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Electron Transport Properties of Strained $In_x Ga_{1-x}As$

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Abstract

The transport properties of bulk materials have been investigated by means of an ensemble Monte Carlo method. The band structure used is a three valley (Γ-L-X) conduction band including non parabolicity for any III-V ternary compound material with position dependent alloy composition. The scattering mechanisms included in the simulation are optical and acoustic phonons, piezoelectric, intervalley scattering, ionized impurities and alloy scattering. As a first approach to the study of strained pseudomorphic materials, we have used a Monte Carlo method to calculate the effect of strain on electron transport properties of bulk InGaAs. Strain-induced velocity reduction is found to be much more pronounced for InGaAs grown on GaAs substrate than for InGaAs grown on InP substrate. The simulation results are in good qualitative agreement with experimental observations, and further demonstrate the power of the Monte Carlo approach to modeling these high field transport processes.

Keywords *: Simulation, Monte Carlo method,Ternary compound, Scattering mechanisms.*

1. Introduction

The properties of electronic devices are often tailored by forming heterostructures of either group IV or III-V alloy. Modern growth techniques give exellent material control and interface quality. Special optical and electronic properties can be obtained by proper alloying of semiconductors. The intoduction of elastic strain through heteroepitaxy of lattice-mismatched materials gives an additional degree of freedom and thus greatly enhances the variability of obtaining desired material characteristics.

We investigate basic properties and low-field transport of the important GaInAs system in view of strain effects and give formulations suited for device simulation[1]. The organisation of this article is as follows. First the effects of alloying and strain on the bulk band structurez are sketched. Then the dependence of the band edge energies and effective masses on temperature and strain is given. Finally the electron velocity is investigated on the basic of Monte Carlo simulation.

2.The Model.

Boltzman transport equation is solved using a standard single electron Monte Carlo method, described by Zimmermann (1985), which requires the knowledge of matrial parameters and scattering rates. Modeling of unstrained $In_xGa_{1-x}As$ assumes a non parabolic three valleys band structure and takes into account the following scattering mechanisms : electron-phnon interactions (polar optic, non polar optic, acoustic, piezoelectric, intervalleys) and alloy

scattering. Values of material parameters are interpolated between those corresponding to the best kown compositions [2](x=0,0.53,1) and alloy scattering potential [3-12].

3. Lattice Mismatch Strain.

Within this section the effects of strain which result from lattice- mismatched epitaxy are considered. A change of the crystal symmetry and hence the band structure can be observed. Strained-layer epitaxy produces biaxial stress parallel to the interface ; in the perponducular direction no stress is built up. The interdependence of stress and strain is assumed to remain completely in the linear range of Hooke's law. The components of the strain tensor are functions of the interface orientation[4] and the lattice misfit.

For an epilayer with lattice constant a on a thick substrate with lattice constant a_0 the misfit is defined as ;

$$f_0 = \frac{a - a_0}{a_0} \tag{1}$$

under the assumption of coherent growth, the in-plane strain in the epilayer and the perpendicular component are ;

$$e_{ii} = \frac{a_0 - a}{a}$$

$$e_{\perp} = -\frac{2c_{12}}{c_{11}} e_{ii} \tag{2}$$

where $e_{ii}, e_{\perp}$ are the componentsof the strain tensor and c_{11}, c_{12} the elastic stiffness constants of InGaAs.

4. Band Edges.

4.1Temperature effects

the characteristic thermal behavior of the band gaps is usually described by Varshini's equation[5] ;

$$E^I(T) = E^i(0) - \frac{A^i T^2}{T + B^i} \tag{5}$$

which is similar to a parabolic dependence at low T , changing into linearity at high T.

4.2 Strain effects

Strain effects on the band edge energies can be described following the defomation potential theory of Brooks[6], Herring and Vogt[7], and Kane[8].

The shift of band edges can be decomposed into a term, further called hydrostatic, affectting the average of a certain degenerate conduction band minimum or the valence band and a term, called uniaxial, influencing each individual minimum(Figure 1).

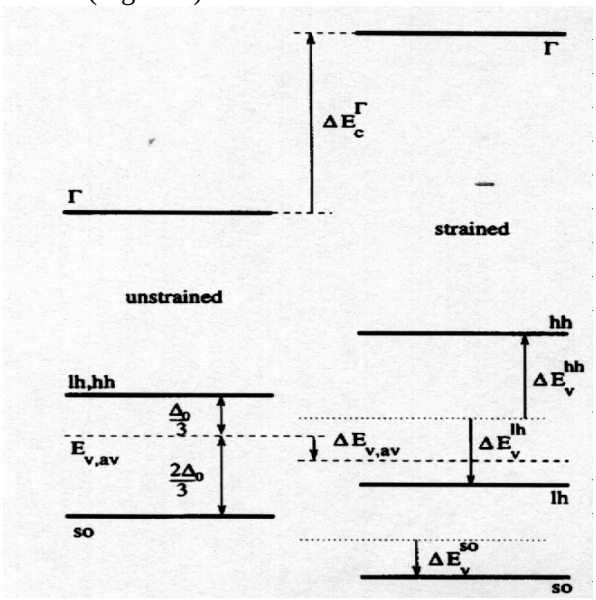

Figure. 1. Band edges for unstrained and strained III-V semiconductors

5. Effective Electron Mass

The effective electron mass can be closely related to fundamental band parameters via **K.p** theory[9]. For the unstrained direct Γ valley holds ;

$$\frac{1}{m^{\Gamma}} = 1 + \frac{E_p}{3}\left(\frac{2}{E^{\Gamma}} + \frac{1}{E^{\Gamma} + \Delta_0}\right) \tag{6}$$

