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Dependence of GaAs and Si surface energy on the misorientation angle of crystal planes

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The paper reports on the dependence of Si and GaAs surface energies on the misorientation angle of Si and GaAs crystal planes in a broad angle range. The energetic balance between GaAs and Si is unfavourable for growth of GaAs on Si substrate. Minima of the surface energy correspond to GaAs/Si heterostructure interface energy minima which indicate preferable crystal orientations for obtaining GaAs layers on Si.

Key words: *III–V semiconductors; interface*

1. Introduction

The growth of GaAs epitaxial layers on Si substrate has been the focus of extensive research in recent years because of their applications for electronic devices. Among many growth methods used to obtain GaAs/Si heterostructure [1–4], liquid phase epitaxy (LPE) seems to be one of the best [5].

Heteroepitaxial growth, like GaAs on Si, is in general more complicated than homoepitaxial growth because of the misfit between the substrate and the layer. Relations between surface energies of the substrate and the layer are crucial for the growth process. The surface energy varies with the orientation of the crystal plane because of variation of atom arrangement on the surface. In consequence, the value of heterostructure interfacial energy depends on the orientation of the substrate plane showing some orientations more preferable for epitaxial growth. This paper presents the dependence of Si and GaAs surface energy on the misorientation angle over a broad range of angles, discussing also the importance of the balance of surface energies.

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2. Theory

It is well known that four primary growth modes of an epitaxial film on a substrate are distinghished [6, 7]: layer-by-layer growth mode, island growth mode, the growth mode where islands grow on the top of an initial smooth layer and the columnar growth mode. The particular growth mode that results depends on a balance between the surface energy of the substrate and epitaxial layer and the lattice mismatch between the layers. In order to obtain the most ideal layer-by-layer growth mode, the following formula has to be fulfilled:

$$\gamma_l + \gamma_{in} - \gamma_s \le 0 \tag{1}$$

where γ_l – surface energy of the layer, γ_{in} – interface energy, γ_s – surface energy of substrate.

The calculations of surface energy are based on the parametrizable model for a tetravalent semiconductor, proposed by Ackland [8]. The model consists of a sum over all atoms of a pair potential and a sum over all valence electrons bond energy:

$$E = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} A\mathrm{e}^{-\alpha r_{ij}} - \frac{1}{2}\sum_{i=1}^{N}\sum_{n=1}^{4} Br_{ik_n}\mathrm{e}^{-\beta r_{ik_n}} \tag{2}$$

where the n sum runs over four electron pairs which have atom i as one of their foci and k_n as the other, and r_{ik} is the separation between the two ions on which the electron orbital is centred. Pairwise repulsion is represented by an exponent. The strength of the covalent bond is represented by the radial part of the hydrogenic p wave function. A, B, α, β are fitting parameters. In the Ackland model these paremeters have been determined for Si. In our recent study, the values of A, B, α, β parameters were determined for GaAs [9], thus the model can now be used in calculations for both Si and GaAs.

The energy described by Eq. (2) can be used in calculations of the surface energy. We have performed numerical calculations by using a computer program [10]. The energy described by Eq. (2) was divided by the number of atoms taken into account, the result being referred to as E_w. The following formula for the surface energy [11] was used:

$$\gamma_{(hkl)} = E_w \rho_{(hkl)} z_{(hkl)} \tag{3}$$

where $\rho_{(hkl)}$ is the density of atoms on the crystal plane, $z_{(hkl)}$ – number of broken bonds for one atom in this plane.

3. Results

First, the analysis of surface energy was performed for typical low-index Si planes: (001), (011), (111) and (113). The density of atoms and number of broken bonds for one atom for each plane were determined by taking into account the geometry of Si crystal [10]. The results are presented and compared with literature data in Table 1.

Table 1. Surface energies [mJ/m^2] of Si planes γ_1 found in this work compared to the values γ_2 and γ_3 obtained by other authors

Si plane	γ_1	γ_2	γ_3
(001)	2512	2537^1	2310^1, 1488^2
(011)	1776	1794^1	1601^1, 1721^2
(111)	1467	1465^1	1225^1, 1405^2
(113)	2272	2240^1	1380^2

1 – [7], 2 – [12].

