

THEORY OF CRITICAL LAYER THICKNESS OF NONCONSTANT QUANTUM-WELL WIDTH PRODUCED BY INTERDIFFUSION AND ITS OPTOELECTRONICS CONSEQUENCE

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ABSTRACT

In this paper, the concept of critical layer thickness is applied to the interdiffused quantum well (DFQW) structure. For the as-grown InGaAs/InP lattice matched quantum well, the interdiffusion process will induce in-plane strain into the DFQW forming a lattice mismatched system. The relation between the as-grown well width (L_z) and the diffusion length (L_d) for formation of dislocation is presented.

INTRODUCTION

Heteroepitaxy in lattice-mismatched systems is becoming more and more important for achieving high-performance electronic and optoelectronic devices. The fabrication of lattice mismatched semiconductor epitaxial layers in heterostructure is required to consider the critical layer thickness (CLT). When epitaxial layers of two different materials with their own lattice constants are grown on each others forming the strain layers QW material systems. The concept of CLT is essential for realising dislocation-free pseudomorphic QW materials. The CLT exists beyond which coherently strained pseudomorphic growth alters the growth with misfit dislocations. This restricts the design of device structures. In the theoretical calculations, Van der Merwe [1] calculated the CLT based on energy considerations in 1963. However, the first accepted model introduced by Matthews and Blakeslee [2] in 1974 is based on the mechanical equilibrium. Later, two models were further developed by several research groups [3, 4]. Both of the models are generally in agreement with experimental data. Recently, thermally induced composition intermixing in heterostructure quantum wells (QW) is becoming a popular choice in order to design multi-wavelength optical devices applications. [5] The intermixing process involves the interdiffusion of the constituent atoms of the heterostructure, the processing temperature, and time. During the process the as-grown square-QW compositional profile is modified to a graded profile thereby altering the confinement profile and subband structure in the interdiffused QW (DFQW). The CLT of the DFQW structures is not clearly defined by conventional methods. The conventional way to determine the CLT of a strained QW is to consider the abrupt interface while the DFQW has a graded compositional profiles of the interface. Therefore, it is difficult to define the QW width for DFQW. In this paper, the proposed theoretical model for tackling the CLT in DFQW is now considered. The theory is based on the equilibrium of two type of energies: the strain relief energy and the self-energy of misfit dislocation. These two energies can be calculated with the graded and continuous profile of the DFQW.

THEORETICAL MODEL

QW Interdiffusion

In our calculation, we consider the lattice matched $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}$ as-grown QW lattice matching to InP substrate. [6] After interdiffusion, group-III and group-V sublattices move across the interface of the heterostructure, so that the interdiffused QW structure may or may not be lattice matched to InP. Therefore, a strained-layer structure may result after interdiffusion. The constituent atoms interdiffusion has been modeled by an error function distribution. The group-III and group-V interdiffusion processes can be modeled by two different diffusion lengths. The diffusion of In and Ga atoms is characterized by a diffusion length, L_d^{III} , which is defined as $L_d^{\text{III}}=(D^{\text{III}}t)^{1/2}$, where D^{III} is the diffusion coefficient of group-III atoms and t is the diffusion time; the diffusion of As and P atoms is characterized by the diffusion length $L_d^{\text{V}}=(D^{\text{V}}t)^{1/2}$. The QW structure to be modeled consists of an as-grown InGaAs square well sandwiched between thick InP barriers. When the intermixing of QW occurs, the concentration of the diffusion atoms across the QW structure is assumed to have an error function distribution. The constituent atom compositional profiles can be represented as the group-III sublattice and group-V sublattice. In the group-III sublattices, the In concentration after interdiffusion is described by

$$x_{\text{In}}(z) = 1 - \frac{1-x}{2} \left[\text{erf} \left(\frac{L_z + 2z}{4L_d^{\text{III}}} \right) + \text{erf} \left(\frac{L_z - 2z}{4L_d^{\text{III}}} \right) \right] \quad (1a)$$

where L_z is the as-grown well width, z is the growth direction, and the QW is centered at $z=0$. In the group-V sublattices, the As concentration after diffusion is given by

$$y_{\text{As}}(z) = \frac{y}{2} \left[\text{erf} \left(\frac{L_z + 2z}{4L_d^{\text{V}}} \right) + \text{erf} \left(\frac{L_z - 2z}{4L_d^{\text{V}}} \right) \right] \quad (1b)$$

where x and y are the as-grown In and As concentration, respectively.

