INFLUENCE OF ELASTIC STRAINS ON ZONE ENERGY DIAGRAM OF $In_{1-x}Ga_xAs/GaAs$ HETEROSTRUCTURE

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Abstract— The paper consists of calculation of strains in the $In_{1-x}Ga_xAs/GaAs$ heterostructure and their dependence on relation between the thicknesses of contacting semiconductors. It also features the examination of how concentration of components and relation between the thicknesses of layers influences the key parameters of the zone energy diagram of heterostructure.

Keywords— *strained heterostructure, Gallium Arsenide, Indium Gallium Arsenide, deformation, strains, zone diagram.*

I. INTRODUCTION

The possibility of management of a certain set of physical properties through the change of the grade of deformation, strains, concentrations of components and relation between thicknesses of the contacting layer and substrate of strained heterostructures on the basis of III-V compounds is still attracting interest among researchers. Issues related to the influence of deformations on a separate semiconductor are widely covered in literature comprising experiments and theoretic researches [1,2,3]. The literature examines deformations and provides a thorough representation of shift of energetic levels in $In_{1-x}Ga_xAs/GaAs$ semiconductor crystals [4]. Still there is no model that takes into account how internal deformations in strained structures affect the key parameters of heterojunctions depending on the concentration of components and thicknesses of layer and substrate. This paper will show the dependence of elastic strains and deformations as well as changes in zone energy diagram of the $In_{1-x}Ga_xAs/GaAs$ structure depending on the concentration of components and thicknesses of layer and substrate.

II. THEORY

Symmetry of semiconductor decreases in case of deformation leading to change in the electron spectrum [5]. In case of small deformations strain tensor ε_{ik} equals

$$\varepsilon_{ik} = \frac{1}{2} \left(\frac{du_i}{dx_k} + \frac{du_k}{dx_i} \right),$$

where u_i, u_k are defined as components of crystal lattice displacement vector at strain.

Assume that heterostructure occurs by means of coalescence in direction [001]. The misfit between the constant lattice parameters of layer and substrate causes mechanical stresses, whereby the lattice spacing of $In_{1-x}Ga_xAs$ layer depends on the concentration x according to the Vegard's rule and the lattice spacing of GaAs substrate remains constant. Because of the decrease in symmetry of layer and substrate one needs to introduce constant lattice

spacings for directions [100], [010] - a_p , [001] - $a_{\perp}$ and use idealization of uniformity of deformations in substrate and layer. As it is known from the theory of elasticity [6] strain values of substrate and layer can be expressed in terms of constant lattice spacings a_s , a_l and substrate and layer thicknesses h_s , h_l :

$$\tau_{s,l} = \frac{E_{s,l} (a_p - a_{s,l})}{(1 - \nu_{n,c}) a_{s,l}} h_{s,l},$$

where $E_{s,l}$ and $\nu_{s,l}$ - respective Young's modules and Poisson's ratios of substrate (s) and layer (l). Young's module and Poisson's ratio of layer are defined depending on the concentration x by the linear interpolation of values for the correspondent binary compounds. Constant lattice spacings of substrate and layer along the contact surface a_p and in the out-of-plane direction $a_{\perp,s,l}$ are obtained from the equilibrium condition for mechanical strains $\tau_s + \tau_l = 0$:

$$a_p = \frac{\frac{E_s}{1-\nu_s} h_s + \frac{E_l}{1-\nu_l} h_l}{\frac{E_s}{1-\nu_s} h_s + \frac{E_l}{1-\nu_l} h_l} \cdot \frac{a_s}{a_l} + \frac{2\nu_{s,l}}{1-\nu_{s,l}} \left(a_{s,l} - \frac{\frac{E_s}{1-\nu_s} h_s + \frac{E_l}{1-\nu_l} h_l}{\frac{E_s}{1-\nu_s} h_s + \frac{E_l}{1-\nu_l} h_l} \right);$$

subsequently the components of strain tensor can be defined as follows [7]:

$$(\varepsilon_{s,l})_{11} = (\varepsilon_{s,l})_{22} = \frac{(-1+\nu_{s,l})E_{l,s}(a_{s,l}-a_{l,s})}{E_{l,s}(-1+\nu_{s,l})a_{s,l} + h^{\left[\frac{1,at,l}{-1,at,s}\right]}E_{s,l}(-1+\nu_{l,s})a_{s,l}},$$

$$(\varepsilon_{s,l})_{33} = \frac{\nu_{s,l}E_{l,s}(a_{l,s}-a_{s,l})}{E_{l,s}(-1+\nu_{s,l})a_{s,l} + h^{\left[\frac{1,at,l}{-1,at,s}\right]}E_{s,l}(-1+\nu_{l,s})a_{l,s}},$$

where indexes 11, 22, 33 define the respective directions [100], [010], [001].

