New approach to the high quality epitaxial growth of lattice-mismatched materials

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(Received 16 April 1986; accepted for publication 22 May 1986)

We have reconsidered the problem of the critical layer thickness h_c for growth of strained heterolayers on lattice-mismatched substrates, using a new approach which allows us to determine the spatial distribution of stresses in a bi-material assembly and include the effects of a finite size of the sample. The possibility of dislocation-free growth of lattice-mismatched materials on porous silicon substrates is discussed as an example of a more general problem of heteroepitaxial growth on small seed pads of lateral dimension l, having a uniform crystal orientation over the entire substrate wafer. It turns out that for a given mismatch f, the critical film thickness h_c^l strongly depends on l, rising sharply when the latter is sufficiently small, $l \lesssim l_{\min}$. The characteristic size $l_{\min}(f)$ below which, effectively, $h_c^l(f) \to \infty$, is determined in terms of the experimentally known (or calculated for growth on a monolithic substrate) function $h_c^\infty(f) \equiv h_c(f)$. When $l \lesssim l_{\min}$, then the entire elastic stress in the epitaxial film will be accommodated without dislocations.

There exists a tremendous interest in the possibility of growing high quality epitaxial layers of foreign materials on lattice-mismatched semiconductor substrates. In pursuing this direction, the objective is to enhance the range of useful devices available with a given substrate. When utilization of the heterointerface is not required, one is willing to tolerate various intermediate layers, so long as the top working layers are of desired device quality. Of the many pitfalls in the path of this development, some (such as the possible chemical incompatibility of the two materials or their different lattice symmetry) are not directly related to the lattice mismatch. The latter (which is our sole concern in this paper) manifests itself adversely by generating misfit dislocations, which thread the epitaxial layers, thus degrading their quality.

We shall confine our discussion to the Ge_xSi_{1-x}/Si system—a prototype lattice-mismatched heterostructure which is perfectly compatible in all other respects. It is well known[1] that thin Ge_xSi_{1-x} alloy layers can be grown pseudomorphically (i.e., without dislocations) on a silicon substrate and capped by another silicon layer. The maximum thickness h_c of the alloy layer decreases with the increasing Ge content x. People and Bean[2] have calculated $h_c(x)$ for a film grown on a large wafer (effectively infinite lateral dimension) on the assumption that the film grows initially without dislocations, which are then generated at the interface, as the strain energy density per unit area of the film exceeds the areal energy density associated with an isolated dislocation. Their result, which implicitly gives $h_c(x)$ in (Å) by the equation

$$x^2 h_c = 10.8 \ln(h_c/4), \tag{1}$$

is in excellent agreement with the empirical data. Unfortunately, in order to grow even a 100-Å-thick Ge_xSi_{1-x} film without dislocations, one has to limit the Ge content to $x \lesssim 0.5$.

In this letter, we describe a radically new approach to strained-layer growth based on reducing the stress energy in the epitaxial film by limiting the strained zone to a narrow layer adjacent to the interface. The key idea is illustrated in Fig. 1. Suppose the substrate surface is patterned prior to growth, so that the "rigid" contact between the film and the substrate is confined to "seed" pads of characteristic linear dimension $2l$. In between the pads we assume no adhesion, as if the film could freely slip with respect to the substrate. (This can be visualized by imagining that the seed pads are separated by trenches, sufficiently deep and wide; at the end of the paper we shall discuss the possibility of using for the patterned substrate *porous silicon*[3,4] films.) Consider the stress field in a film loaded as described in Fig. 1, assuming that the film contains no dislocations or any other plastic deformation. Solutions to such boundary value problems with sources of finite lateral extent (separated sufficiently far that the strain fields from different sources do not interfere effectively) typically have an exponentially decaying dependence on the distance z from the source plane, with a characteristic length h_e of the decay (the effective height of the strained film) being of the order of the source dimension. We can expect, therefore, that the total strain energy per unit area of the film will remain finite for any film thickness exceeding h_e, and for a sufficiently small pad size it will never exceed the threshold energy for generating dislocations.

Quantitatively, these ideas can be expressed by using the methods developed by one of us[5,6] for treating the mechanical properties of finite bi-material assemblies. In a film loaded with a misfit strain f (for Ge_xSi_{1-x}/Si systems $f = 0.042x$) along a segment $(-l, l)$ in y direction, the normal stress $\sigma_y \equiv \sigma(y,z)$ can be approximately expressed in the form

$$\sigma(y,z) = f\frac{E}{1-\nu}\chi(y,z)e^{-\pi z/2l}, \tag{2}$$

where E is the Young modulus of the film, ν its Poisson ratio, and the function χ, which characterizes the lateral stress distribution, is given by

$$\chi(y,z) = \begin{cases} 1 - \dfrac{\cosh ky}{\cosh kl} & z \lesssim h_e \\ 1 & z \gtrsim h_e \,. \end{cases} \tag{3}$$

