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Mechanical relaxation of strained semiconducting stripes: Influence on optoelectronic properties

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The mechanical relaxation of strained semiconducting stripes is studied. The deformation tensor is calculated using a classical approach of elasticity problem with predeformations; the electronic band structure is then simulated using an 8 band **kp** model including strain. To confirm the models developed, compressively and tensely strained stripes were fabricated and characterized by photoluminescence measurements. Theoretical and experimental results are in very good agreement and show the importance of mechanical anisotropic relaxation phenomena in optoelectronic devices like waveguide structures, modulators, or lasers. © 1997 American Institute of Physics. [S0003-6951(97)04637-8]

The use of strained semiconductors offers new possibilities in terms of the design of optoelectronic devices. On the one hand, stress can be intentionally introduced into a semiconductor layer by the use of a stressing overlayer.¹⁻⁴ On the other hand, in the case of layers strained on their substrate, parasitic elastic stresses can frequently be induced during the technological fabrication of the devices, particularly at the edges of the patterns (mesa, stripes, etc.).⁵ In both cases, inhomogeneous strain fields occur. These resulting stress and strain distributions give rise to modulation of the electronic and optical properties of the materials constituting the final devices. In order to show the importance of nonhomogeneous elastic stresses field induced by the devices fabrication, this letter presents a theoretical and experimental study of stress relaxation of compressively and tensely strained stripes. A complete model describing the mechanical relaxation of the stripes and its influence on the electro-optic properties was developed.

Two structures grown by molecular beam epitaxy on a (001) semi-insulating InP substrate were analyzed. They were comprised of a 2000-Å-thick pseudomorphic In_xGa_{1-x}As layer on a 4000-Å-thick In_{0.52}Al_{0.48}As buffer layer. In the first structure, $x=0.58$ corresponds to a lattice mismatch $\alpha=(a/a_0)-1$ (a being the lattice parameter of the material and a_0 the lattice parameter of the substrate) of +0.33% [compressively strained stripe (CS)]. In the second one, $x=0.485$ leads to a lattice mismatch of -0.32% [tensely strained stripe (TS)]. InGaAs-based stripes of 50 μm in width with 50 μm spacing between two adjacent stripes were patterned using selective CH₄/H₂ reactive ion etching.⁶

Models were developed first in order to simulate the structures. Then, to confirm these models, theoretical results were compared to experimental photoluminescence measurements. Figure 1 shows a schematic view of half the stripe (along the lateral axis). A mechanical analysis is performed first. It consists of a classical elasticity problem with predeformations. The reference configuration, defined by reducing in each material the lattice parameter a to the value a_0 of the

substrate material, leads to a fictitious and stressed reference condition but allows a simple formulation of the mechanical problem. Considering Fig. 1, the boundary conditions are the following: no motion at the edge of the substrate (OAD), no horizontal motion (OBE), and free surface elsewhere (EFCD). For the stripes studied here, the substrate and the layer are supposed to have the same elastic properties, and to be different only through their lattice parameter.

Practically, calculations are done in the area defined in Fig. 1. $X=0$ is a symmetry plane for the stripe, and along the Y direction there is a continuous translation symmetry. An aspect ratio, width over thickness, of 50 is chosen in order to have a fully strained region (i.e., no strain relaxation) around $X=0$ (i.e., the center of the stripe). A rectangular mesh is used, namely, 10 elements along the Z axis and 50 elements along the X axis in the layer. The e_{xx} and e_{zz} strain tensor components and the shear deformations e_{xz} are given in Fig. 2 for the CS stripe. Calculations are done in each element of the mesh, but for better understanding, the results are given in terms of variations of these deformations along the X axis (corresponding to the stripe width) for several vertical coordinates in the stripe ($Z=0.05$, $Z=0.55$, and $Z=0.95$; $Z=1$ corresponding to the top stripe surface). Relaxation phenomena clearly occur near the stripe edges, over distances of a few stripe thicknesses. Results are thus only depicted near the edges of the stripes. In the middle of the stripe, the deformations are those related to the pseudomorphic layer, namely, $e_{xx}=-0.0033$, $e_{yy}=-0.0033$, and $e_{zz}=+0.0034$, shear deformations e_{xz} being obviously equal to 0; all these

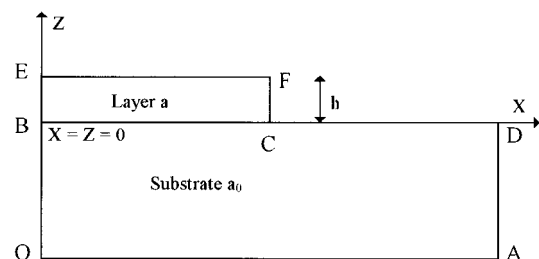


FIG. 1. Schematic view of the stripe.