Knowing the components of strain tensor one can define the strains occurring in layer (l) and surface (s) along the respective directions [100], [010], [001] (corresponding to the indexes 11, 22, 33) and depending on the relation between the thickness of substrate and layer $h = \frac{h_l}{h_s}$ on the basis of generalized Hooke's law and law on elastic change of volume [8]:

$$(\sigma_{s,l})_{cp} = \frac{E_{s,l}}{3(1-2\nu_{s,l})} \left((\varepsilon_{s,l})_{11} + (\varepsilon_{s,l})_{22} + (\varepsilon_{s,l})_{33} \right),$$

where

$$(\sigma_{s,l})_{ik} = \frac{E_{s,l}}{(1+\nu_{s,l})} \left((\varepsilon_{s,l})_{ik} + \frac{\nu_{s,l}}{1-2\nu_{s,l}} \left((\varepsilon_{s,l})_{11} + (\varepsilon_{s,l})_{22} + (\varepsilon_{s,l})_{33} \right) \right)$$

where $i = k = 1, 2, 3$.

Knowing the values of strain tensor components one can define the shift of energy levels in strained substrate and layer. Simple compression or stretching in $\text{In}_{1-x}\text{Ga}_x\text{As}$ and in GaAs leads to the equal shift of energy minimums of conductivity zone in equivalent directions $\langle 111 \rangle$ $\Delta E_c = a_c (\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33})$ [4]. Change of valence band due to deformation is represented as [4] $\Delta E_v = a_v (\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}) \pm b_v |\varepsilon_{11} - \varepsilon_{33}|$, whereby the sign "+" corresponds to light holes and "-" - to heavy holes.

The calculated shifts of conductivity zone edges and valence band splittings on substrate and layer allow definition

of the dependence in change of the forbidden bandwidth ΔE_g of substrate (s) and layer (l) in the presence of deformation from relation h and concentration x :

$$\Delta E_{gs}(x, h) = \Delta E_{cs}(x, h) - \Delta E_{vs}(x, h) =$$

$$= (a_{cs} - a_{vs}) \left((\varepsilon_s)_{11}(x, h) + (\varepsilon_s)_{22}(x, h) + (\varepsilon_s)_{33}(x, h) \right) \mp$$

$$\mp b_v \left| (\varepsilon_s)_{11}(x, h) - (\varepsilon_s)_{33}(x, h) \right|$$

$$\Delta E_{gl}(x, h) = \Delta E_{cl}(x, h) - \Delta E_{vl}(x, h) =$$

$$= (a_{cl}(x) - a_{vl}(x)) \left((\varepsilon_l)_{11}(x, h) + (\varepsilon_l)_{22}(x, h) + (\varepsilon_l)_{33}(x, h) \right) \mp$$

$$\mp b_v(x) \left| (\varepsilon_l)_{11}(x, h) - (\varepsilon_l)_{33}(x, h) \right|$$

III. RESULTS AND THEIR DISCUSSION

Values of parameters of equations at $T = 300K$ [9, 10, 11, 12].

Fig.1. Deformation of a layer

Fig. 2 Dependence of the layer stresses on the ratio of the substrate and layer thicknesses and the concentration of the components

Fig. 3. Dependence of the layer stresses on the ratio of the substrate and layer thicknesses and the concentration of the components

Fig. 4. The change in the width of the forbidden band of heavy holes in the layer, depending on the concentration of the components and on the ratio of the thicknesses of the substrate and the layer

Fig. 5. The change in the width of the forbidden band of light holes in the layer as a function of the concentration of the components and the ratio of the thicknesses of the substrate and the layer

Fig. 6. The change in the width of the forbidden band of heavy holes in the layer, depending on the concentration of the components and on the ratio of the thicknesses of the substrate and the layer

Fig. 7. The change in the width of the forbidden band of light holes in the layer as a function of the concentration of the components and the ratio of the thicknesses of the substrate and the layer

Fig. 8. Deformation of a substrate

Fig. 9. Dependence of the stresses of the substrate on the ratio of the thicknesses of the substrate and the layer and the concentration of the components

Fig. 10. Dependence of the stresses of the substrate on the ratio of the thicknesses of the substrate and the layer and the concentration of the components

Fig. 11. The change in the width of the forbidden band of light holes in the substrate as a function of the concentration of the components and the ratio of the thicknesses of the substrate and the layer

Fig. 12. The change in the width of the forbidden band of heavy holes in the substrate as a function of the concentration of the components and the ratio of the thicknesses of the substrate and the layer

Fig. 13. The change in the width of the forbidden band of light holes in the substrate as a function of the concentration of the components and the ratio of the thicknesses of the substrate and the layer

Fig. 14. The change in the width of the forbidden band of heavy holes in the substrate as a function of the concentration of the components and the ratio of the thicknesses of the substrate and the layer

The occurring strains lead not only to the quantitative but also to the qualitative changes in the zonal structure which

respectively should lead to a significant change of electronic properties of the $\text{In}_{1-x}\text{Ga}_x\text{As}/\text{GaAs}$ strained heterostructure.

IV. CONCLUSION

Taking into account the aforementioned, the elastic state of $\text{In}_{1-x}\text{Ga}_x\text{As}/\text{GaAs}$ heterostructure results in significant changes in the energetic zone structure. Selection of correlation between thicknesses of substrate and layer provides for prognosis and subsequent management of zone diagram parameters and, correspondingly, electronic properties of $\text{In}_{1-x}\text{Ga}_x\text{As}/\text{GaAs}$ heterostructures. The formula practically determined for ΔE_g permits an analysis of the forbidden bandwidth change depending on concentration of components and correlation between the thicknesses of layer and substrate in an elastically strained heterostructure.

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