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Computer simulation of Si and Ge adatoms and thin layers on Si substrates

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Abstract. The molecular dynamics method is used to determine minimum energy configurations of Si and Ge adatoms on a Si surface. Results for thin layers of Ge on Si substrates and Si–Ge superlattices are also presented.

1. Introduction

Modern crystal growth techniques like molecular beam epitaxy (MBE) have been shown to be very useful in the preparation of group IV, III–V and II–VI semiconductors and also of superlattice structures. Besides lattice matched heterostructures, it has also become possible to grow strained layer superlattices and other more complicated structures. In order to understand fully the process involved in the growth and evolution of these structures, it is desirable to complement the experimental work with computer simulation studies.

Recently there has been considerable activity in this area ranging from the simulation of epitaxial growth of Si [1] to the simulation of strained layer structures [2]. Molecular dynamics (MD) and Monte Carlo (MC) methods have been the principal tools in these simulations. Although MC simulations can be computationally faster, MD has the advantage of being able to track the trajectory of the individual particles by solving the classical equations of motion. However this technique requires interatomic potentials between the various atoms in the system. In considering epitaxial growth of semiconductor structures, it is essential to take into account the effect of chemical bonds as well as surface diffusion and nucleation. In the case of strained structures, the method must be able to accommodate the formation of misfit dislocations to relieve strain. Thus it is clear that some kind of energy formulation where bonding effects are considered needs to be employed. In this paper we have attempted to test the appropriateness of some potentials to model adsorption sites and strained configurations.

2. Interatomic potentials

In recent years empirical interatomic potentials have been shown to be useful in the study of surface reconstructions in silicon. Stillinger and Weber (SW) [3] constructed a two- and a three-body potential for silicon which minimised the energy for the diamond

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Table 1. Parameters for Si–Ge interaction (in reduced units, $\varepsilon = 2.050$ eV, $\sigma = 2.124$ Å).

A	7.049556277	a	1.80
B	0.6022245584	γ	1.20
p	4.0	$\lambda_{\text{Si-Si-Ge}}$	24.33333
q	0.0	$\lambda_{\text{Ge-Ge-Si}}$	27.66667

Table 2. Interlayer separations for $(Si)_4(Ge)_4$ superlattic on Si(001) substrates (Å).

	Our calculation	[9]
d (Si–Si)	1.3575	1.3546
d (Si–Ge)	1.3992	1.3811
d (Ge–Ge)	1.4908	1.428

structure. The two parts of the potential can be thought of as extensions to the bond stretch and bond bending forces of the Keating model. Ding and Andersen [4] constructed potentials of the same form to describe condensed phases of germanium. Following the suggestion of Abell [5] that coordination number is an important factor that needs to be considered, various potentials were proposed for silicon, the most significant being that of Tersoff (T) [6]. This has since been improved upon by Khor and Das Sarma (KD) [7]. For the silicon–germanium system we have constructed potentials in the form of SW potential. The three-body interaction consists of two terms—one describing the Si–Si–Ge interaction and the other the Si–Ge–Ge interaction. The parameters were optimised to give the equilibrium lattice spacing of the $Si_{0.5}Ge_{0.5}$ alloy and are tabulated in table 1. The MD method used in this work is that used in earlier studies on the evolution of defects in metals [8].

3. Results

3.1. Si–Ge superlattices

To test whether or not the potentials could be useful in describing strained behaviour, we calculated the interlayer separation in relaxed $(Si)_n(Ge)_n$ ($n = 1, 6$) superlattices on Si (001) and (111) substrates. The results for the (001) substrates can be directly compared with that obtained from a Keating model, where the parameters were fitted to reproduce *ab initio* results [9]. As can be seen from table 2, the SW-type potential for Ge under-estimates the strain energy but the separation at the interface is reasonably well described.

As a basis for comparing the SW and T potentials with respect to strain, we have calculated the interlayer separation for Si expanded onto a Ge (001) substrate. We find the separation to be 1.2625 Å for SW and 1.1625 Å for T. Thus it is clear that T potentials under-estimate the strain energy even more than the SW type.

3.2. Si and Ge adatoms on Si(111) surfaces

The SW potential is not capable of predicting the correct reconstruction of the (111) surface. This is not surprising as there is no mechanism to take account of the reduced

Table 3. Interatomic distances for $\sqrt{3} \times \sqrt{3}$ H_3 and T_4 adatom sites (A). Numbering of atoms as in [10].