Critical Layer Thickness of DFQW

In the square QW epitaxial growth, the problem of lattice mismatch is due to a barrier-layer with different lattice constants of well-layer. This is generally accommodated by a combination of coherent strain and misfit dislocations. A lattice misfit parameter is defined as $f = |a_w - a_b|/a_w$, where a_w and a_b are the lattice constants of well and barrier, respectively. The CLT (h_c) for pseudomorphic epitaxy is derived by considering the thickness dependence of the strain energy and dislocation energy, and by minimizing the total energy. The CLT is obtained by [2]

$$h_c = \frac{b(1 - \gamma \cos^2 \Theta_{ab}) \left[\ln \left(\frac{h_c}{b} \right) + 1 \right]}{8\pi(1 + \gamma)f \cos \lambda} \quad (2)$$

where γ is Poisson's ratio, Θ_{ab} is the angle between the dislocation line and its Burgers vector (b), and λ is the angle between the slip direction and that line in the interface plane which is normal to the line of intersection between the slip plane and the interface. This model is only valid for

calculating the CLT of the square-QW structure. It cannot be applied in the DFQW structure. In the DFQW structure, the thickness of well layer is not clearly defined because the abrupt interface is changed to the continuous distribution. The in-plane strain could not be uniformly induced in the QW layers.

The in-plane strain, $\epsilon(x, y)$, across the well will vary with DFQW so that the strain effects are also z-dependent. Assuming that the growth direction z is along $\langle 001 \rangle$, then for the biaxial components parallel to the interface of the strain components, after interdiffusion, are given by:

$$\epsilon_{xx} = \epsilon_{yy} = \epsilon(x, y) = [a_w(x, y) - a_b] / a_w(x, y), \quad (3a)$$

$$\epsilon_{zz} = -2[c_{12}(x, y) / c_{11}(x, y)]\epsilon(x, y), \quad (3b)$$

$$\epsilon_{xy} = \epsilon_{yz} = \epsilon_{zx} = 0, \quad (3c)$$

where $a_w(x, y)$ and a_b are the lattice constant of the well layer and the *InP* substrate materials, respectively. $\epsilon(x, y)$ is defined to be negative for compressive strain, $c_{ij}(x, y)$ is an elastic stiffness constant and ϵ_{ij} is a strain component.

For the zincblende structure semiconductor, the strain energy density is given by [7]

$$U_{st} = \frac{1}{2}c_{11}(\epsilon_{xx}^2 + \epsilon_{yy}^2 + \epsilon_{zz}^2) + c_{44}(\epsilon_{yz}^2 + \epsilon_{zx}^2 + \epsilon_{xy}^2) + c_{12}(\epsilon_{yy}\epsilon_{zz} + \epsilon_{zz}\epsilon_{xx} + \epsilon_{xx}\epsilon_{yy}). \quad (4)$$

Substituting equations (3) into (4), we get

$$U_{st} = \left(c_{11}(x, y) + c_{12}(x, y) - \frac{2c_{12}^2(x, y)}{c_{11}(x, y)} \right) \epsilon^2(x, y). \quad (5)$$

The dislocation energy density is calculated by elastic theory. For a 60° dislocation, the energy density is given by [7]

$$U_{dis} = \frac{\mu b^2}{4\pi(1-\nu)} (1 - \nu \cos^2 \alpha) \ell n \left(\frac{B}{b} \right), \quad (6)$$

where μ is the shear modulus and is equal to $\frac{1}{2}(c_{11}-c_{12})$, ν is Poisson's ratio and is equal to $c_{12}/(c_{11}+c_{12})$, B is the extent of the distortion produced by a dislocation and $\alpha=60^\circ$ for the 60° dislocation. For the strain energy large than dislocation energy, it is energetically favourable to form dislocations and the mismatch is accommodated by a combination of coherent strain and misfit dislocations.

RESULTS AND DISCUSSIONS

In our calculation, an undoped $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ single QW layer sandwiched between *InP* barriers is considered. The as-grown structure is lattice matched and the effects of interdiffusion on the QW structure are considered both for group-III and group-V sublattice intermixing. The parameters were generally determined by interpolating scheme between the binary parameters at room temperature and listed in the Table 1. [8]

Table 1 : Material parameters for InGaAsP DFQW at room temperature.