E_p denotes the squared conduction (Γ) to valence band momentum matrix element. Terms resulting from higher bands can be negleted for III-V

compound since their gaps are much larger and the matrix elements are small. The polynomial approximation of ( ) for Ga_x In_{1-x} As
at low temperature ;

$$m^{\Gamma}(x,0) = 0.0237 + 0.031x + 0.0122x^2 \qquad (7)$$

shows a small deviation of m^{Γ} from linearity. The effects of temperature can be calculated using (5). The dependence on T is rather weak, so an Asatz with a linear material independent temperature coeficient is sufficient ;

$$m^{\Gamma}(x,T) = m^{\Gamma}(x,0) - 1.2.10^{-5}\frac{T}{K} \qquad (8)$$

5.1 Strain Effects

In the strained case m^{Γ} becomes anisotropic. An extension of (6) leads to different masses parallel and perponducular to the interface[1-10] ;

$$\frac{1}{m_{\perp}^{\Gamma}} = 1 + \frac{E_p}{3}\left(\frac{3}{2E^{\Gamma-hh}} + \frac{1}{2E^{\Gamma-lh}} + \frac{1}{E^{\Gamma-s_o}} + \frac{2\delta E}{\Delta_0}\left(\frac{1}{E^{\Gamma-lh}} - \frac{1}{E^{\Gamma-s_o}}\right)\right)$$

(9)

$$\frac{1}{m_{ii}^{\Gamma}} = 1 + \frac{E_p}{3}\left(\frac{2}{E^{\Gamma-lh}} + \frac{1}{E^{\Gamma-s_o}} - \frac{4\delta E}{\Delta_0}\left(\frac{1}{E^{\Gamma-lh}} - \frac{1}{E^{\Gamma-s_o}}\right)\right)$$

(10)

where $E^{\Gamma-hh}$ is the difference $E^{\Gamma} - E^{hh}$ under strain. The meaing of the differences $E^{\Gamma-lh}$, $E^{\Gamma-s_o}$ is analogous. The strained mass parameters can be written as ;

$$m_{ii}^{\Gamma} = m^{\Gamma} + \Delta m_{ii}^{\Gamma}$$

$$m_{\perp}^{\Lambda} = m^{\Gamma} + \Delta m_{\perp}^{\Gamma} \qquad (11)$$

The density of state (DOS) mass can be expressed in the same way ;

$$m_d^{\Lambda} = \left(\left(m_{ii}^{\Gamma}\right)^2 m_{\perp}^{\Gamma}\right)^{1/3} = m^{\Gamma} + \Delta m_d^{\Gamma} \qquad (12)$$

6. Results and Discussions.

The model has been used to compute the room temperature velocity of $In_xGa_{1-x}As$ under strain corresponding to pseudomorphic growth on GaAs. Figure. 2.shows the velocity-field characteristics of strained and unstrained $In_{0.25}Ga_{0.75}As$ as together with those of the host material GaAs. The velocity in the strained material is lower than that in the unstrained material. An intersting fact is that, as long as only the velocity is concerned, strained $In_{0.25}Ga_{0.75}As$ and GaAs exhibit almost the same behavior.

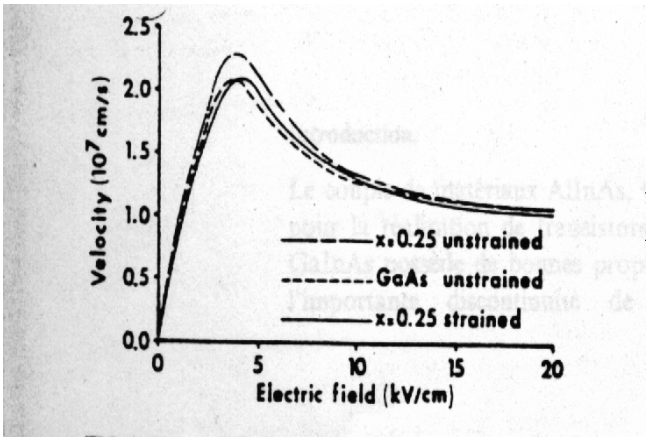

Figure . 2. Velocity- field characteristic of $In_{0.25}Ga_{0.75}As$ under strain corresponding to pseudomorphic growth on GaAs.

