Strained interface of lattice-mismatched wafer fusion

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(Received 28 January 1997)

A model has been developed for the periodic strain field near the wafer-fusion interface of lattice-mismatched single crystals. A solution has been found that satisfies the elastic mechanical equilibrium and the boundary conditions. It reveals a wavy interface with the amplitude of the atomic displacement rapidly decaying a short distance from the interface. The model is consistent with the experimental observations of nearly defect-free material except at the interface. The strong alternating strains along the interface have implications for its electronic energy-band structure and electrical characteristics. [S0163-1829(97)05219-3]

There has been considerable recent interest in a ''wafer-fusion'' process in which single-crystal wafers are pressed together at elevated temperatures for the formation of covalent bonds along the interface.[1–15] The process is similar to sintering but occurs in a more macroscopic scale. It further allows grown single-crystal layers to be transferred and monolithically integrated onto a substrate of a different lattice parameter or of a different crystal orientation to form novel optoelectronic devices. Except at the interface, virtually no dislocations have been found in the wafer-fused materials,[2,6–8,12] in sharp contrast with the direct heteroepitaxial growth of the materials on lattice-mismatched substrates.[16–18] The realization of this long-sought capability has a potential for an entirely new class of optoelectronic and electronic devices. Indeed, a number of high-performance devices with good reliability have already been developed.[2–5,8–10,12] One example of these rather interesting applications is a practical manufacturing of highly efficient $(Al_xGa_{1-x})In_{0.5}P$ light-emitting diodes, in which a transparent GaP substrate is wafer fused to replace the absorbing GaAs.[10,11] However, considerable strain is still present near the wafer-fusion interface and needs to be examined to better understand the nature of the interface and to facilitate further applications. In particular, the strain modification of the electronic energy-band structure can have significant implications for the electrical characteristics or other physical properties of the interface.

Several groups have obtained high-resolution transmission-electron-microscope cross-sectional views of the GaAs/InP wafer-fused interface and have observed an array of misfit dislocations along the interface with a regular spacing as expected from the amount of lattice mismatch.[2,6,8,12] Based on this observation, we have developed in this work a comprehensive model of the strain field near the interface. We consider the periodic compressive and tensile strains along the interface and describe a solution that satisfies the mechanical equilibrium and the boundary conditions. The model shows that the strain is highly localized to the interface and is consistent with the experimental observations of virtually defect-free materials and reliable high-performance devices.

The present model of lattice-mismatched wafer fusion is illustrated in Fig. 1. The two semi-infinite perfect crystals prior to the bond formation are illustrated in Fig. 1(a). The lattice parameters of the upper and lower wafers are a and $(1+\varepsilon)a$, respectively, and the x and z axes are parallel and perpendicular to the interface, respectively. Figure 1(b) illustrates the bond formation between the two crystals after wafer fusion. The lattice mismatch ε is usually a few percent and gives rise to misfit dislocations with a regular spacing of

$$\Lambda = a/\varepsilon. \tag{1}$$

In the upper wafer, in regions near the dislocation cores, there is compressive strain in the lateral direction, whereas in