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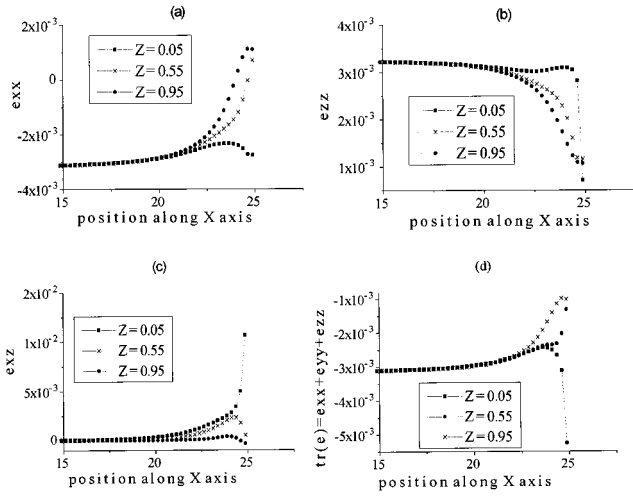


FIG. 2. Variations of the e_{xx} (a), e_{zz} (b), and e_{xz} (c) strain tensor components, and variations of the hydrostatic part ($e_{xx} + e_{yy} + e_{zz}$) (d) for the compressively strained stripe structure.

components significantly change near the edges. For Z larger than about half of the stripe thickness, there is a phenomenon of overrelaxation along the X axis: the strain tensor component, e_{xx} , which is at first negative, becomes weakly positive. This is due to the stress singularity which appears at corner C (Fig. 1). These well known singularities can be studied from an analytic point of view, leading to an asymptotic expression for the displacement u_i and the stress σ_{ij} :

$$u_i = r^\alpha U_i(\theta), \quad \sigma_{ij} = \frac{1}{r^{1-\alpha}} \varphi_{ij}(\theta), \quad (1)$$

where r and θ are the polar coordinates around C. The eigen-shapes $U_i(\theta)$ and $\varphi_{ij}(\theta)$ can be obtained through the solution of an appropriate spectrum. The characteristic exponent α has been roughly estimated as 0.7.⁷

The strain tensor components corresponding to the TS stripe are the opposite of the CS stripe ones for directions X , Y , and Z whereas shear deformations keep the same values in both cases.

Once the strain tensor components are known, the electronic band structure calculation can be performed. The electronic states and the energy levels are found by solving the Schrödinger equation. An 8 band **kp** model, based on Kane's formalism⁸ including the spin-orbit interactions is used. Strain states have been introduced by Bahder⁹ by repeating the original derivation given by Bir and Pikus.^{10,11} At each point of the material the strain tensor components are known and electronic properties can thus be calculated.

Calculations were done for both structures. The results are presented in Fig. 3 for the CS stripe. Variations of the mean band gap [$E_{g \text{ mean}} = (E_g(\text{HH}) + E_g(\text{LH}))/2$, HH, and LH corresponding to the heavy and light holes, respectively] are plotted along the X axis for the three Z coordinates defined previously. HH/LH splitting is also represented. Far from the edges, for both strain cases, the energy transitions corresponding to the pseudomorphic layer band gaps are obtained. When a layer is under compressive (tensile) biaxial strain, the uniaxial component increases the heavy (light) hole band level. The band gaps are thus $E_g(\text{HH}) = 0.689$ eV

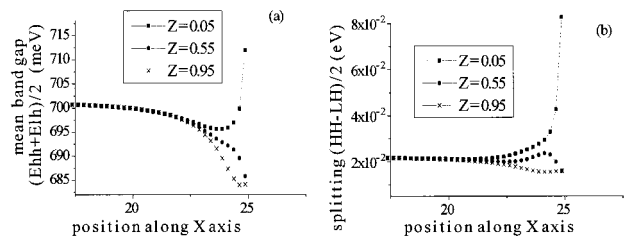


FIG. 3. Variations of the mean band gap (a) and variations of HH/LH splitting (b) for the compressively strained stripe structure.

for the CS stripe, and $E_g(\text{LH}) = 0.741$ eV for the TS stripe. In order to understand the change of the mean band gap and HH/LH splitting versus the strain relaxation, approximated analytic expressions from Ref. 12 can be used. The mean band gap is directly related to the hydrostatic part of the strain:

$$E_{g \text{ mean}} = E_g + a_g(e_{xx} + e_{yy} + e_{zz}), \quad (2)$$

where E_g is the band gap of the unstrained material, and a_g is the hydrostatic deformation potential.

HH/LH splitting, $E_s = \text{HH} - \text{LH}$ is given by

$$E_s = \left\{ \frac{b_v^2}{2} [(e_{xx} - e_{yy})^2 + (e_{xx} - e_{zz})^2 + (e_{yy} - e_{zz})^2] + d_v^2 e_{xz}^2 \right\}^{1/2}, \quad (3)$$

where b_v is the valence band deformation potential associated with strain along the $[100]$ direction, and d_v is the shear deformation potential for strain along the $[111]$ direction.

