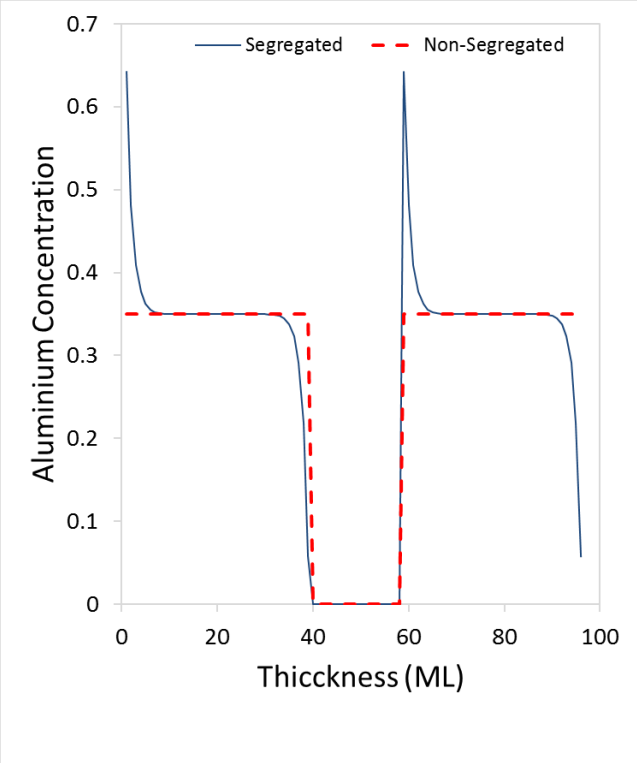

Figure 1. Al concentration profile for both non-segregated (dashed line) and segregated (solid line) for 19 MLs of GaAs sandwiched between 39 MLs of $Al_{0.35}Ga_{0.65}As$ SQW at a growth temperature of 710^{o}C and growth rate of 0.1 ML/s.

Based on KM, reducing growth temperature and/or increasing growth rate can reduce Ga segregation and result on an atomic concentration profile closer to non-segregated profile. However, lower growth temperature and higher growth rate result on rougher interfaces and broaden energy band gap which is not desirable. This is why we need to compensate the segregation effect at high temperature by readjusting the energy bandgap by changing the GaAs well thickness.

2.2 Energy Bandgap Modeling

For energy bandgap calculation, we used ETBM considering the spin-orbit, first-nearest-neighbor and sp^3s^* orbitals which is more accurate modeling method compared with other methods such as k.p especially when our thickness variation is only few MLs. Similar to previous work, we

assumed that $Al_{0.35}Ga_{0.65}As$ Hamiltonian matrix elements have the same value as the corresponding matrix elements in the AlAs or GaAs bulk after considering corrections for ternary materials. Therefore, we obtained the ternary ETBM numerical fitting parameters from AlAs and GaAs bulk energy band-structures [19-22].

3. RESULTS AND DISCUSSION

We started from a unite cell consists of 39 MLs of $Al_{0.35}Ga_{0.65}As$ and 19 MLs of GaAs. Considering 5 states of sp^3s^* for each atom with both spin-up and spin-down states, the Hamiltonian for such a unit cell become a 1160X1160 elements matrix. Based on this Hamiltonian, for a non-segregated material (ideal case), the predicted bandgap energy is expected to be 1.53 eV which is equivalent to a wavelength of 808 nm.

When we consider Ga segregation, the $Al_{0.35}Ga_{0.65}As$ interfaces no longer stay abrupt. The deformed interfaces modify the $Al_{0.35}Ga_{0.65}As$ barrier height and alters the energy bandgap and optoelectronic properties of the desired quantum structure. The ETB energy bandgap modeling shows that the Ga segregation in $Al_{0.35}Ga_{0.65}As$/GaAs system causes a 0.1 eV redshift and decreases the energy bandgap from 1.53 eV to about 1.43 eV at a growth temperature of 710^{o}C and growth rate of 0.1ML/s.

