Stress relaxation in laterally small strained semiconductor epilayers

P. Van Mieghem, S. C. Jain, J. Nijs, and R. Van Overstraeten
Interuniversity Micro Electronics Center (IMEC), Kapeldreef 75, B3001 Leuven, Belgium

(Received 25 August 1992; accepted for publication 27 August 1993)

The stress field in laterally small strained semiconductor epilayers has been studied by the finite element method. The reaction of the epilayer on the substrate and the bulging-out effect caused by shear forces in the side wall boundaries play an important role. Analytical approximate methods are shown to be deficient. The normal stresses relax faster than a simple exponential with height z and virtually complete relaxation occurs at a height $h_{\rm eff} \approx \sqrt{ab}/2$ (where a and b are the width and length, respectively, of the parallellopipidial epilayer) which is in good agreement with recent experiments. An equivalent lattice spacing f_m as a function of $z/\sqrt{ab}$ is defined and calculated.

Equilibrium theories of elastic stress relaxation in epilayers are valid only when the lateral dimension a,b of the layers is much larger than its height h.[1,2] Currently there is a lot of interest in small layers ($a,b<h$). Both in Ge/Si[3,4] and GaInAs/GaAs[5] systems, where the strain is 4% to 5%, the growth is islandic after a few monolayers. In both cases the initial strain relaxes not by the introduction of dislocations but by the islandic deformation. Small layers have also been grown using selective growth techniques.[6,7] Again, strain in these layers is found to relax without the introduction of misfit dislocations. Pioneering work to calculate approximately the strain relaxation in small layers was done by Suhir *et al.*[8,9] In this communication, the stress field in small layers using the finite element method (FEM) is calculated with SYSTUS[11] showing the deficiencies of analytical approximations. Our results agree well with the recent experiment of Eaglesham *et al.*[4,5]

The simplest geometry that may represent an epilayer island is a parallelopiped. Even in this simple shape no analytical solution seems available to determine the elastic stress distribution due to the interfacial lattice mismatch because it requires[10] the simultaneous solution of nine partial differential equations. A sufficiently accurate solution of the problem is obtained by the FEM, which is extremely well suited since the parallelopiped is divided into elements (or unit cells) and into nodes (or atoms).

We consider parallelopipida with an interfacial plane $-a/2\leqslant x\leqslant a/2$, $-b/2\leqslant y\leqslant b/2$ and a height $0\leqslant z\leqslant h$, where $z\leqslant b$. To achieve high accuracy we chose elements containing 20 nodes, with the height depending exponentially on the z coordinate as the stress distribution changes rapidly near the interface. This accuracy constraint limits the one to one correspondence of the physics (atoms and unit cells) with the FEM (nodes and elements) in the z direction. The numerical results apply to pure Ge on Si but are easily extended to other materials. The lateral length of a unit cell equals the lattice spacing of Ge (5.65 Å). As a boundary condition, all nodes (atoms) in the interface plane ($z=0$) are displaced to cause a uniform biaxial strain of 4.17% (the lattice mismatch between Ge and Si). In addition, we restrict their motion in the z direction ($u_z(x,y,0)=0$). This constraint is the only assumption made and is believed to be reasonable (it is supported by Fig. 2 in Ref. 4 and will be discussed further).

For $a=b=h=8$ unit cells, we have simulated the elastic stress distributions as a function of z. A plot of a deformed parallelopiped is inserted in Fig. 1. The results in the cross section $x=y$ from the center to the corner of the parallelopiped are shown in Figs. 1 and 2. Due to symmetry, we have $\sigma_x=\sigma_y$, $\tau_{xz}=\tau_{yz}$, and $u_x=u_y$ for nodes in the plane $x=y$. As expected, the normal stresses σ_x (Fig. 1) decrease along the diagonal for sufficiently high z. Near the interface an opposite behavior is observed. The lattice mismatch forces the epilayer to bend, which is prohibited by our boundary condition $u_z(x,y,0)=0$ for all $-a/2\leqslant x\leqslant a/2$, $-b/2\leqslant y\leqslant b/2$. As a result, large normal stresses σ_z (Fig. 1) originate, influencing the normal stress σ_x through the Poisson effect. From these high interface stresses we conclude that the substrate is locally deformed by the lattice mismatched epilayer and that the boundary condition $u_z(x,y,0)=0$ should be relaxed. For the higher values of z the normal stress σ_x changes sign and becomes even weakly tensile. The shear stresses parallel with the interface, τ_{xy}, happen to be two orders of magnitude smaller than the other stress components and are almost zero in the center. This means that the form of the squarial interface is well maintained. The shear stresses τ_{xz} (Fig. 2), on the other hand, are comparable to the normal stresses and increase toward the corner causing the "bulging-out" effect. The displacements u_x (Fig. 2) at $z=0$ reflect the boundary interface condition of 4.17% strain. The displacement u_z (Fig. 2) shows how the cross section along the diagonal bends but flattens toward the top which is of technological interest.