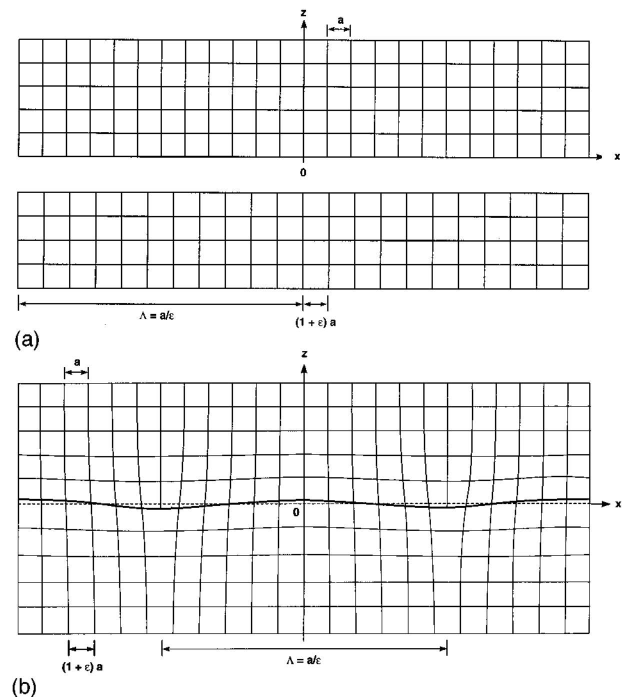

FIG. 1. Schematic drawing of the present model of the interface of lattice-mismatched wafer fusion. Part (a) shows the two starting semi-infinite perfect single crystals of two different lattice parameters, and part (b) shows the bond formation after wafer fusion. The mismatch results in a periodic array of misfit dislocations as illustrated in (b). The strain field can be found by solving the elastic mechanical equilibrium equations for the given boundary conditions. The model reveals a wavy atomic displacement perpendicular to the interface. It also shows that the strain field is highly localized to a thin region along the interface.

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regions between the dislocations the strain becomes tensile. The opposite is true in the lower wafer. This periodic strain field must also satisfy the mechanical equilibrium condition, i.e.,

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xz}}{\partial z} = 0, \tag{2}$$

and

$$\frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{zz}}{\partial z} = 0, \tag{3}$$

where σ_{xx} and σ_{zz} are the normal stresses, and σ_{xz} is the shear stress. (For simplicity, the crystal has been approximated as a continuum.) This simple two-dimensional case is considered first, and an extension to the more realistic three-dimensional case will be given later. Equations (2) and (3) state that at equilibrium there is no net force acting on any given volume element. With the additional boundary condition of diminishing strain away from the interface, a solution can readily be found (by first considering the Airy stress function[19]) for the upper wafer, i.e.,

$$\sigma_{xx} = -\sigma_{zz} = \sum_{m=1}^{\infty} A_m e^{-m\varsigma} \cos(m\xi) \tag{4}$$

and

$$\sigma_{xz} = -\sum_{m=1}^{\infty} A_m e^{-m\varsigma} \sin(m\xi), \tag{5}$$

where

$$\xi \equiv \frac{2\pi x}{\Lambda}, \tag{6}$$

$$\varsigma \equiv \frac{2\pi z}{\Lambda}, \tag{7}$$

and the A_m's are the coefficients to be determined by matching to the atomic arrangement along the interface. The solution for the lower wafer is similar but with some opposite signs. A simplification of retaining only the fundamental term of $m=1$ will be considered first for an illustration of the principles.

For elastically isotropic materials, the strains are given by

$$\varepsilon_{xx} = \frac{1}{2\mu(1+\nu)} (\sigma_{xx} - \nu\sigma_{zz}) = \frac{A}{2\mu} e^{-\varsigma}\cos\xi, \tag{8}$$

$$\varepsilon_{zz} = \frac{1}{2\mu(1+\nu)} (\sigma_{zz} - \nu\sigma_{xx}) = -\frac{A}{2\mu} e^{-\varsigma}\cos\xi, \tag{9}$$

and

$$\varepsilon_{xz} = \frac{1}{2\mu} \sigma_{xz} = -\frac{A}{2\mu} e^{-\varsigma}\sin\xi, \tag{10}$$

where μ is the shear modulus and ν is the Poisson's ratio. The coefficient A can now be determined by matching to the strain in regions in between the dislocations, such as that near the origin in Fig. 1(b); where a symmetry consideration places the strain at $\varepsilon/2$, i.e.,

$$\varepsilon_{xx}(0,0) = \varepsilon/2. \tag{11}$$

Note that correction will be needed for any deviation from the symmetry assumption of equal elastic constants in the two materials. By comparing Eq. (11) with Eq. (8), we have

$$A = \varepsilon\mu. \tag{12}$$

Substitution of Eq. (12) into Eqs. (8)–(10) yields the strain field.