Figure 2 shows growth temperature and growth rate dependencies of the $Al_{0.35}Ga_{0.65}As$/GaAs calculated energy bandgap due to the Ga segregation. From that, we can see how increasing the growth temperature results on a redshift. At high growth rate of 1 ML/s, increasing the temperature from 500^{o}C to 710^{o}C results on <0.04 eV redshift; while, at low growth rate of 0.1 ML/s, it causes greater redshift of about 0.1 eV. This is because when we increase the growth temperature, the Ga segregation energy will be increased; therefore, the segregation rate will be increased and energy bandgap of the system will be decreased.

Figure 2 also reveals that in a range of 500-710^{o}C, increasing the growth rate reduces the Ga segregation and increases the energy bandgap of the system. At low growth temperatures, the growth rate has minimal effect on the energy bandgap. As we increase the temperature from

500°C to 710°C, growth rate effect on energy bandgap becomes more significant. For example, at a growth temperate of 500°C, altering growth rate 0.1-1 ML/s can result in <0.01 eV; whereas, the same growth rate range can alter the energy bandgap 0.07 eV at 710°C. This is because when we increase the growth rate, the time that Ga needs for segregation will be decreased; therefore, the segregation rate will be decreased and as a result of that we see less energy bandgap variation.

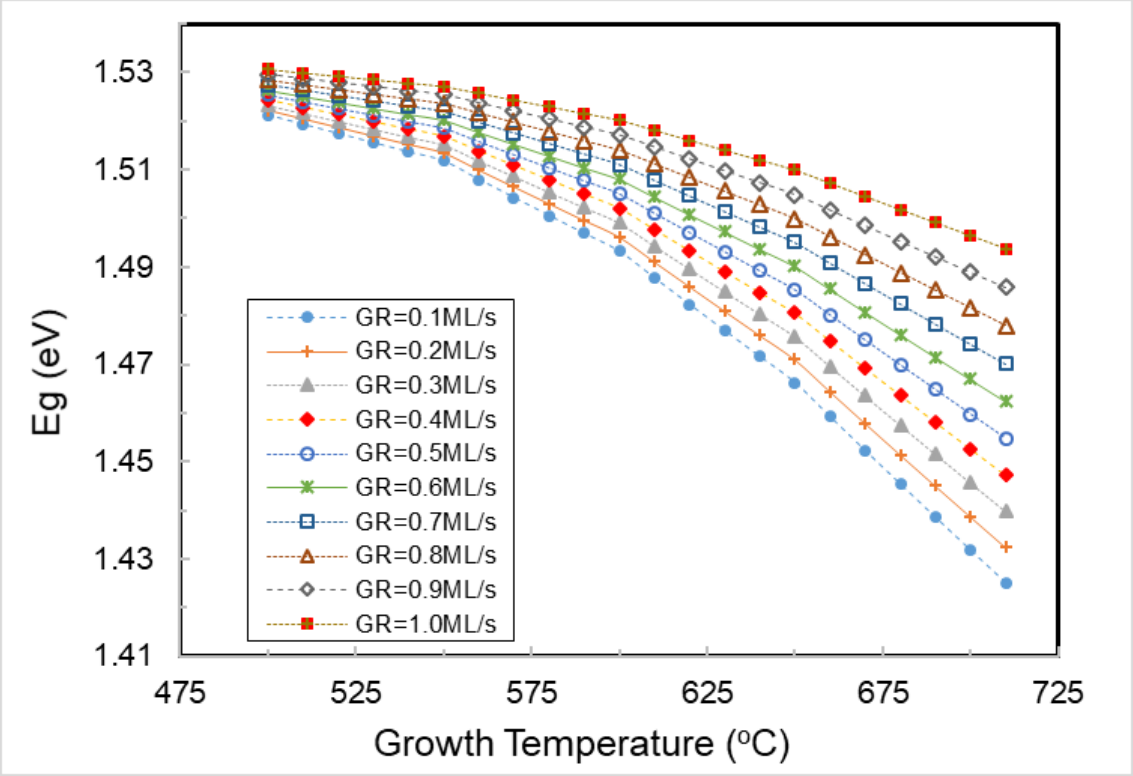

Figure 2. The growth temperature and growth rate dependencies of the $Al_{0.35}Ga_{0.65}As/GaAs$ calculated energy bandgap due to the Ga segregation.

