Comment on "Fabrication of strained silicon on insulator by strain transfer process" [Appl. Phys. Lett. 87, 051921 (2005)]

R. L. Peterson[a)]
Princeton Institute for the Science and Technology of Materials (PRISM)
and Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544

K. D. Hobart and F. J. Kub
Naval Research Laboratory, Washington, D.C. 20375

J. C. Sturm
Princeton Institute for the Science and Technology of Materials (PRISM)
and Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544

In a recent letter, Jin *et al.*[1] demonstrated a new technique for achieving biaxially tensile strained silicon on insulator (SOI). An unstrained SOI film is capped with a commensurately strained SiGe layer and the sample is ion implanted with nitrogen. A postimplant anneal creates a superviscous interface between the silicon and the underlying oxide, which allows the strain to transfer from the SiGe into the silicon. An equation is given (derived in part from Ref. 2) for the final silicon and SiGe strains achieved by this strain equalization process. The purpose of this Comment is to point out inconsistencies in the given strain transfer equations.

When an elastic thin film is subject to a biaxial in-plane strain, the strain energy density of the film, E, is given by[3,4]

$$E = hB\epsilon_{\text{biaxial}}^2, \tag{1}$$

where h is the film thickness, $\epsilon_{\text{biaxial}}$ is the film's biaxial strain, and $B = c_{11} + c_{12} - 2c_{12}^2/c_{11}$, where c_{11} and c_{12} are film elastic stiffness coefficients.

For a bilayer of epitaxial SiGe and silicon, as in Refs. 1, 2, and 5, the silicon and SiGe layers have a coherent interface between them. The SiGe layer has an initial biaxial compressive strain of ϵ_o (for $Si_{0.8}Ge_{0.2}$, $\epsilon_o = -0.8\%$) and the silicon is unstrained. Coherency requires that the strained in-plane lattice constants of the two films be equal, that is, $a_{r,\text{SiGe}}\Delta\epsilon_{\text{SiGe}} = a_{r,\text{Si}}\Delta\epsilon_{\text{Si}}$, where a_r is the relaxed cubic lattice constant of the film, and the strain is defined as $\epsilon \equiv (a_{\text{strained, in-plane}} - a_r)/a_r$. Upon high temperature annealing, the silicon/oxide interface becomes viscous (using a variety of techniques[1,2,5]), allowing the SiGe to partially relax and reduce its compressive strain, thereby stretching the underlying silicon so it becomes tensile. Strains in the two films are related by

$$\epsilon_{\text{SiGe}} = \epsilon_o + \frac{a_{r,\text{Si}}}{a_{r,\text{SiGe}}}\epsilon_{\text{Si}}. \tag{2}$$

Note that even if the lattice constant factor is neglected, this differs from the equation given in Ref. 1, $\epsilon_o = \epsilon_{\text{SiGe}} + \epsilon_{\text{Si}}$, that is said to be valid "since the alloy composition remains constant throughout the relaxation process" (where subscripts 1 and 2 in Ref. 1 represent Si and SiGe). If correct, this equation would imply that as one layer becomes more tensile, the other becomes more compressive. Obviously this is not physically possible for coherently linked layers.

We now comment on the final equilibrium state of the bilayer films under the conditions that the two layers remain coherent and planar. Combining Eqs. (1) and (2), one can solve for the total energy of the strained bilayer,

$$E_{\text{total}} = \sum_{\text{all films}} E_{\text{film}}$$
$$= h_{\text{Si}}B_{\text{Si}}\epsilon_{\text{Si}}^2 + h_{\text{SiGe}}B_{\text{SiGe}}\left(\epsilon_o + \frac{a_{r,\text{Si}}}{a_{r,\text{SiGe}}}\epsilon_{\text{Si}}\right)^2. \tag{3}$$

The equilibrium condition of the bilayer will be its minimum energy state, which can be determined by differentiating Eq. (3) with respect to ϵ_{Si}. [Since ϵ_{Si} and ϵ_{SiGe} are linearly related via Eq. (2), it does not matter which is the variable of differentiation.] What results is

$$\frac{h_{\text{Si}}B_{\text{Si}}\epsilon_{\text{Si}}}{a_{r,\text{Si}}} + \frac{h_{\text{SiGe}}B_{\text{SiGe}}\epsilon_{\text{SiGe}}}{a_{r,\text{SiGe}}} = 0. \tag{4}$$

Since $a_{r,\text{Si}}/a_{r,\text{SiGe}} = 1 + \epsilon_0$, to first order in ϵ one can drop the lattice constants in the denominator of Eq. (4). Using the relation between stress and strain in the biaxially strained films of $\sigma_{\text{biaxial}} = B\epsilon_{\text{biaxial}}$, one arrives at the well-known force balance condition,

$$h_{\text{Si}}\sigma_{\text{Si}} + h_{\text{SiGe}}\sigma_{\text{SiGe}} = 0. \tag{5}$$

Simply put, Eq. (5) states that a bilayer reaches equilibrium when the total net force on the bilayer in the plane is zero. When combined with Eq. (2), this yields a strain in the Si layer of[6]

$$\epsilon_{\text{biaxial,Si}} = -\frac{\epsilon_o}{1 + (h_{\text{Si}}/h_{\text{SiGe}})(B_{\text{Si}}/B_{\text{SiGe}})}. \tag{6}$$

In contrast, in the paper of Jin *et al.*[1] they give the condition, repeated here,

[a)]Current address: Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK; electronic mail: rlp38@cam.ac.uk

$$E_{\text{total}} = E_{\text{Si}} + E_{\text{SiGe}} = 0, \tag{7}$$

stating that the equilibrium state is determined by zero total energy, not by minimum energy as described by Eq. (4) above. Later, the authors instead use the condition of equal energy between the two films, $E_{\text{Si}} = E_{\text{SiGe}}$, or

$$h_{\text{Si}} B_{\text{Si}} \epsilon_{\text{Si}}^2 - h_{\text{SiGe}} B_{\text{SiGe}} \epsilon_{\text{SiGe}}^2 = 0 \tag{8}$$

to solve for the equilibrium strain, a concept that they reference from Eq. (1) of Ref. 2. The major differences between Eqs. (8) and (4) are clear: the strain terms go from ϵ^2 to ϵ, and there is a change in sign. The physical basis for Eqs. (7) and (8) is not clear.

Accepting the stress balance condition for coherent films as the final equilibrium state and applying Eq. (6) to the experimental conditions of Ref. 1 ($h_{\text{Si}} = 50$ nm, $h_{\text{SiGe}} = 75$ nm of $Si_{0.8}Ge_{0.2}$, $\epsilon_o = -0.8\%$) and using the c_{11}, c_{12} values from Ref. 7, one finds an expected biaxial tensile strain in silicon of +0.47%. The reported experimental strain in the silicon is +0.72%, which is substantially greater than this. Note that if the layers did not remain coherent, one would expect less strain in the silicon layer than that expected by stress balance, not more. Therefore a new strain generation mechanism beyond force balance may be responsible for the observed results.

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