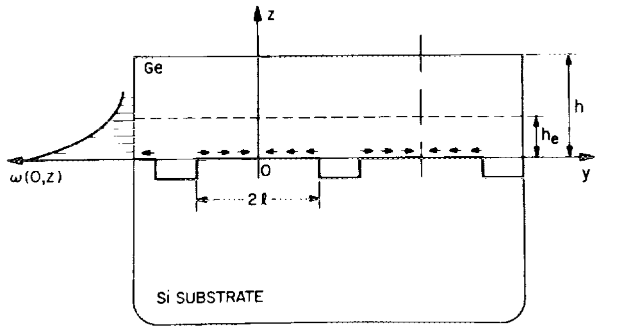

FIG. 1. Illustration of the discontinuous boundary value problem considered in this work. It is assumed that the initial epitaxial growth occurs on seed pads of lateral linear dimension (half-length) l with no adhesion of the films between the pads. The strain energy profile, $\omega(0, z)$, for the pad mid cross section is shown on the left.

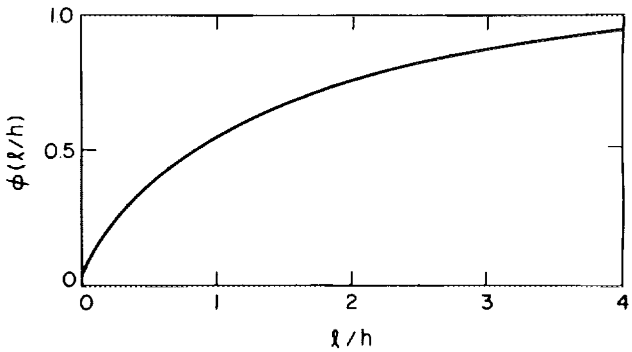

FIG. 2. Reduction factor $\phi(l/h)$ defined by Eq. (7). The limiting cases: $\phi \sim 1 - \operatorname{sech}(\zeta l/h)$ for $l \gg h$ and $\phi \sim \xi(l/\pi h)^{1/2}$ for $l \ll h$.

The interfacial compliance parameter k in our case can be estimated by the following formula:

$$k = \left(\frac{3}{2}\,\frac{1-\nu}{1+\nu}\right)^{1/2}\frac{1}{h_e} \equiv \frac{\zeta(\nu)}{h_e}. \qquad (4)$$

For Ge_xSi_{1-x} alloys ($\nu \approx 0.27$) one has $\zeta \approx 0.93$. One assumption underlying the derivation of Eqs. (2)–(4) is that trenches separating the pads are sufficiently wide ($\gtrsim h_e$) to ensure that adjacent stress zones do not interfere significantly. The thickness h_e, which defines the effective extent of the stress zones in z direction, is determined below self-consistently.

The strain energy density ω per unit volume is of the form

$$\omega(y,z) = \frac{1-\nu}{E}\sigma^2. \qquad (5)$$

Clearly, ω is highest in the plane $y = 0$. The maximum strain energy density per unit area is in the middle of the contact zone and is given by

$$\epsilon_S = \int_0^h \omega(0,z)dz \equiv \frac{E}{1-\nu}f^2 h_e. \qquad (6)$$

In the integral in Eq. (6) we can extend the form of χ given by the top line of (3) to all values of z, since the range of $z > h_e$ gives a negligible contribution to the integral. The second equation in (6) defines h_e, viz.,

$$h_e = h\left[\left(1 - \operatorname{sech}\frac{\zeta l}{h_e}\right)^2 (1 - e^{-\pi h/l})\frac{l}{\pi h}\right] \equiv h\left[\phi\left(\frac{l}{h}\right)\right]^2. \qquad (7)$$

The left-hand side equation in (7) determines h_e/h in terms of the ratio l/h, and subsequently the right-hand side identity in (7) defines the "reduction factor" $\phi(l/h)$ which is plotted in Fig. 2. For $l \gg h$, $\phi \to 1$ asymptotically, and for $l \ll h$ one has $\phi \propto (l/h)^{1/2}$. It can be seen from (7) that h_e varies from $h_e \approx h$ when $h \ll l$ to

$$h_e \approx \frac{l}{h}\,[1 - \operatorname{sech}(\zeta\pi)]^2 \equiv \frac{\xi^2 l}{\pi} \qquad h \gg l, \qquad (8)$$

where for Ge_xSi_{1-x} alloys $\xi \approx 0.89$. We see that $h_e \lesssim l/3$ for all values of l and of the film thickness h; this has allowed us to express χ to a good approximation in the simple form (3).