At high growth temperature and/or low growth rate, still we can compensate for Ga segregation by altering the GaAs QW thickness. Figure 3 shows calculated energy bandgap at a growth temperature of 710°C and a growth rate of 1ML/s for different GaAs QW thicknesses. From figure 3, we can see by reducing 4 ML of the GaAs QW thickness down to 15 ML, we can achieve 1.53 eV bandgap for a wavelength of about 808nm which is close to the reported experimental results on the similar systems [23, 24].

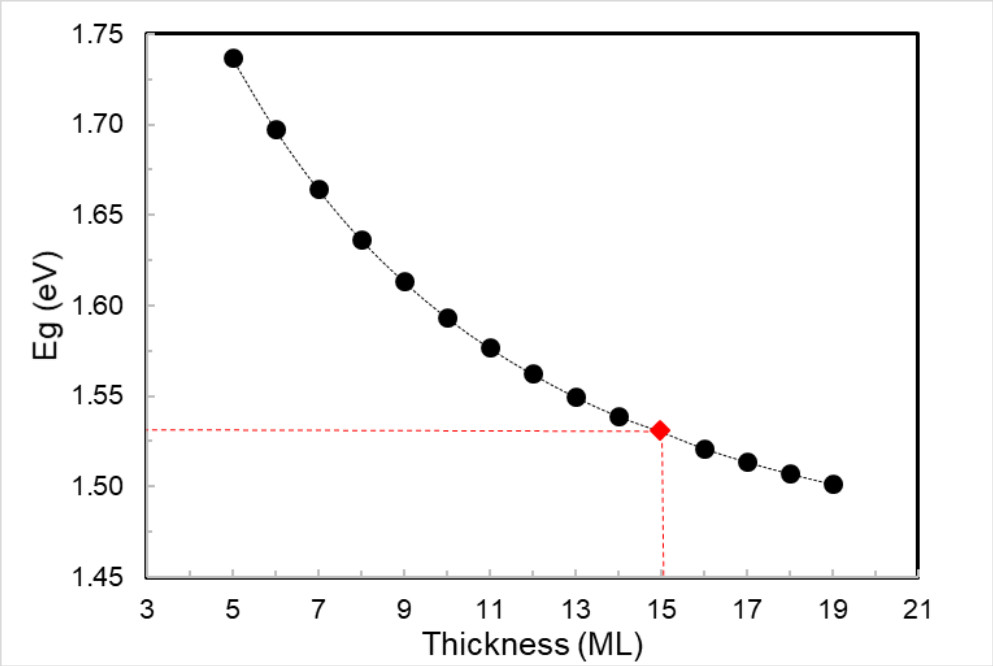

Figure 3. $Al_{0.35}Ga_{0.65}As/GaAs$ calculated energy bandgap variation for different GaAs thicknesses at a growth temperature of 710°C and growth rate of 1ML/s with considering Ga segregation.

Similarly, one can use the same method to engineer the energy bandgap at different growth temperature and growth rates.

4. CONCLUSION

In conclusion, we used Kinetic model and ETBM to study effect of Ga segregation on energy bandgap of $Al_{0.35}Ga_{0.65}As/GaAs$ SQW system at different growth temperatures (500-710°C) and growth rates (0.1-1 ML/s).

This study shows that how increasing the growth temperature increases the Ga segregation and causes a redshift; whereas, increasing the growth rate decreases the Ga segregation and causes a blueshift. We also predicted in order to compensate for Ga segregation and keep the energy bandgap of $Al_{0.35}Ga_{0.65}As/GaAs$ SQW system at 1.53 eV at high growth temperature of 710°C and growth rate of 1ML/s, we need to reduce 4 ML of the GaAs QW thickness compared with when there is no Ga segregation.

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