	Unit	$\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{P}_{1-y}$
a_w	Å	$5.6533(1-x)y + 6.0583xy + 5.4505(1-x)(1-y) + 5.8687x(1-y)$
C_{11}	$\times 10^{11}$ dynes/cm ²	$11.9(1-x)y + 8.329xy + 14.05(1-x)(1-y) + 10.11x(1-y)$
C_{12}	$\times 10^{11}$ dynes/cm ²	$5.38(1-x)y + 4.526xy + 6.203(1-x)(1-y) + 5.61x(1-y)$

Before calculating the dislocation in DFQW, the model is applied in the case of $\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{P}_{1-y}$ square QW structure. A critical layer thickness of 104Å is found in the well layer for $x=0.2$. The value is agreed with the experimental results. [9]

For InGaAs/InP DFQW system of group-III interdiffusion, Ga atoms diffuse out to the InP barrier layer and In atoms diffuse into the well layer, and a thin and graded InGaP/InGaAs interface is formed. The distribution of the In and Ga atoms are described by the error function distribution, while the As and P concentration profiles do not change. The In compositional profiles are shown in Fig.1(a). In the early stages of the interdiffusion, the In atoms near the interface diffuse into the well, while Ga atoms diffuse into the barrier, but at the well centre the In concentration change slightly. As the interdiffusion process, the In concentration at the well center is changed from 0.53 to 0.85 as $L_d \rightarrow 120\text{Å}$. Thus, the intermixing of In and Ga atoms will result in a change of structural properties such as in-plane strain. The as-grown square well structure due to the intermixing of atoms will gradually change from an abrupt interface to a non-continuous profile.

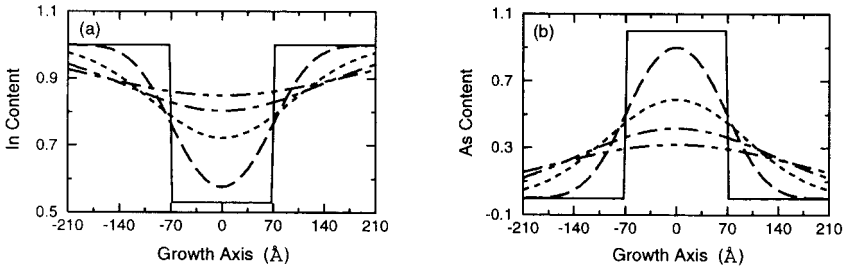


Fig.1 The (a) Indium and (b) Arsenic compositional profiles of InGaAs/InP DFQW with as-grown well width of 140 Å for various diffusion lengths. As-grown (—); $L_d=30\text{Å}$ (---); $L_d=60\text{Å}$ (- · - · -); $L_d=90\text{Å}$ (·····); $L_d=120\text{Å}$ (-----).

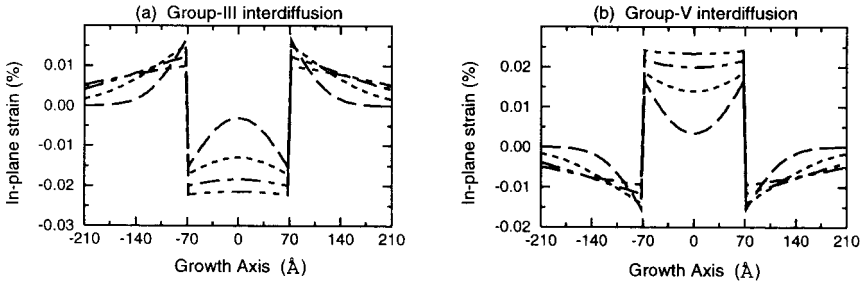


Fig.2 In-plane strain across the (a) group-III and (b) group-V interdiffused QW for various diffusion lengths. These lines are represented to the diffusion lengths same as figure 1.

