RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 30, NUMBER 6 15 SEPTEMBER 1984

Stability of registry in strained-layer superlattice interfaces

Brian W. Dodson
Sandia National Laboratories, Albuquerque, New Mexico 87185

(Received 9 April 1984)

Stability of lattice registry as a function of lattice parameter mismatch has been studied for a single interface. The interface model consists of two two-dimensional lattice systems each 12 atoms high by 120 atoms long. Each of the two lattice systems has a different lattice parameter, but is initially constrained to match at the interface. The atoms interact with their nearest neighbors either through a Lennard-Jones potential or an anisotropic potential designed to more closely simulate covalent bonding. The stability of registry is then determined via Monte Carlo evolution of the initial state of the system. We find that registry is stable to extremely large mismatches (> 15%), from which one can infer that the observed loss of registry above a few percent mismatch is not due to instability of an initially perfect superlattice, but rather to an inability to grow perfect interfaces.

Strained-layer superlattice (SLS) systems such as GaAs-$\mathrm{GaAs}_{1-x}\mathrm{P}_x$ are currently of great interest in device applications. When the lattice mismatch between the layers is small (1–2%), the unit cells undergo homogeneous deformation into a state of compressive uniaxial strain in one layer, and tensile uniaxial strain in the other, leading to a constant unit-cell dimension parallel to the layer interface. The opposed uniaxial strains in the two layer materials lead to a system band gap which can be varied by control of the lattice mismatch and of the layer thickness, which allows significantly more flexibility for design of semiconductor devices.

The applicability of SLS systems to devices is limited by an instability of lattice registry which develops at larger mismatches. Although maintenance of registry in a very low defect SLS has been limited, as a practical matter, to systems possessing 1–2% mismatch, the mechanism leading to the loss of registry has not been identified. The present work seeks to determine whether the loss of registry is due to a fundamental instability in an initially perfect SLS, or is related to the failure of epitaxial growth of perfect, lattice-matched interfaces.

In this Rapid Communication the choice was made to study the stability of a single interface between two similar atomic systems as a function of lattice parameter mismatch. Each of the layers consists of a two-dimensional (2D) slab with 12 atoms perpendicular to the interface and 120 atoms parallel to the interface. Thus, the total simulation involves a system of 2880 atoms, each of which interacts only with its nearest neighbors, through a continuous interatomic potential which will be described in detail later. Both layers are isotropically compressed or expanded so that the unit cells have identical dimensions. The layers are then assembled so that an atomically perfect interface is formed, which may then remain perfect upon removing external constraints from the system. The system then has completely free boundary conditions, so that only a section of 2D interface 24 atoms by 120 atoms is modeled. If this perfect SLS state were unstable, the evolution from the initial system would lead to a defective interface and lattice. The relaxation of the initial state is performed through a Monte Carlo technique,[1] carried out at zero temperature, with a total of 2×10^3 Monte Carlo steps/spin needed to reach a long-lived metastable state. The SLS interface is clearly metastable, but the energy needed to nucleate a dislocation is very large.[2] Accordingly, the metastable state is the condition of interest. Previous atomistic simulations indicate that temperatures up to ~20% of melting do not significantly alter threshold strains for lattice damage,[3] and thus the approximation of a zero temperature calculation seems justified. Similarly, the use of a two-dimensional lattice is justified by differences of ~20% in damage thresholds found in atomistic simulations of two- and three-dimensional lattices subjected to uniaxial strain.[4]

Simulations have been performed using two different continuous nearest-neighbor interatomic potential functions. The first was a Lennard-Jones (LJ) potential, which models spherically symmetric molecular systems bound by van der Waals forces. This potential is thus a function only of the distance between any pair of neighboring atoms, where, in scaled units, the potential becomes

$$\tilde{\phi}(\tilde{r})=\tilde{r}^{-12}-\alpha\tilde{r}^{-6} \ . \tag{1}$$

Here the scaled potential energy $\tilde{\phi}=\phi/4E$, where E is an energy characteristic of the strength of the LJ potential, and $\tilde{r}=r/\sigma$, where σ represents the range of the potential. The interaction is truncated at $\tilde{r}=3.0$. In two dimensions, this potential leads to a hexagonal-close-packed structure at zero temperature and no applied stress.[2] The parameter α in Eq. (1) is used to vary the equilibrium bond length. Thus $r_{\mathrm{eq}}=(2/\alpha)^{-6}$. A 10% reduction in equilibrium lattice parameter requires that α change from 1.0 to 1.8813.

Although the LJ interatomic potential is quite realistic for a certain class of materials, it is not suitable for modeling of semiconductors, which are bonded covalently, and typically exhibit a rather open lattice and directional bonding forces. At present, little work has been done on calculating covalent bond energies away from the ground state, e.g., in strained lattices. In addition, a pairwise interaction approximation does not work well for covalently bonded materials.[5] The second potential used herein has therefore been designed to include the principle characteristic of covalent bonding, that is, the dependence of the magnitude of the attractive part of the potential upon angular orientation. The form of this directional Lennard-Jones (DLJ) potential, in scaled units, is

$$\tilde{\phi}_{12}(\tilde{r},\theta_1,\theta_2,\theta)=\tilde{r}^{-12}-\alpha\beta\gamma\tilde{r}^{-6} \ , \tag{2}$$