	H_3		T_4	
	1–2	1–3	1–2	1–3a
Si (SW)	3.57	4.22	3.62	3.65
Si (T)	2.42	3.12	2.42	2.39
Si [10]	2.55	3.05	2.49	2.49
Ge	3.62	4.23	3.60	3.63

coordination of the surface and adatoms. The T potential finds the 7×7 reconstruction is of lower energy but, like the SW potential, finds the $H_3\sqrt{3} \times \sqrt{3}$ configuration to be of lower energy than the $T_4\sqrt{3} \times \sqrt{3}$ arrangement. This is in contradiction with the *ab initio* results of Northrup [10]. In table 3 we present the results for Si adatoms on Si substrates using the T and SW potentials. Also shown are the results for Ge adatoms. The migration energy of Si adatoms on the T_4 site has been calculated by the method described by Matthai [11]. The value of 1.25 eV is approximately the magnitude of the diffusion energy used in MC simulations [2].

3.3. Simulation of Si–Ge interfaces

It is of interest to see if dislocations will form at strained interfaces to relieve strain, and if so to determine the Burgers vector and the dislocation core position. To investigate this we have performed simulations of layers of Ge on Si(111) substrates. The number of layers perpendicular to the interface needs to be greater than 25 to account for the

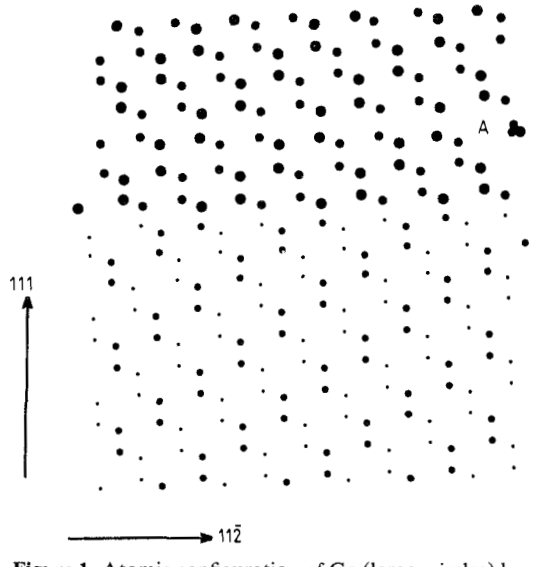

Figure 1. Atomic configuration of Ge (larger circles) layers on Si (smaller circles) obtained after heating and subsequent quenching. The Si region is periodically infinite.

mismatch. The Ge layers were 'free' surfaces on three sides so that it had 'room' to expand, and they were heated up to different temperatures. The final quenched configurations for 10 double layers and an initial temperature of ~2000 K is shown in figure 1. The Ge atoms have moved into a lower-energy configuration and a closer analysis reveals that the Ge–Ge separation parallel to the interface remains the same as the Si–Si separation. The Ge–Ge separation perpendicular to and away from the interface expands to ≈2.5 Å, which is the value obtained for strained Ge in the Si–Ge superlattice. Thus it is clear that for this particular case the strain energy is not sufficient for dislocations to form. However, there appears to be a dislocation forming with the core centred at A, three layers above the interface (see figure 1) and with Burgers vector = $\frac{1}{2}(110)$.

4. Discussion

For the two types of potentials studied, the SW type are best suited to describe strained layers and the T type appears best for surface structures. However, both types have to be improved upon before they can be used in studies of growth simulation. We have also shown that strained interfaces could result in the formation of dislocations with the core centred away from the interface. The Burgers vector of the dislocation is that with the lowest energy. Work is now under way to construct better potentials for use in larger systems and for growth simulations.

Acknowledgments

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References

[1] Schneider M, Schuller I K and Rahman A 1987 *Phys. Rev.* B **36** 1340–3
[2] Kobayashi A and Das Sarma S 1988 *Phys. Rev.* B **37** 1039–42
[3] Stillinger F and Weber T 1985 *Phys. Rev.* B **31** 5262–71
[4] Ding K and Anderson H C 1987 *Phys. Rev.* B **34** 6987–91
[5] Abell G C 1985 *Phys. Rev.* B **31** 6184–96
[6] Tersoff J 1988 *Phys. Rev.* B **37** 6991–7000
[7] Khor K E and Das Sarma S 1989 *Phys. Rev.* B **39** 1188–93
[8] Matthai C C and Bacon D J 1985 *J. Nucl. Mater.* **135** 173–80
[9] Froyen S, Wood D M and Zunger A 1988 *Phys. Rev.* B **37** 6893–907
[10] Northrup J E 1986 *Phys. Rev. Lett.* **57** 154–7
[11] Matthai C C 1985 *Phil. Mag.* A **52** 305–8