Edge strain relaxation in quantum wells grown on the cleaved edge of a strained semiconductor superlattice

C. Priester
IEMN, Département ISEN, Avenue Poincaré, Boîte Postale 69, F-59652 Villeneuve d'Ascq Cédex, France

S. J. Sferco
INTEC, Güemes 3450, 3000 Sante Fe, Argentina

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In this Brief Report we address, from a theoretical point of view, the question of the existence and the localization of strain-induced quantum wires when one deposits a strained quantum well on the cleaved edge of a strained superlattice (such as a CdTe quantum well on the cleaved edge of a $CdTe/Cd_xZn_{1-x}Te$ superlattice). For systems in which ternary layers are made of perfectly homogeneous composition alloys, and with no width fluctuation, we show a very strong decay of the strain modulation versus the distance to the cleavage interface. We also demonstrate a strong strain relaxation near the edge of the structure. [S0163-1829(97)05311-3]

In strained semiconductor systems surface effects are often intimately bound to strain-relaxation effects. This is the case for quantum wires grown directly from molecular-beam epitaxy (MBE). Such systems, which are very attractive due to their potential optoelectronic applications, were initially proposed in Ref. 1. They result from a two-step growth process. During the first step a strained superlattice is deposited on a substrate in the [001] direction. The sample is then cleaved. The second step is the growth of three layers (a quantum well sandwiched between two barriers) above the [110] cleaved interface. Such structures were first grown with III-V systems[1] and more recently with CdTe-$Cd_xZn_{1-x}Te$ layers, the superlattice being strain compensated.[2,3] In such systems, the strain present in the superlattice is generally supposed to induce lateral confinement in the [110] quantum well resulting from strain modulation in the in-plane lattice constant of the overgrown quantum well. Quantum wires should result from this lateral confinement. Photoluminescence (PL) measurements clearly show three different typical PL spectra, obtained from three different regions of the sample.[2,3] The PL obtained from the quantum well above the superlattice is a broad band shifted by about 20 meV to the red relative to the PL spectrum from the quantum well above the substrate. This experimental result supports the assumption of carrier localization by strain modulation in the quantum well. Some calculations have been performed, within the so-called zero-attenuation assumption (ZAA), i.e., assuming that the strain modulation present within the superlattice is entirely transferred to the [110] quantum well. The resulting calculated energy shift is in good agreement with the experimental shift obtained during excitement at low-power density.[4]

However, the ZAA is bound to lead to an overestimation of the strain modulation in the overgrown quantum well, as emphasized by Kash *et al.*[5] Their description within continuous elasticity theory, using a standard finite-element method, has led to the conclusion that for the III-V structure described in Ref. 1, the attenuation lowers the strain modulation by two orders of magnitude, relative to the ZAA.

The first point that we want to address here is, for the II-VI structures studied in Refs. 2 and 3, the strength of the attenuation of the strain modulation and which are the leading parameters for this attenuation. The second issue is, in case this attenuation cannot be avoided, to propose an alternative explanation for the PL ''wire signal.''

To resolve these questions it is important to know the strain distribution all over the structure. We have calculated this using a microscopic description described hereafter.

The microscopic elastic energy is treated within a valence force field (VFF) approach[6] or, more precisely, the Keating model for the present calculation.[7] This choice of a VFF framework to calculate elastic energies allows, due to its simplicity, the treatment of systems with a great number of atoms, up to 10^6 per period. We calculate the atomic positions that minimize the elastic energy of the system via a conjugate gradient method.[8] As we consider systems where surfaces are supposed to be perfectly planar, we have chosen not to take into account surface reconstruction or dimerization (whose effect, in these purely two-dimensional surfaces, has made three atomic planes completely vanish from the surface).

The structures studied here are made of layers typically 50, 100, or 200 Å wide. Such systems do not require the use of a microscopic model: the layers are wide enough for continuous elasticity to be efficient. In other words, due to the large number of atoms considered, we do not expect that our atomic description differs significantly from the standard finite-element methods of continuous description used by Kash *et al.*[5] The Keating parameters were taken from fits on the elastic constants for the pure, stoichiometric CdTe and ZnTe semiconductors.[9] Keating parameters for $Cd_xZn_{1-x}Te$ alloys have been calculated as concentration-weighted averages of the parameters for binary compounds. From the atomic positions in the relaxed system, we can derive the local strain state or, equivalently, ϵ_{XX}, ϵ_{YY}, ϵ_{ZZ}, ϵ_{YZ}, ϵ_{XZ}, and ϵ_{XY}, the components of the local deformation tensor. The structures we are interested in were grown on a $Cd_{0.88}Zn_{0.12}Te$ [001] substrate. The strained

