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STRAIN-GENERATED ELECTRIC FIELDS IN [111] GROWTH AXIS STRAINED-LAYER SUPERLATTICES

D. L. Smith

Los Alamos National Laboratory
Los Alamos, NM 87545, USA

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We show that the internal strains in [111] growth axis strained-layer superlattices generate polarization fields by the piezoelectric effect. The electric fields produced by these polarization fields can be very large. For example, in GaAs - $Ga_{0.8}In_{0.2}As$ superlattices, which have a 1.4% lattice mismatch, the fields are greater than 10^5V/cm. The fields are oriented in the [111] direction and have opposite signs in the two materials if the piezoelectric coefficients of the two constituent materials have the same sign. Such strain-induced fields do not occur for [100] growth axis superlattices.

Semiconductor superlattices made from two materials with significantly different lattice constants are of current interest.[1] It has been shown that these strained-layer superlattices can be grown with a high degree of crystalline perfection.[2-4] For sufficiently thin layers, the lattice mismatch is accommodated by internal strains rather than by the formation of dislocations. Most studies of strained-layer superlattices have been performed in III-V semiconductor systems with the growth axis being along a [100] direction. It is well-known, however, that epitaxial growth with a [111] growth direction is also possible for III-V semiconductors. Recently, there have also been studies of II-VI semiconductor superlattices with $\lesssim 0.6\%$ lattice mismatch and a [111] growth direction. The purpose of this communication is to show that for strained-layer superlattices made from zincblend structure semiconductors with a [111] growth direction, large internal electric fields are generated by the piezoelectric effect. These fields do not occur for a [100] growth direction.

Zincblend structure semiconductors are piezoelectric materials. Off-diagonal strains induce an electric polarization given by[5]

$$P_i = e_{14}\,\epsilon_{jk}\ , \qquad (1)$$

where P is the induced polarization, e_{14} is the piezoelectric constant, and ϵ_{jk} is a symmetrized strain component.[6] However, diagonal strains (e.g., ϵ_{xx}) do not induce a polarization (i.e., $e_{11} = 0$) in these materials.[5] A strained-layer superlattice with a [100] growth direction will have only diagonal strains induced,[1] but with a [111] growth direction off-diagonal strains also occur. Thus, [111] growth axis strained-layer superlattices will have strain-induced polarization fields, whereas [100] growth axis materials will not.

To determine the magnitude and direction of the polarization, it is necessary to calculate the lattice-mismatch-induced strains in the two superlattice constituents. By the symmetry of the problem, it is clear that the three diagonal strain components are equal and the three off-diagonal strain components are equal in each material. Thus, there are four unknowns: a diagonal and an off-diagonal strain component in each material. Requiring that the strain-distorted lattice-translation vectors of the two materials have equal projections on the plane normal to the growth direction, gives

$$(1 + \epsilon^a_{xx}) - \frac{\epsilon^a_{xy}}{2}\,a^a = (1 + \epsilon^b_{xx}) - \frac{\epsilon^b_{xy}}{2}\,a^b \qquad (2)$$

where a^i is the lattice constant of material i. The mechanical energy density[7] of the superlattice is minimized with respect to the strain components subject to the condition of Eq. (2). This procedure gives (to first order in the difference in lattice constants)

$$\epsilon^a_{xx} = \frac{a^b/a^a - 1)}{[(1 + A^a) + (1 + A^b)\,B(h_a/h_b)]}\ , \qquad (3a)$$

$$\epsilon^b_{xx} = -\frac{h_a}{h_b}\,B\,\epsilon^a_{xx}\ , \qquad (3b)$$

$$\epsilon^a_{xy} = -2A^a\,\epsilon^a_{xx}\ , \qquad (3c)$$

and

$$\epsilon^b_{xy} = -2A^b\,\epsilon^b_{xx}\ . \qquad (3d)$$

where

$$A^i = \frac{C_{11}^i + 2C_{12}^i}{4C_{44}^i} , \quad (3e)$$

and

$$B = \frac{C_{11}^a + 2C_{12}^a}{C_{11}^b + 2C_{12}^b} , \quad (3f)$$

h_i is the layer thickness of material i and the C's are the elastic constants. Because the three off-diagonal stress components are equal, the components of the polarization vector are equal and the polarization vector is in the [111] direction. The sign of the polarization vector in a material depends on whether it has the larger or smaller lattice constant and on the sign of the piezoelectric coefficient. The common III-V semiconductors have a negative piezoelectric coefficient and the common II-VI semiconductors have a positive piezoelectric coefficient.[8,9] A III-V semiconductor with the larger lattice constant in a [111] strained-layer superlattice will have the polarization vector pointing from the A (cation) to the B (anion) face. A III-V semiconductor with the smaller lattice constant will have the polarization point from the B to the A face. For II-VI semiconductors, the direction of the polarization vectors will be reversed. Thus, for a strained layer superlattice with a [111] growth axis of two III-V or two II-VI semiconductors, polarization vectors along the growth axis, and of opposite sign in the two materials, are induced by the piezoelectric effect. If one were to grow a superlattice of a III-V and a II-VI semiconductor, the polarization vectors in the two materials would have the same sign.