where θ_1 and θ_2 are the orientation angles of particles 1 and 2, and θ is the angle of the vector connecting particle 1 with particle 2, where all angles are measured relative to a coordinate system wherein a vector parallel to the interface has an angle of either $\pi/2$ or $3\pi/2$. $\tilde{r}$ is the magnitude of this same vector. α is defined as in Eq. (1), and β and γ are functions describing the angular dependence of the interaction between pairs of particles. β is defined by $\beta = |\sin[3(\hat{\theta}_1 \cdot \hat{r}_{12})/2]|$, where a $\hat{}$ represents a unit vector parallel to the direction defined by the variable. Thus, we have defined a three-lobed potential dependent on the orientation of the atom. (γ is defined identically to β, by replacing all reference to θ_1 with θ_2.) The net result is an interatomic potential having a radial dependence similar to that of Eq. (1), but with an angular dependence which encourages the formation of three bonds with the maxima of β and γ corresponding to bond alignment. The DLJ potential is more strongly oriented than a realistic covalent bond, since the possibility of distorting a single bond to improve bond strength does not exist within DLJ. However, modeling the current problem with both LJ and DLJ potentials should bracket the actual angular dependence characteristic of covalent bonds. The equilibrium crystal structure for the DLJ potential is found to be an open system of empty hexagons, sometimes known as a two-dimensional honeycomb lattice. At equilibrium, $\beta = \gamma = 1$, so the bond lengths are identical to those of the LJ potential.

As described earlier, the initial state for our simulation is one where homogeneous compression or expansion of the two lattice materials has resulted in a perfectly registered structure, but where the lattice parameter perpendicular to the interface needs to relax considerably in the process of equilibration. This initial system is relaxed to a metastable equilibrium using a Monte Carlo procedure, and the resulting lattice configuration is inspected for damage or loss of registry.

The results of this analysis were unexpected, as neither the LJ nor the DLJ superlattice interface models showed any sign of loss of registry up to 15% lattice mismatch, the largest mismatch value considered. The significance of this result becomes clear when one considers that the total lattice strain energy involved in matching an interface with a 15% mismatch will be approximately 100 times that occurring with a 2% mismatch. Thus, the theoretical stability of an SLS interface is much greater than the practical results achieved to date.

It is instructive to consider some details of the equilibrium states of our interface models. For example, how does the DLJ model with 10% lattice mismatch accommodate to such large strains? Very little of the accommodation occurs through changes in average bond length, which are 2.8% elongation in the more dense material, and 0.9% compression in the less dense material, numbers resulting from a direct study of the atomic positions in the equilibrated lattices. The strain is relieved primarily through changes in bond angle. The residual uniaxial strain is split approximately evenly between the SLS layers. In the 10% DLJ model, the less dense layer exhibits 4.3% compressive uniaxial strain parallel to the interface, and the more dense material exhibits 6.5% tensile uniaxial strain in the same direction, resulting in a unit-cell dimension parallel to the interface which varies by less than 1% from the arithmetic mean of the equilibrium cell dimensions of the two layer materials.

In prior work by the present author,[6] a two-dimensional perfect LJ lattice has been subjected gradually to uniaxial strain by a simulation technique which ensures that the system remains near a local equilibrium. The damage threshold in that case was found to be at 8.5% uniaxial strain, and the mechnaism for producing lattice damage was the accumulation of sufficient strain energy to nucleate dislocations. Both the more open structure of the DLJ model and the ability to change bond angles to accommodate uniaxial strain suggest that the threshold for damage of a perfect DLJ lattice might be considerably higher. Combining these results on mechanical yield strain with the observation that the layers of the SLS share the strain associated with lattice registry about equally, one concludes that the LJ model should show instability of registry not far above 15% mismatch, and the DLJ model should retain registry to considerably larger values of mismatch.

The theoretical results presented in this Rapid Communication clearly suggest that the practical limits on SLS stability are not due to any fundamental instability of an SLS interface. We must therefore look toward two possibilities. First, a large mismatch between the layer materials may make the growth of a perfect interface impossible. This would result in interface vacancies which would serve as nucleation centers for damage, resulting in instability of registry at much smaller mismatch values than in the perfect interfaces. Second, the interfaces may be imperfect owing to factors which are subject, at least in principle, to experimental control. Thus, it is conceivable that there may exist new surface treatments aimed at producing a more perfect substrate, combined with specific combinations of substrate temperature and deposition rate, which will result in access to a larger regime of acceptable lattice mismatch. The present author is currently evaluating the first of these possibilities through simulation of the layer growth between mismatched materials.

This work was performed at Sandia National Laboratories supported by the U.S. Department of Energy under Contract No. DE-AC04-76DP00789.

---

[1] K. Binder, *Monte Carlo Techniques in Statistical Physics* (Springer-Verlag, New York, 1979).

[2] B. W. Dodson and P. A. Taylor, Phys. Rev. B (to be published).

[3] P. A. Taylor and B. W. Dodson (unpublished).

[4] B. W. Dodson (unpublished).

[5] A. M. Stoneham and J. H. Harding, in *Computer Simulation of Solids,* edited by C. R. A. Catlow and W. C. Mackrodt (Springer-Verlag, New York, 1982).

[6] P. A. Taylor and B. W. Dodson (unpublished).