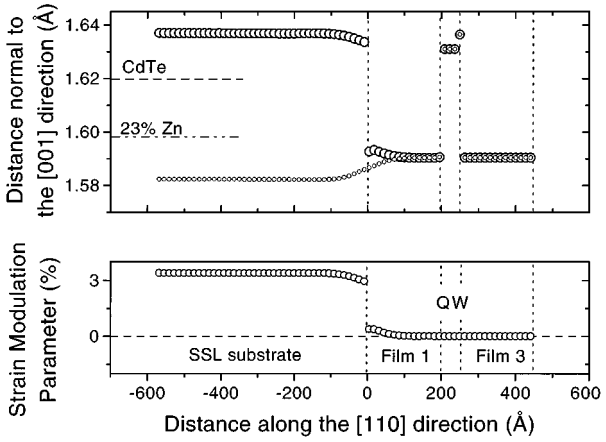

FIG. 1. Strain distribution in a system modeled with an infinite superlattice (with the origin of the distance in the [110] direction being placed at the cleavage with the superlattice). Top: distance between adjacent planes normal to the [001] direction at the center of the CdTe superlattice layers (big circles) and at the center of the $Cd_{0.77}Zn_{0.23}Te$ superlattice layers (small circles), as a function of the distance in the growing [110] direction. As a reference, we indicate the same distances for bulk CdTe (dashed line) and the bulks of Zn atoms, respectively. Bottom: strain modulation parameter (as defined in the text as a function of the distance in the [110] direction. The zero value (dashed lines) indicates that the modulation strain is completely lost.

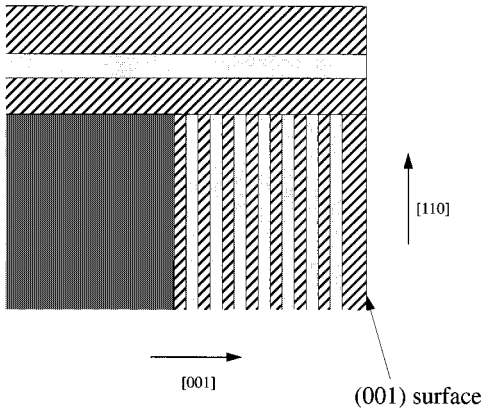

FIG. 2. Schematic representation of the modeled system. The dark gray area corresponds to the $Cd_{0.88}Zn_{0.12}Te$ substrate, the middle gray areas represent CdTe layers, and the hached areas show $Cd_{0.77}Zn_{0.23}Te$ layers.

compensated superlattice is made of 150 periods of [100 Å $Cd_{0.77}Zn_{0.23}Te$/100 Å CdTe]. The first barrier separating the [110] quantum well from the cleavage interface is 100 or 200 Å wide. One idea for modeling such a system is to consider that the superlattice with 150 periods is very large and to assimilate it to an *infinite* superlattice. This way we *neglect the effect of the [001] lateral surface*. This model has been used in Ref. 5. One gets thus a periodic system, the period being 200 Å along the [001] axis and equal to the substrate lattice parameter along the [110] axis. We have calculated the strain relaxation for four different structures described in Ref. 10. Figure 1 provides an overview of the strain distribution for the structure corresponding to a 50-Å-wide CdTe [110] quantum well sandwiched between two 200-Å-wide $Cd_{0.77}Zn_{0.23}Te$ layers. In the upper plot, big and small circles represent the variations of the local in-plane parameter in the [001] direction when one describes a [110] axis located at the center of CdTe (big circles) and $Cd_{0.77}Zn_{0.23}Te$ (small circles) superlattice layers. The ZAA would have provided horizontal lines all over the structure (no attenuation). Figure 1 clearly indicates that, in the structure model here, the strain modulation is totally attenuated in the [110] quantum well: the atoms have elastically rearranged in such a way as to equally distribute the strain in the [110] quantum well. Figure 1 also shows that relaxation occurs in a few monolayers near the cleavage interface. Roughly, we can consider the distance of 100 Å as sufficiently far from the interface to find the system presenting no more differences in the strain state for atoms above each component of the superlattice. This ''quenching distance'' is typically the width of the superlattice layers. In order to emphasize this result, we have calculated what we call the ''strain modulation parameter,'' defined as [(distance in the central plane of CdTe layers) $-$(distance in the central plane of $Cd_{0.77}Zn_{0.23}Te$ layers)]/(the average of both distances), expressed in percent. Figure 1 (bottom) shows the variations of this parameter as a function of the position in the [110] direction. When this parameter vanishes, the strain modulation is completely lost. This is what happens all over the CdTe quantum well. We obtained this for the four calculated systems.[10] Of course, a complete description of the strain state implies the knowledge of all the components of the local strain tensor for all atoms. We have also calculated this, and the loss of strain modulation is confirmed by these calculations.

