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Erratum: "Analyzing the growth of $In_xGa_{1-x}N$/GaN superlattices in self-induced GaN nanowires by x-ray diffraction" [Appl. Phys. Lett. 98, 261907 (2011)]

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In our original paper, the effect of lateral relaxation in axial nanowire superlattices (SLs) on the average out-of-plane lattice parameter was given incorrectly.[1] This leads to an underestimation of the In content by approximately 30% of the given values, otherwise our findings remain valid. We derive here the correct expression that replaces Eq. (2) of the original paper.

Symmetric Bragg x-ray diffraction probes the vertical (normal to the layers) lattice constants of strained layers in a heterostructure. For coherent epitaxial growth without plastic relaxation, all layers attain a common in-plane lattice parameter. In case of a planar heterostructure on a bulk substrate, all layers have the same lateral lattice parameter as the substrate. The resulting average vertical lattice parameter of the heterostructure is governed by the Poisson effect, and the well-known result is given below in Eq. (9). In a nanowire, however, the heterostructure is free to relax laterally, and the in-plane lattice parameter is obtained from a balance between layers. If the requirement of the stress-free side surface is satisfied on average, the Poisson effect is compensated and the average vertical lattice parameter is given by Eq. (11) below.

To derive this not obvious result, let us consider a periodic superlattice stack made from two materials, 1 and 2. Material 1 is taken as a reference for all strain values and material 2 possesses an eigenstrain ε_0 with respect to it. We take the lateral and the vertical eigenstrain components equal to each other. Thus, the lattice constants c_1^0 and c_2^0 in the fully relaxed state are related by $\varepsilon_0 = (c_2^0 - c_1^0)/c_1^0$. For the coherent growth considered here, the in-plane lattice parameter can be approximated to assume a constant value throughout the whole stack, so that the in-plane total strain $\varepsilon_{1xx} = \varepsilon_{2xx} = \varepsilon_{xx}$. The same condition holds for the yy components, the axes x and y are in the lateral plane.

For the lateral relaxation of the SL, we distinguish two cases

$$\begin{aligned} &\text{I. planar SL:} && \varepsilon_{xx} = 0 \\ &\text{II. nanowire SL:} && \xi_1\sigma_{1xx} + \xi_2\sigma_{2xx} = 0 \end{aligned} \tag{1}$$

For a planar superlattice on a bulk substrate, lateral relaxation is absent, $\varepsilon_{xx} = 0$. In contrast, for an axial nanowire superlattice, the lateral stress σ_{xx}, averaged over the superlattice period, vanishes as in Eq. (1). ξ_1 and ξ_2 are the thickness fractions of the two materials ($\xi_1 + \xi_2 = 1$).

In both cases considered above, the superlattice is free to expand vertically and experiences no vertical stress, $\sigma_{zz} = 0$. Then, Hooke's law relates the strain components and allows to calculate the vertical strain. For material 1, where $\varepsilon_0 = 0$, we obtain

$$\sigma_{1zz} = \sigma_0[(1-\nu)\varepsilon_{1zz} + \nu\varepsilon_{1xx} + \nu\varepsilon_{1yy}] = 0, \tag{2}$$

where $\sigma_0 = E/[(1+\nu)(1-2\nu)]$. The Young modulus E and the Poisson ratio ν are taken to be identical for both materials. Since $\varepsilon_{xx} = \varepsilon_{yy}$, we have

$$\varepsilon_{1zz} = -\frac{2\nu}{1-\nu}\varepsilon_{xx}. \tag{3}$$

In material 2, only the difference between the total strain ε and the eigenstrain ε_0 leads to stress, and instead of Eq. (3), we have

$$\varepsilon_{2zz} - \varepsilon_0 = -\frac{2\nu}{1-\nu}(\varepsilon_{xx} - \varepsilon_0). \tag{4}$$

For the case of nanowires, the lateral strain ε_{xx} can be found by calculating the in-plane stress

$$\sigma_{1xx} = \sigma_0[(1-\nu)\varepsilon_{xx} + \nu\varepsilon_{yy} + \nu\varepsilon_{1zz}],$$

$$\sigma_{2xx} = \sigma_0[(1-\nu)(\varepsilon_{xx} - \varepsilon_0) + \nu(\varepsilon_{xx} - \varepsilon_0) + \nu(\varepsilon_{2zz} - \varepsilon_0)]. \tag{5}$$

Substituting these expressions into Eq. (1), we arrive at the simple result

$$\varepsilon_{xx} = \xi_2\varepsilon_0, \tag{6}$$

which means that the degree of relaxation of material 2 is proportional to its contribution to the superlattice period.

The average out-of-plane lattice constant, which determines the x-ray diffraction peak positions, is

$$c_{avg} = \xi_1 c_1 + \xi_2 c_2 = \xi_1 c_1^0(1 + \varepsilon_{1zz}) + \xi_2 c_1^0(1 + \varepsilon_{2zz}). \tag{7}$$

For the case of planar layers on bulk substrate, where $\varepsilon_{xx} = 0$, we substitute the out-of-plane strain from Eqs. (3) and (4) into Eq. (7), which becomes

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$$c_{avg} = c_1^0(1 + \xi_2 \varepsilon_{2zz}) = c_1^0\left(1 + \frac{1+\nu}{1-\nu}\xi_2\varepsilon_0\right). \quad (8)$$

For GaN/$In_xGa_{1-x}N$ superlattices, Vegard's law defines $\varepsilon_0 = x(c_{InN} - c_{GaN})/c_{GaN}$. With the average superlattice composition $x_{avg} = \xi_2 x$, this yields the familiar result

$$\text{I. planar SL:} \quad \frac{c_{avg} - c_{GaN}}{c_{InN} - c_{GaN}} = \frac{1+\nu}{1-\nu}x_{avg}. \quad (9)$$

Contrarily, for nanowires, Eq. (6) holds, and Eq. (7) becomes

$$c_{avg} = c_1^0(1 + \xi_2\varepsilon_0). \quad (10)$$

This means that c_{avg} is not subject to the Poisson effect

$$\text{II. nanowire SL:} \quad \frac{c_{avg} - c_{GaN}}{c_{InN} - c_{GaN}} = x_{avg}. \quad (11)$$

This is the correct form of Eq. (2) in the original paper. A detailed solution of the anisotropic elastic problem in a cylinder shows that Eq. (11) remains valid as long as the height of the whole heterostructure is not much smaller than the nanowire diameter.[2]

[1]M. Wölz, V. M. Kaganer, O. Brandt, L. Geelhaar, and H. Riechert, Appl. Phys. Lett. **98**, 261907 (2011).
[2]V. M. Kaganer and A. Yu. Belov, Phys. Rev. B **85**, 125402 (2012).