The strain-induced electric polarizations will lead to electric fields given by[5]

$$D_i = \epsilon_0 E_i + \epsilon_0 \chi E_i + e_{14}\epsilon_{jk} , \quad (4)$$

where χ is the susceptibility and D is the displacement. If there are no external charges, D vanishes, leaving

$$E_i = -\frac{e_{14}\epsilon_{jk}}{\epsilon_0 \epsilon} , \quad (5)$$

where $\epsilon = 1 + \chi$ is the low-frequency dielectric constant. If there are free carriers in the superlattice layers, the strain-induced fields will be screened by these carriers (i.e., the low-frequency dielectric function will be large because of the free carrier screening). If one or both of the superlattice layers is devoid of free carriers, large strain-induced electric fields result.

In Fig. 1, we show calculated results for the magnitude of the polarization and electric fields in GaAs - $Ga_{0.8}In_{0.2}As$ superlattices with a [111] growth direction as a function of the ratio of the layer thicknesses. This strained-layer superlattice has been grown with a [100] growth direction.[4] The lattice mismatch is about 1.4%. The piezoelectric constant and the elastic constants of the alloy were taken to be an average of the alloy constituents. The piezoelectric constants of GaAs and InAs were taken from Ref. (8) and the elastic constants from Ref. (10). The first thing to notice is the large magnitude of the induced fields. In particular, electric fields greater than 10^5 V/cm can be generated. These fields are comparable to or larger than those that occur in the depletion region of a p-n junction and are approaching breakdown fields (~$3.5 \cdot 10^5$ V/cm in GaAs). A field of 10^5 v/cm causes a 100 meV energy drop across a 100 Å superlattice layer. This is a large energy compared to typical subband energy splittings in a superlattice or multiple quantum well. Thus, these strain-generated fields can be expected to significantly modify the subband structure. As one would expect, the fields tend to be larger in the thinner material because there the strain is largest. Although the polarization fields in the two materials are of opposite signs, they do not, in general, cancel to zero. Thus, the superlattice has a net macroscopic polarization like a ferroelectric. For comparison, we state the spontaneous polarizations of two common ferroelectrics: KDP - $5.3 \cdot 10^{-2}$ c/m^2 and Rochelle salt - $2.6 \cdot 10^{-3}$ c/m^2. The strain-induced polarizations in the GaAs -$Ga_{0.8}In_{0.2}As$ superlattice layers are smaller than the spontaneous polarization in KDP and comparable to that in Rochelle salt.

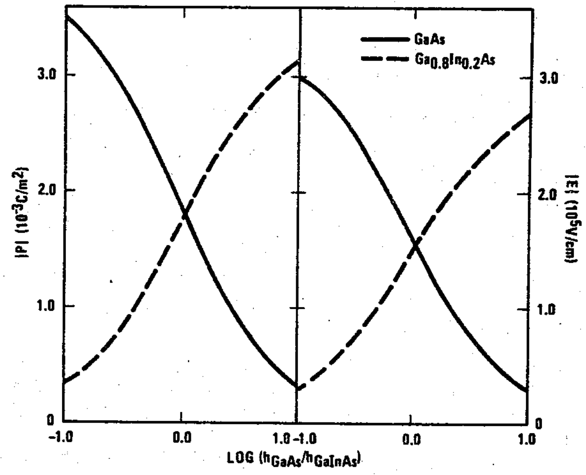

Fig.1. Magnitude of strain-induced polarization (left panel) and corresponding electric field (right panel) in the (111) GaAs - $Ga_{0.8}In_{0.2}As$ superlattice as a function of the logarithm of the ratio of layer thicknesses. The solid lines are the fields in GaAs and the dash lines are the fields in the alloy.

The large alternating strain-induced electric fields should significantly influence the properties of a [111] strained-layer superlattice. For example, these fields should lead to sizable Stark shift in the optical response. Free carriers generated by photoabsorption would screen the fields and reduce the Stark shifts. Thus, nonlinear optical phenomena are also expected to result from the strain-induced fields. Because the internal fields can approach breakdown fields, they might be expected to influence carrier multiplication processes in the materials.

In summary, we have shown that the internal strains in a [111] growth direction strained-layer superlattice generate large electric polarization fields. If not screened by free carriers, these polarization fields cause internal electric fields which can be of the order 10^5V/cm. The fields point in the [111] direction. For a superlattice of two III-V or two II-VI materials, the signs of the fields are opposite in the two materials. Although of opposite signs in each material, the net polarization does not, in general, cancel to zero. Thus, the [111] strained-layer superlattices will have a net macroscopic polarization. In a [111] strained-layer superlattice made from a III-V and a II-VI semiconductor, the polarization fields in both materials would have the same sign. Large net macroscopic polarizations could also be achieved with a superlattice of a III-V or II-VI semiconductor and a group IV semiconductor (e.g., GaAsP-Si). Finally, we note that strained-layer superlattices with growth directions other than [111] can also have large piezoelectric polarizations induced. Similar strain-induced polarizations can occur for superlattices with crystal structures other than zincblend. The [100] growth direction in zincblend structure semiconductors is rather special in that lattice mismatch only causes stress components that do not induce a polarization for this growth direction.

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