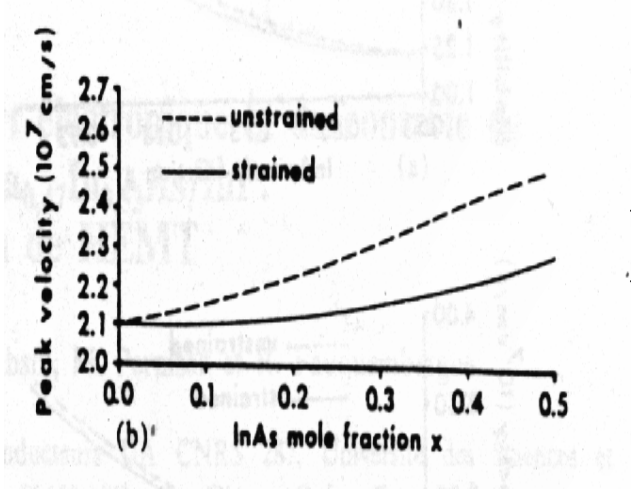

Figure. 3. Peak velocity as a function of x for $In_xGa_{1-x}As$.

This remains true for the whole range of composition x=0-0.25. as shown in Figure. 3, a noticeable improvement of the peak velocity could only be obtained at high x values. Unfortunately, when a GaAs substrate is used, these compositions are unsuitable for device applications owing to the low critical thickness.

The room temperature transport properties of $In_xG_{1-x}As$ (x>0.53), pseudomophically strained on InP, have also been studied. As shown in Figure. 4, the velocity-field characteristic of strained $In_{0.78}Ga_{0.22}As$ is much closer to that of the unstrained material than to that of the lattice matched $In_{0.53}Ga_{0.47}As$. this situation is in strong contrast with that of $In_{0.25}Ga_{0.75}As$ on GaAs, corresponding to the same lattice mismatch. Looking at the peak velocity shown in Figure. 5, we observe that increasing the indium composition significantly improves the transport properties of both strained and unstrained InGaAs.

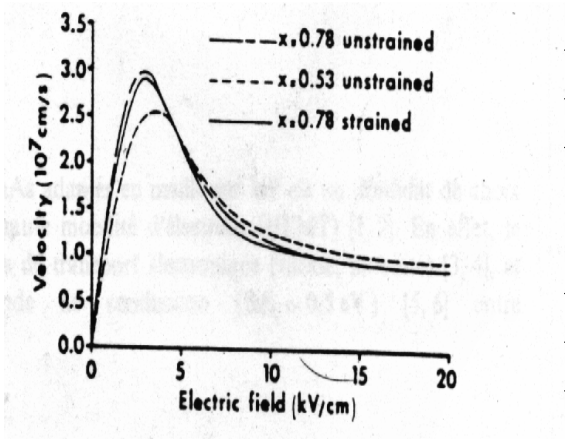

Figure . 4. Velocity- field characteristic of $In_{0.78}Ga_{0.22}As$ under strain corresponding to pseudomorphic growth on InP.

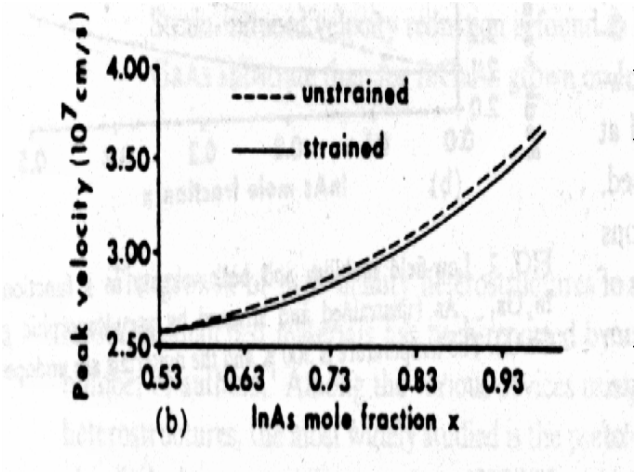

Figure. 5. Peak velocity as a function of x for $In_xGa_{1-x}As$.

Transport properties of unstrained $In_xG_{1-x}As$ are improved when x is increased, owing to the decrease of the Γ valley effective mass and increase of the Γ-L energy spacing. But this evolution is lower at low x, especially when the mobility is concerned. This is explained by an increase of scattering rates with x at low x, mainly due to polar optic and alloy scattering rates, the latter varying roughly as x(1-x). at high x, both effective mass and scattering rates decrease, yielding a more pronounced improvement of transport properties.

7.Conclusion.

The compressive strain leads to several effects, such as increase of effective mass and decrease of intervalley spacing, which are prejudicial to the velocity, for given strain, these effects are less pronunced at high x, owing to the variation of material parameters between GaAs and InAs.as a result, in all cases the compressive strain leads to a velocity degradation which competes the effect of increased indium composition. The relative important of these two effects is strongly dependent on indium composition, the former being dominant at low x and the latter at high x. thE compressive strain such as that encountered in pseudomorphic layers, leads to a degradation of the room

temperature transport properties of InGaAs. The key point is that this effect is much more pronounced for InGaAs(x<0.53) grown on InP. This suggests that the latter material is a good candidate for HEMT Aapplication as confirmed by experimental results.

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