In Table 1, our calculations of Si surface energies γ_1 have been compared with the surface energies based on the nearest neighbour broken-bond model γ_2 [7] and other literature data γ_3 [12]. There is a very good agreement between our results γ_1 and the literature data γ_2. In our study, we considered unrelaxed and unreconstructed surfaces and that is why the values of the surface energies obtained by us are higher than the values for reconstructed surfaces γ_3. In semiconductors, bond directionality is of great importance, thus reconstruction and relaxation decrease the value of surface energy, even by1000 mJ/m^2 [12,13].

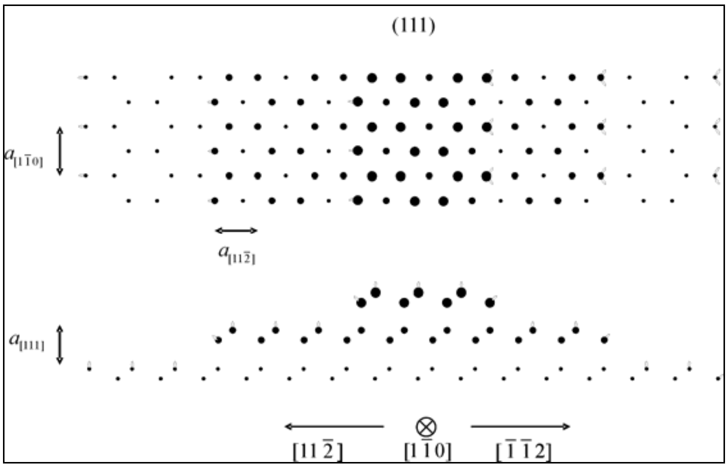

Fig. 1. Atomic model of the (111) plane tilted in $[11\bar{2}]$ and [$[\bar{1}\bar{1}2]$ direction. The small elliptic features indicate broken bonds

The dependence of Si and GaAs surface energy on the angle of misorientation of crystal planes (θ) was studied. The values of surface energy were calculated according to Eq. 3 in which the density of broken bonds was a function of misorientation angle. In order to find the dependence between the density of broken bonds and misorientation angle we have performed the analysis of atom arrangement on vicinal planes. First, we considered the (111) plane (Fig.1) tilted in $[\bar{1}\bar{1}2]$ and $[11\bar{2}]$ directions and we have found the expression for broken bonds density l as a function of the misorientation angle θ:

$$l=\frac{\left(3a_{[111]}+ua_{[11\bar{2}]}\tan\theta\right)\cos\theta}{3a_{[111]}a_{[1\bar{1}0]}a_{[11\bar{2}]}} \tag{4}$$

where $a_{[111]}$, $a_{[11\bar{2}]}$, $a_{[1\bar{1}0]}$ are the lattice constants of the surface unit cell (Fig. 1), $u = 4$ when θ goes in the $[\bar{1}\bar{1}2]$ direction and $u = 2$ when θ goes in the $[11\bar{2}]$ direction.

We also performed the analysis for other crystal planes. The relation between broken bonds density and misorientation angle was found for (011) plane tilted in [001] direction, (001) plane tilted in [011] and (001) plane tilted in [010] direction.

Our model assumes that vicinal surfaces consist of regular steps with a well defined height. In fact, clean vicinal Si surfaces usually consist of irregularly distributed steps, there are some cases, however, when it is possible to obtain their regular distribution [14–16]. The model can be applied to surfaces with irregularly distributed steps if we consider the obtained broken bond density the as average value for the whole surface. Figures 2–5 show the results of the calculations of the surface energy versus the surface plane misorientation angle for all the mentioned planes.

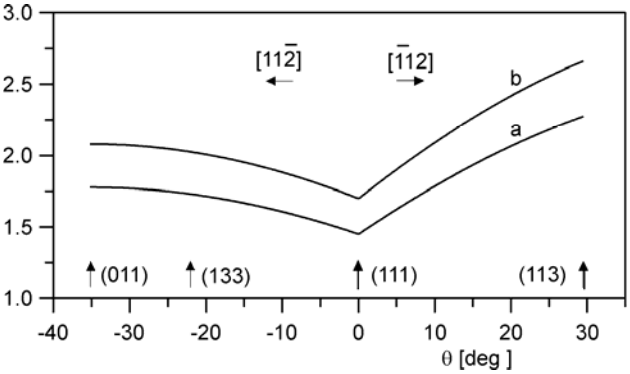

Fig. 2. The dependences of surface energies of Si (a) and GaAs (b) on the misorientation angle θ of (111) plane to $[11\bar{2}]$ direction

According to the presented model, the (111) plane has the lowest value of surface energy and (001) plane has the highest value. The results of this study agree with our analysis [9] of GaAs/Si heterostructure interface energy showing the importance of the balance between the surface energy of the substrate and the layer. The interface energy depends on the surface energy of the substrate and the layer and its minima indicate crystallographic planes that can be favourable for the growth of the layer.