The homogeneous elastic energy[10] in a slab parallel to the interface plane between z and $z+\Delta z$, $E_h(z)$ is calculated as

$$E_h(z)=\sum_{(z-\Delta z_{\rm el}<z_{\rm el}<z)} [I_l^2(z_{\rm el})-2(1+\nu)I_2(z_{\rm el})]\frac{ab\Delta z_{\rm el}}{2E}, \tag{1}$$

with the stress invariants

$$I_1=\sigma_x+\sigma_y+\sigma_z, \tag{2}$$

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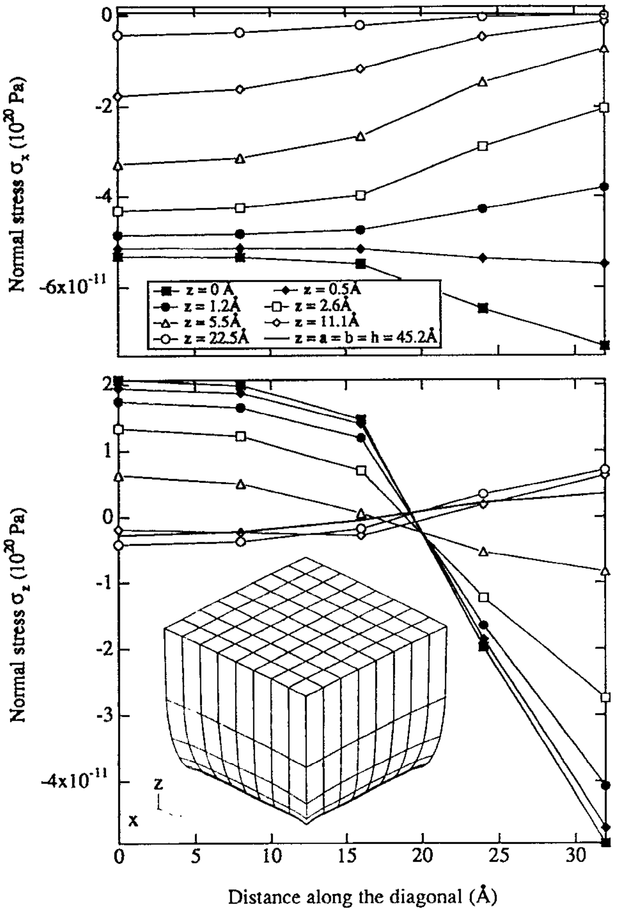

FIG. 1. The normal stresses σ_x and σ_z for various heights z, as a function of distance from the center along the diagonal to the corner in a parallelopiped ($a=b=h=45.2$ Å), for which the deformed mesh is drawn in the insert.