The atomic displacements u_x and u_z, parallel and perpendicular to the interface, respectively, can now be evaluated by integrating Eqs. (8)–(10), i.e.,

$$u_x = \frac{a}{4\pi} e^{-\varsigma}\sin\xi \tag{13}$$

and

$$u_z = \frac{a}{4\pi} e^{-\varsigma}\cos\xi. \tag{14}$$

Note that Eq. (14) leads to a wavy interface, i.e.,

$$u_z(x,0) = \frac{a}{4\pi} \cos\frac{2\pi x}{\Lambda}. \tag{15}$$

This is reflected in Fig. 1(b), but with an exaggeration by a factor of 2, so that the wavy feature can be more clearly seen. Also note that the amplitude of the wavy atomic displacement quickly decays a short distance from the interface due to the exponential factor $e^{-2\pi z/\Lambda}$ in Eqs. (13) and (14). The present picture of a strong periodic strain field along the interface is in general agreement with the cross-sectional transmission-electron-microscope observations, especially those in Ref. 2.

The present two-dimensional solution can be generalized to the more realistic three-dimensional case by superposition. With the additional orthogonal y axis, it can readily be verified that the three-dimensional solution as represented by the set of atomic displacements

$$u_x = \frac{a}{4\pi} e^{-\varsigma}\sin\xi, \tag{16}$$

$$u_y = \frac{a}{4\pi} e^{-\varsigma}\sin\eta, \tag{17}$$

and

$$u_z = \frac{a}{4\pi} e^{-\varsigma}(\cos\xi + \cos\eta), \tag{18}$$

with

$$\eta \equiv 2\pi y/\Lambda, \tag{19}$$

satisfies the mechanical equilibrium and boundary conditions.

While the present solution appears to be accurate for regions between the dislocations, the strain in regions closer to

the dislocations is probably significantly underestimated. More accurate solutions can be obtained by including the higher-order terms in the Fourier expansion, but would require more detailed knowledge of the atomic arrangement there. These higher-order terms would nonetheless represent effects that are even more short ranged or localized as can be seen in the exponential factors in Eqs. (4) and (5). It should be noted, however, that the present consideration based on linear elasticity theory is not applicable to the dislocation core regions.

The rapidly diminishing strain away from the interface implies a minimal disturbance to the bulk of the materials during the wafer-fusion process, despite the considerable strain introduced to the interface. This is consistent with the experimental observation of virtually no dislocation generation in the wafer-fused materials. This is also consistent with the good device performance and reliability obtained, which are virtually identical to those on the original lattice-matched substrate. Such a result is rather different from the heteroepitaxial growth of thick layers on lattice-mismatched substrates, in which the strain relaxation resulted in high densities of threading dislocations in the grown layers.[16–18] Thus, the wafer fusion process is a viable alternative for integration with lattice-mismatched substrates without material degradation. The highly localized strain further precludes any stress-enhanced long-range diffusion and therefore ensures a long-term stability and reliability of the materials and devices.

The present model may also provide insight into the electronic structure and the electrical characteristics of the mismatched interface. Since strain alters the crystal symmetry and shifts the electronic energy bands, the strong alternating strains along and across the interface should result in considerable modulation of the band structure and may lead to interesting phenomena. Potential wells may be formed and lead to ''quantum dots'' and ''quantum wires.'' The electronic behaviors will probably be affected by the presence of dislocations. The coherent array of dislocations along the wafer-fused interface may make it simpler for investigating such effects. The interface strain pattern, and hence the electronic structures, can be altered by choosing the degrees of lattice mismatch, misorientation (i.e., angle-polished, off-axis wafers), or rotation between the two single-crystal wafers. Further experimental and theoretical studies will be needed to explore these possibilities.

The author wishes to thank S. H. Groves and R. M. Osgood for discussions that have stimulated this work. Support from the Department of the Air Force under Contract AF19628-95-C-0002 is gratefully acknowledged.

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