These results, similar to those of Ref. 5, do not support the formation of quantum wires in the CdTe quantum-well region due to strain-induced modulation from the superlattice. Observation of Fig. 1 could suggest the possibility of a strain-induced creation of a quantum wire just near the interface, in the CdTe layers of the superlattice. However, this confinement should be rather weak (as the strain modulation just below the interface is very weak too), and this hypothesis is not supported by recent experimental data,[11] which have demonstrated that the PL wire signal is bound to the presence of the [110] quantum well (if there had been interface wires they should be observed, even in the absence of the [110] quantum well, which is not the case).

At this point it is interesting to reconsider the model used and to modify it in order to include the effect of the [001] lateral surface. For this we now consider the system schematized in Fig. 2. In this case both the initial [001] substrate and the [001] surface are now explicitly taken into account. Obviously, in order to keep a finite number of ''nonfrozen atoms,'' we have modeled [001] and [110] frozen bottom planes ''far enough'' from the edge, indicating that the substrate is very wide compared to the grown surstructure. The strain modulation corresponding to this system is given in Fig. 3(a). Here we have chosen to represent the local deformations ϵ_{XX}, ϵ_{ZZ}, and ϵ_{XZ} at the center of the [110] CdTe quantum well; the directions (X,Y,Z) are not the crystallographic ones but ([001],[1,1,0],[110]). ϵ_{YY} is fixed by $Cd_{0.88}Zn_{0.12}Te$ to -0.73% and, due to the symmetry of the system, ϵ_{XY} and ϵ_{YZ} vanish. The vertical dotted lines refer to the lower superlattice interfaces (for the sake of legibility, we