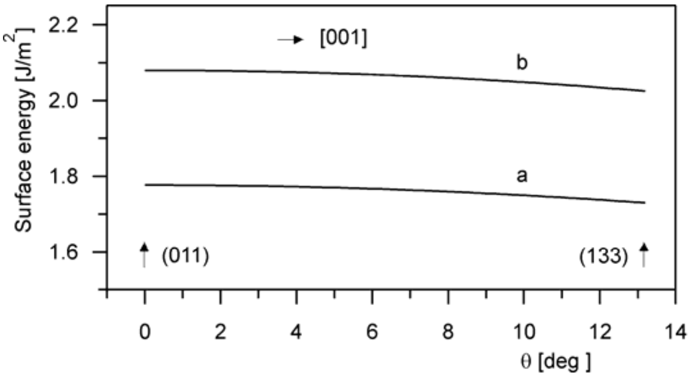

Fig. 3. The dependences of surface energies of Si (a) and GaAs (b) on the misorientation angle θ to (011) plane in [001] direction

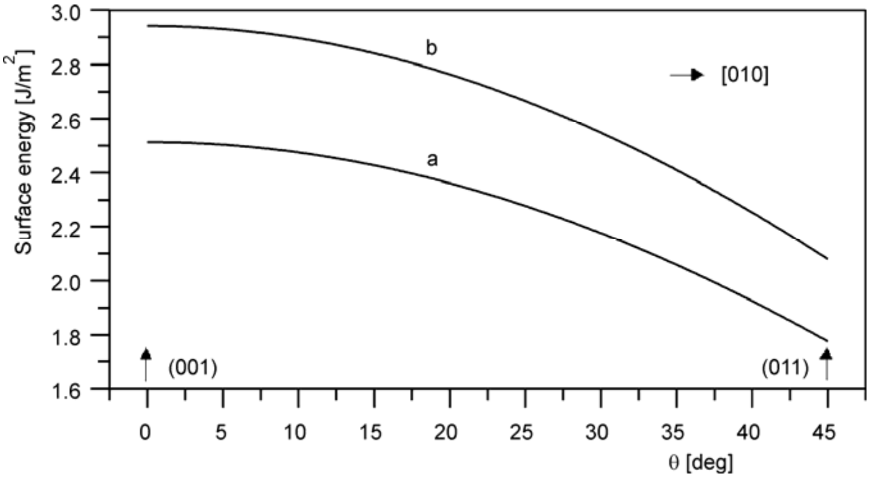

Fig. 4. The dependences of surface energies of Si (a) and GaAs (b) on the misorientation angle θ from (001) plane to (011) plane in [010] direction

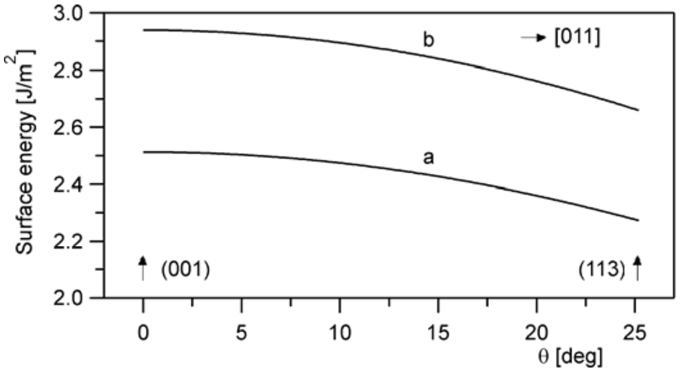

Fig. 5. The dependences of surface energies of Si (a) and GaAs (b) on misorientation angle θ to (001) plane in [011] direction

4. Conclusions

GaAs surface energy is higher than that of Si surface energy hence the energetic balance is unfavourable for the growth of GaAs on Si substrate. However, for some crystallographic planes Si and GaAs surface energies have minima and GaAs/Si heterostructure interface energy has corresponding minima that indicate planes of better growth conditions.

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