Following People and Bean,[2] we can find the critical h (which we denote by h_c^l) for generating plasticity effects by comparing (6) with the areal energy density ϵ_D associated with a single linear dislocation located at a distance h from the free surface of the film,

$$\epsilon_D = \frac{Gb^2}{10\pi a\sqrt{2}}\ln\frac{h}{b}, \qquad (9)$$

where $G = E/2(1+\nu)$ is the shear modulus of the film material, $b \approx 4$ Å is the Burgers vector of the dislocation, and $a \approx \langle a(x)\rangle = 5.54$ Å is the bulk lattice constant of the alloy film. The result, evident from the form of Eqs. (6) and (7), is given by

$$h_c^l(f) = h_c[\phi(l/h_c^l)f]. \qquad (10)$$

For large $l \gg h$ one has $\phi \to 1$ (cf. Fig. 2) and $h_c^l \to h_c^\infty \equiv h_c$, as can be expected. When l decreases, h_c^l increasingly deviates from h_c.

In the opposite limit, $h \gg l$, when h_e is described by (8), the energy density associated with a linear dislocation is no longer of the form (9). Indeed, the factor $\ln(h/b)$ arises as an infrared cutoff in the divergent integral describing the energy per unit length of an infinitely long dislocation parallel to a free surface. When the length of the dislocation is less than the distance h from the free surface, then it is that length ($\approx l$) which serves as the integration cutoff.[7] Thus, in the limit $h \gg l$, substituting l instead of h in Eq. (9), using (8) in Eq. (6), and equating ϵ_S with ϵ_D, we obtain

$$\frac{(\xi f)^2}{\pi}\,l \approx \frac{1-\nu}{1+\nu}\,\frac{1}{20\pi\sqrt{2}}\,\frac{b^2}{a}\ln\frac{l}{b}, \qquad (11)$$

which is an equation determining $l = l_{\min}$. We see that Eq. (11) is of the form of the People–Bean equation [Eq. (1) above or modified Eq. (9a) of Ref. 2], but with a reduced $f_{\text{eff}} = \xi f/\sqrt{\pi}$. It follows that the value of $l_{\min}$ is given by

$$l_{\min}(x) = h_c(\xi x/\sqrt{\pi}). \qquad (12)$$

Figure 3 shows the dependence $l_{\min}(x)$, calculated on the basis of the experimental results[1] for Ge_xSi_{1-x} alloy layers on Si, as well as the predicted dependence of h_c^l on the pad size l. Qualitatively, the latter dependence is described by the two asymptotes h_c and $l_{\min}$.

Consider the case of a pure Ge, $x = 1$. Our theory predicts that Ge films of arbitrary thickness can be epitaxially grown without dislocations on a Si substrate, provided the

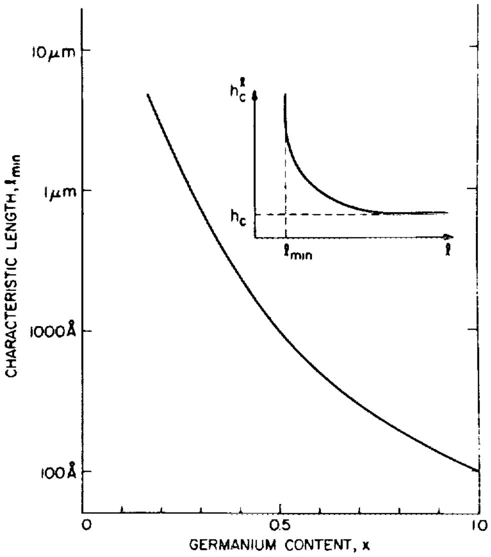

FIG. 3. Dependence of the minimum half-length l_{min} of the pads, below which $h_c^l(x)$ is effectively infinite, on the Ge content x in the epitaxial Ge_xSi_{1-x} film. The insert shows the predicted dependence of h_c^l on the pad size l, with two asymptotes [at $l_{min}(x)$ and $h_c(x)$] shown by the dashed lines.

latter surface is patterned with pads of half-length $l \lesssim l_{min}(1) \approx h_c(0.5) \approx 100$ Å, separated by "trenches" wider than at least l/π. This is probably beyond the reach of any lithography. However, an attractive possibility is to use *porous silicon* (PS) substrates,[3,4] which have been considered so far only for homoepitaxial growth with the intent to subsequently oxidize PS and thus obtain a silicon-on-insulator structure. According to the investigators of this technology,[8] the PS films look microscopically like a sponge with ~35 Å walls and voids. The PS surface therefore naturally satisfies the most stringent conditions for the type of growth proposed in the present work.

It may be worthwhile to emphasize that one of the underlying assumptions of the present theory is that the epitaxial growth on the patterned surface is dominated by the seed pads rather than by the trenches. This condition may not be easy to realize, since the area of the pads cannot much exceed that of the trenches, since the latter must be wider than $\approx l/\pi$, which leaves only a factor of six margin for the area ratio. Our assumption that the trenches do not present themselves as sources of lateral strain can be expected to be best applicable to the situation when the trenches are deep or their surface is made amorphous. The experimental fact[4] that Si films of good crystalline quality can be grown on PS substrates is quite encouraging, since the growth of Ge cannot be expected to present any special difficulties beyond those considered in this letter.

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