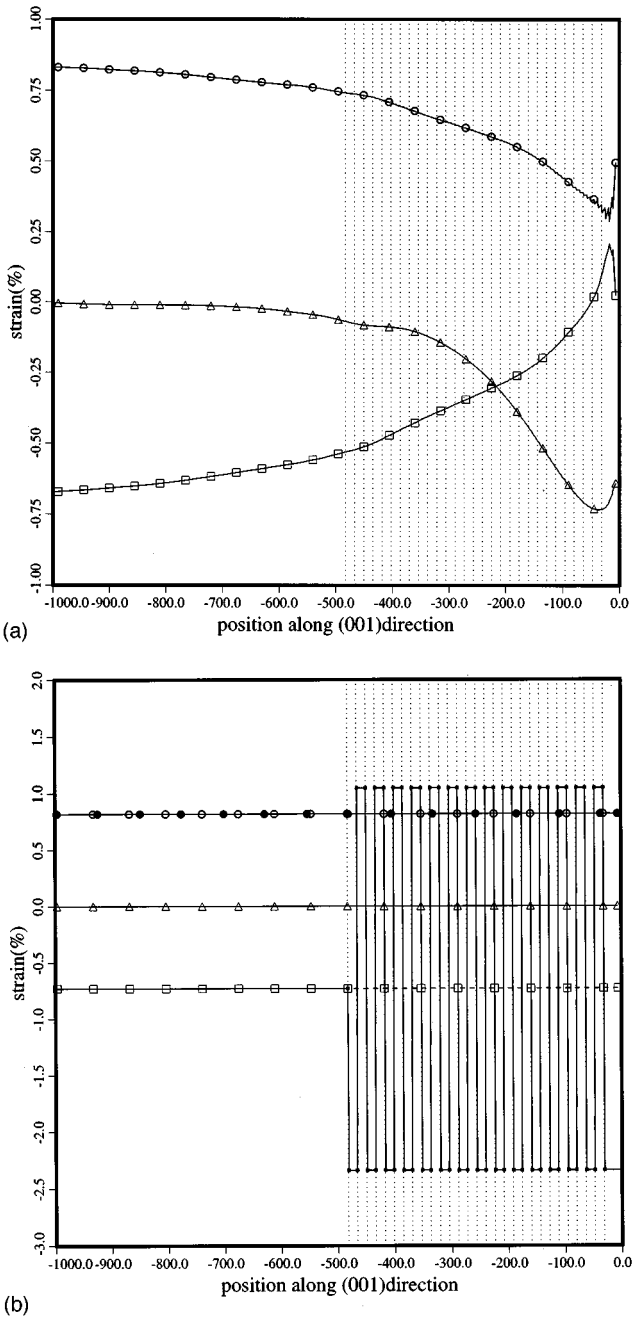

FIG. 3. (a) ϵ_{XX} (squares), ϵ_{ZZ} (circles), and ϵ_{XZ} (triangles) deformations at the center of the [110] CdTe quantum well; the directions (X,Y,Z) are not the crystallographic ones but ([001], [1,1,0],[110]). The origin of the [001] axis is chosen at the lateral surface. (b) Same quantities in the zero attenuation approximation (full lines, close symbols) and far away from the surface as in the infinite superlattice case (dashed lines, open symbols).

have represented a structure with only 14 CdTe layers in the superlattice). For comparison, Fig. 3(b) displays the same quantities in the ZAA case (full lines) and in the infinite system case (dashed lines). Figure 3 gives evidence of a strong edge relaxation: in the vicinity of the lateral [001] surfaces one observes strong variations of the deformations. This phenomenon has been artificially hidden in previous models (ZAA and infinite superlattice). It is interesting to note that this edge relaxation does not depend on the presence of the superlattice (as far as it is ''strain compensated''). Obviously, far enough from the lateral surface, one recovers the strain state calculated previously. However, the decay of the strain relaxation from the surface to the core of the sample appears to be rather slow.

The last step is to correlate the strain modulation in the [110] quantum well to a band edge profile. For this we have calculated, within a two-conduction-band–four-valence-band $\mathbf{k}\cdot\mathbf{p}$ description, the corresponding bulk band edges for CdTe in the strain state we obtained near the [001] surface. We have obtained a slightly smaller gap (only 10 meV lower, the difference being mainly 90% in the conduction band) than in the purely biaxially strained CdTe, far away from the [001] surface. This allows us to consider the possibility of having a very broad surface quantum wire, which could explain the PL wire signal. However, this hypothesis still has to be supported by two further studies: (i) a theoretical one that would calculate the complete electronic structure of the system (this is not trivial due to the continuously varying strain all over the structure) and (ii) an experimental one that would check whether the PL wire signal is still observed in a structure without the strained superlattice. If this is confirmed, one would have one single surface wire instead of the multiple expected strain modulated wires.

Up to this point, we have considered ideal systems in which ternary layers are made of perfectly homogeneous composition alloys and with no width fluctuation. We have shown that, in this case, for usual design parameters there is no periodic lateral strain modulation in the [110] quantum well. The only way to get such a modulation would be to strongly modify design parameters so that the [110] quantum well draws closer to the cleavage interface. Greatly reducing the width of the first barrier requires one to carefully get rid of defects at the cleavage interface. This would imply the sample to be cleaved *in situ* and, just after the cleavage, to check the quality of the regrowth surface. The alternative of widening the superlattice layers, possibly making use of a gradually composition modulated layers in order to avoid problems of plastic relaxation (so that the [110] quantum well becomes relatively closer, in regard to the superlattice layer width, to the cleavage interface), is no more satisfying: the strain modulation period would become so wide that the quantum size effect would be lost.

Moreover, we have emphasized the edge relaxation near the [001] lateral surface. If this phenomenon proves to significantly affect the electronic structure, one should also take it into account when considering wires and dots fabricated by etching.[12]

Finally, one still has to question the validity of considering perfectly homogeneous composition alloys and perfectly flat layers. The question of nonuniform growth on the cleaved surface, leading to surface roughening and the formation of wires, has already been evoked in Ref. 5. It would also be very interesting to study the possibility of strain-induced surface segregation during the second growth state: due to the strain modulation at the cleavage surface, one could get composition modulated [110] barriers. From this a strain redistribution all over the surstructure would result, which could also lead to lateral confinement. This could be

an alternative explanation of the PL wire signal. These two last hypotheses need to be confirmed by additional experimental information on the structural qualities of the layers deposited onto the cleavage interface. At last we can say that the so-called quantum wires with strain-induced lateral confinement are typical strained systems in which both strain relaxation effects and surface effects are intimately coupled.

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