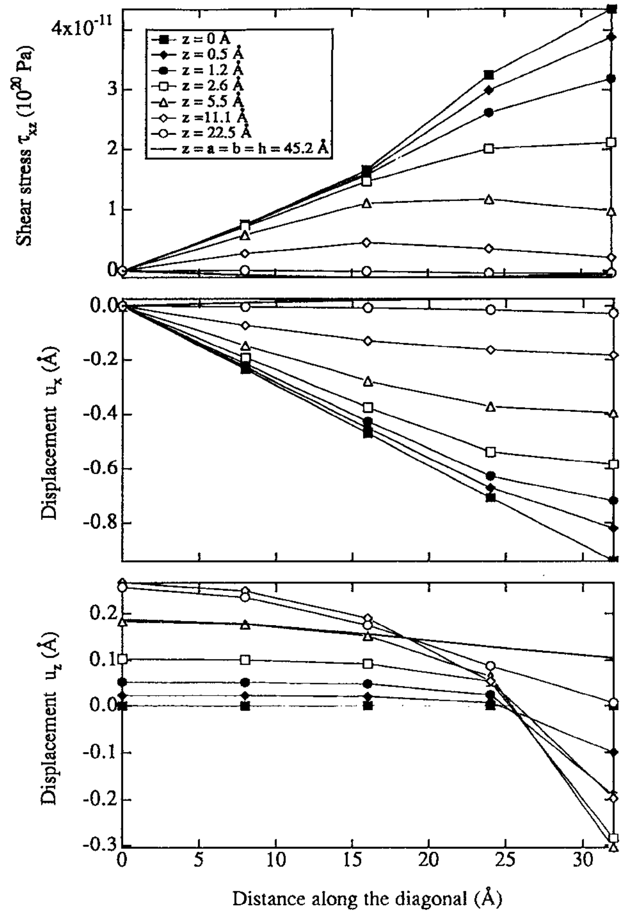

FIG. 2. The shear stress t_{xz} and displacements u_x and u_z for various heights z as a function of distance from the center along the diagonal to the corner ($a=b=h=45.2$ Å).

$$I_2=\sigma_x\sigma_y+\sigma_x\sigma_z+\sigma_y\sigma_z-\tau_{xy}^2-\tau_{xz}^2-\tau_{yz}^2, \tag{3}$$

and the Young's modulus, $E=1.08\ 10^{-9}$ N/Å^2, the Poisson modulus $\nu=0.249$, Δz_{el} the projection of the element of the z axis, z_{el} the z coordinate of the center of the element. In the case of plane biaxial stresses,[10] Eq. (1) reduces to

$$E_{h;\,\mathrm{plane}}(z)=\frac{E}{1-\nu}\epsilon_x^2\,\Delta z_{\mathrm{el}}ab. \tag{4}$$

We define an equivalent strain $f_m(z)$ as

$$f_m(z)=\sqrt{\frac{E_h(z)(1-\nu)}{E\Delta z_{\mathrm{el}}ab}} \tag{5}$$

to compare strain relaxation in islands with the corresponding biaxial strain. In Fig. 3, $f_m(z)$ is shown as a function of the dimensionless ratio $z/\sqrt{ab}$. For low values of $z/\sqrt{ab}, f_m(z)$ exceeds 4.17%, as the deformation energy is larger than for the corresponding biaxial deformation because the corners of the parallellipipidum are distorted and shear stresses are important. Moreover, the influence of the normal stress σ_z (Fig. 1) at the interface, intensified by our boundary condition $u_z(x,y,0)=0$, increases the total elastic energy. When $z/\sqrt{ab}$ increases the bulging-out of the parallelopiped decreases the total deformation energy. For $z/\sqrt{ab}\approx 1/2$, f_m saturates around 1.5%. Eaglesham *et al.*[3,4] have estimated from experiment that islandic growth would reduce the strain to about 2%. From this saturation threshold, we find an effective height of the strained layer $h_{\mathrm{eff}}\approx\sqrt{ab}/2$, in good agreement with the onset of dislocations found in islands (Fig. 4 of Ref. 3)

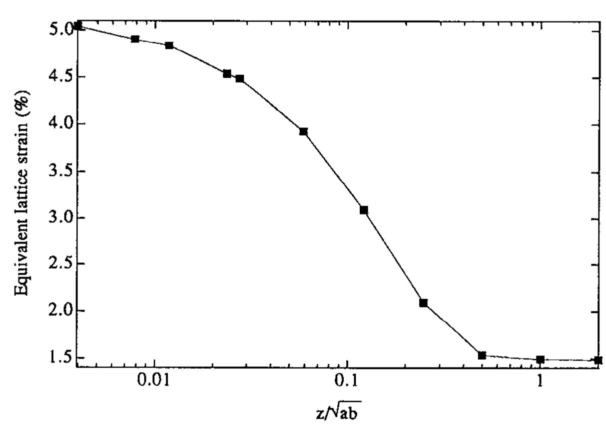

FIG. 3. The equivalent lattice strain f_m plotted vs the ratio of height z upon the square of the interface area $\sqrt{ab}$.