For the CS stripe, variations of the mean band gap near the edges of the stripe are directly related to the change of $tr(\bar{e}) = (e_{xx} + e_{yy} + e_{zz})$. This part is clearly demonstrated by a comparison between Fig. 2(b) and Fig. 3(a). For $Z = 0.05$, i.e., near the interface between the stripe and the substrate, the mean band gap is drastically reduced close to the edge due to the singularity at the point called C in Fig. 1, where the tensor components become infinite. The compressive character of the strain is intensified through e_{xx} and $tr(\bar{e})$ thus becomes strongly negative. For $Z = 0.55$ and $Z = 0.95$, where an overrelaxation phenomenon occurs near the edges, the e_{xx} component becomes positive and $tr(\bar{e})$ is finally increasing, inducing an increase of the mean band gap near the edges.

HH/LH splitting includes two terms, the first related to the normal strains (e_{xx} , e_{yy} , and e_{zz}), and the second that depends on shear deformation e_{xz} . In our case, the first term is found to be much smaller than the second one. Variations of HH/LH splitting are thus close to variations of shear deformation e_{xz} . This is in agreement with the results presented in Fig. 4. Around the middle of the stripe, the splitting is independent of Z and corresponds to the strain state of the pseudomorphic layer. For $Z = 0.05$, near the singularity C, the splitting is greatly enhanced as a result of the increase in the e_{xz} stress tensor component. On the other hand, for larger Z , near the edges, the splitting varies weakly according to the small change of e_{xz} .

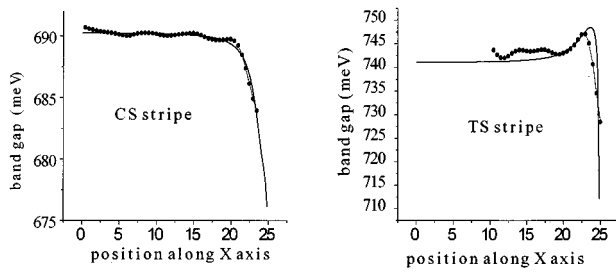


FIG. 4. Variations of the average over the stripe thickness of the theoretical and measured band gap energies for the compressively and the tensely strained stripe structures; the solid line (circle) corresponds to the calculated (measured) values.

As expected with regard to the TS stripe, the tensor components have the same magnitude as that of the CS stripe; the only difference lies in the signs of the normal components, which are opposite. Variations of the mean band gap are thus opposite to those of the previous case, but the same splitting is obtained, the splitting being solely related to the magnitude of the tensor components.

To confirm the theoretical models, the samples were investigated using spectral scanning photoluminescence (SR-SPL) carried out at room temperature, using as the light excitation, a focused He–Ne laser spot. The lateral resolution of measurement is $1 \mu\text{m}$. Since the absorption depth of the light is on the order of the thickness of the stripe, it is considered that the entire depth of the stripe contributes equally to the photoluminescence spectra. Calculations show that the energy band gap variation along the Z axis is less than kT . Therefore, it can be assumed that the photoluminescence measurement is related to the average (E_{av}) over the stripe thickness of the simulated energy band gaps. According to Ref. 13, the measured energy variations at half-width peak (Ehwp) at the low energy side correspond to the energy band gap variations. The average over the stripe thickness of the measured energies at half width peak at low energy side (Ehwp), in comparison with E_{av} , is shown in Fig. 4 for both samples and shows very good agreement between theory and experiments. For the CS stripe, the measurements of the band gaps were shifted by 2 meV. This value corresponds to the slight difference between the 58% theoretically considered composition and the real composition which is 57.4% as derived from DDX investigation. In the middle of the stripe,

the calculations and measurements give the same results. Theoretical and experimental variations are also in good agreement near the edges: the calculated shift between the center and the edges of the stripe, about 15 meV, is confirmed by these measurements. For the TS stripe, the agreement is quite good too although a small discrepancy appears between theory and experiment.

A model describing the mechanical relaxation phenomena and their effect on electro-optic properties of strained stripes was developed. This model was confirmed by photoluminescence measurements. The observed band gap variations between the center and the edges of the stripes confirm that it is necessary to take into account the mechanical stress relaxation phenomena in the device simulation and it is especially necessary for the design of optoelectronic devices. For the two structures studied in this letter, the initial lattice mismatch was weak, about 0.3%. Fluctuations of the electronic and optical properties are increased when higher lattice mismatches are used in quantum wells, for example, for infrared wave length applications. Work in this direction, including quantum confinement calculation, is currently in progress.

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