The variation of the in-plane strain profile with interdiffusion across the structure is illustrated by Fig.2(a). Since the InP lattice constant is always larger than that of InGaP, tensile strain arises in the barrier near the interface, while the InGaAs well becomes compressively strained due to the increase in In content. Consequently the intermixing process results in a strained QW structure. At the interface of the heterostructure, the strain has its maximum value (compressive in the well and tensile in the barrier). The compressive strain in the well increases with interdiffusion. At the initial stage of interdiffusion, the strain in the well is smaller in the centre as compared with that at the interface. For extensive interdiffusion, such as $L_d = 120\text{\AA}$, the well strain variation between the centre and the interface is reduced. On the other hand, the tensile strain in the barrier layers is a maximum at the interface and then decreases gradually to zero outward away from the interface. When the interdiffusion increases, the barrier strain induced at the interface decrease while that at the outer barrier increase.

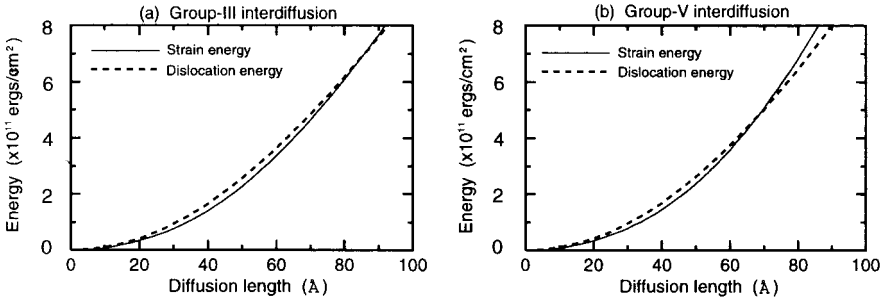


Fig.3 The dislocation energy and strain energy of InGaAs/InP DFQW against the diffusion lengths for (a) group-III and (b) group-V interdiffusion.

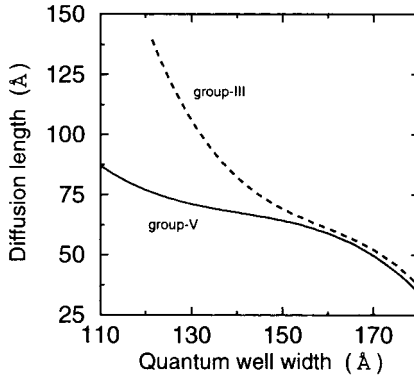


Fig.4 The critical diffusion length forming the dislocation against the as-grown well width for group-III and group-V interdiffusion.

In the case of group-V interdiffusion, only As and P atoms will inter-diffuse with each other between the well-barrier interfaces. Since in the as-grown QW structure, an As atom in the well will move out and a P atom in the barrier will move in, the group-V interdiffusion will result in an InGaAsP/InAsP interface. The distribution of the As and P atoms are also described by the error function distribution in Fig.1(b). The in-plane strain profile is quite different from that of the group-III interdiffusion and is shown in Fig.2(b). Since the InAsP lattice constant is always larger than the InP substrate, the InAsP barrier layer becomes compressively strained due to an increase of the As content. In the well layer, the increase in P content will induce a tensile strain because of a larger lattice constant InGaAsP layer with respect to InP substrate.

The variation of the strain energy and dislocation energy with the diffusion length in the case of group-III and group-V interdiffusion is shown in Fig.3(a)-(b). The strain energy and dislocation energy are represented by the solid line and dash line respectively. The dislocation is generated when the strain energy is larger than the dislocation energy. For example, the dislocation will be created for a diffusion length greater than 86Å and 70Å for a 140Å as-grown well width for group-III and group-V interdiffusion, respectively. The lattice misfit of the well layer for the group-V interdiffusion is larger than for the group-III interdiffusion. Thus, for the group-V interdiffusion it is always easier to create a dislocation than for a group-III interdiffusion. The plot of critical value of diffusion length forming the dislocation against the as-grown well-width is shown in the Fig.4. For the well width below 120Å, not enough strain energy forms for a the dislocation for the group-III interdiffusion. The difference of the critical value of diffusion length between the group-III and group-V interdiffusion is large within a well width of 120Å to 150Å. Above the 150Å well width, the critical value of diffusion length between the group-III and group-V interdiffusion are closer to each others. For the wider well width, a small amount of in-plane strain will make a dislocation.

CONCLUSIONS

In this paper we present the critical layer thickness of lattice mismatched InGaAs/InP DFQW with different well widths and diffusion lengths. The results show that group-V interdiffusion more easily created a dislocation than group-III interdiffusion. Moreover, the model is useful for designing the DFQW structure of optoelectronic devices.

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