TABLE I. Linear and quadratic fits of $\ln \sigma_x(0,0,z)$ vs z for different geometries (a,b).

a (Å)	b (Å)	$\ln \sigma_x(0,0,z) = A + Bz$			$\ln \sigma_x(0,0,z) = C + Dz + Ez^2$			
		A	B	χ^2	C	D	E	χ^2
16.9	113.1	−23.59	−0.3152	0.065	−23.67	−0.2218	−0.00 855	0.000 2
22.6	113.1	−23.62	−0.2295	0.019	−23.66	−0.1793	−0.00 460	0.000 5
28.2	113.1	−23.63	−0.1671	0.013	−23.67	−0.1261	−0.00 375	0.000 3
28.2	56.5	−23.62	−0.1681	0.013	−23.66	−0.1278	−0.00 369	0.000 3
33.9	56.5	−23.63	−0.1392	0.007	−23.65	−0.1080	−0.00 286	0.000 2
39.6	56.5	−23.63	−0.1128	0.005	−23.65	−0.0873	−0.00 234	0.000 08
45.2	45.2	−23.63	−0.0982	0.003	−23.65	−0.0770	−0.00 194	0.000 05

with diameter $D=1400$ Å above 500 Å since $h_{\text{eff}} \approx \sqrt{\pi}\, D_{\text{eff}}/4 = 620$ Å should be reduced somewhat because $D_{\text{eff}} < D$.

The normal stress field σ_x in several geometries (Table I) has been compared with the approximate model of Luryi and Suhir[9] (LS model),

$$\sigma_x(x,y,z) = f\frac{E}{1-\nu}\left[1 - \frac{\cosh(kx)}{\cosh(ka/2)}\theta(h_e - z)\right] e^{-\pi/az}, \qquad (6)$$

with $\theta(z)$ Heavyside's step function and the lattice mismatch $f=0.0417\xi$ (in pure Ge, $\xi=1$). For low z, there is no correspondence with Eq. (6) because of interface reactions. For higher z, the behavior of σ_x as a function of x is similar, except near the edges. The relaxation of σ_x with z is drawn in Fig. 4 but completed in Table I. Limiting $z < h/2$ (above this value the stress field is virtually relaxed), we observe that the stresses relax faster with z than predicted by Eq. (6). Moreover, $\ln \sigma_x(0,0,z)$ is better approximated by a parabola than by a straight line, implying that the stress field in small islands relaxes faster than previously predicted.[9] The fact that $\sigma_x(0,0,z)$ hardly depends on $b(>a)$ agrees with Eq. (6). Further, $\sigma_x(0,0,0)$ turns out to be almost independent of geometry (insert of Fig. 4) in contrast to Eq. (6). All these observations are embodied in an empirical formula ($z < h/2$:$a \leqslant b$, and $a < h$)

$$\sigma_x(0,0,z) \approx f\frac{E}{\sqrt{1-\nu}} \exp\left[-\pi^{3/2}\left(\frac{z}{a^{9/8}}\right) - \frac{1}{\sqrt{\pi}}\left(\frac{z}{a^{3/4}}\right)^2\right]. \qquad (7)$$

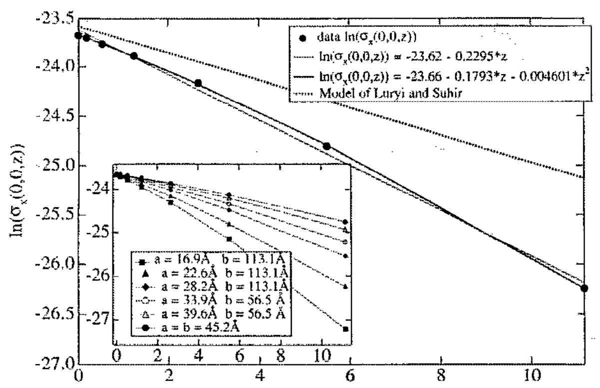

FIG. 4. Comparison of $\ln \sigma_x(0,0,z)$ calculated by the FEM and by the LS model for different geometries.

From Table I and Eq. (6), we deduce that the LS model is reasonably good for small a/b ratios and small z, consistent with the two-dimensional assumption ($a/b=0$) of the LS model. However, for higher $a/b(\leqslant 1)$ the correspondence deteriorates quickly. In addition, we have compared the most favorable line parallel with the z axis, namely, that in the middle of the structure. A similar comparison of the z dependence of the normal stresses near the edges is worse due to the bulging-out effect. We thus infer that the LS model conclusions do not apply for the geometries investigated here and that the error made by using their model can be large.

In conclusion, within the basic approximation $u_z(x,y,0)=0$, an equivalent strain can be defined as a function of $z/\sqrt{ab}$, and $\ln \sigma_x(0,0,z)$ decreases faster (quadratically) with height z than was previously believed (linearally as proposed by Luryi and Suhir). An effective height of the strained layer $h_{\text{eff}} \approx \sqrt{ab}/2$ is obtained and agrees well with experiment.

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