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Materials Science and Engineering B000 (2001) 000–000

MATERIALS SCIENCE & ENGINEERING B

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Oscillation of in-plane lattices constant of Ge islands during molecular beam epitaxy growth on Si

A.I. Nikiforov *, V.A. Cherepanov, O.P. Pchelyakov

Institute of Semiconductor Physics, Russian Academy of Sciences, Siberian Branch, Lavrentjeva 13, 630090 Novosibirsk, Russian Federation

Abstract

Variations in the lattice constant of Ge film were determined by reflection high-energy electron diffraction in the course of the molecular beam epitaxy (MBE) film growth on the silicon surface. Oscillations of the in-plane atomic cell constant were observed for the Ge film growing according to the two-dimensional (2D) mechanism. Variations in the 2D lattice constant at the stage of 2D growth are caused by elastic deformation of edges of 2D islands. © 2001 Published by Elsevier Science B.V.

Keywords: Molecular beam epitaxy; Reflection high-energy electron diffraction; Silicon; Germanium; Quantum dots

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1. Introduction

The germanium on silicon heterosystem is an ideal object for studying the heteroepitaxial growth and the two-dimensional (2D) to three-dimensional (3D) growth mode transition (the Stranski-Krastanow mechanism). Dependence of the island lattice constants on the deposition conditions makes it necessary to provide continuous monitoring the situation at the growth surface of the substrate. The traditionally used technique is reflection high-energy electron diffraction (RHEED). Comparative analysis of the RHEED patterns and the scanning tunnelling microscopy surface images allows the diffraction patterns to be interpreted correctly in the course of the film growth [1]. The RHEED technique was used [2] for plotting phase diagrams of the structures formed at the surface during Ge epitaxy on Si. A variation in the diffraction pattern is a qualitative illustration of morphological rearrangements of the growing film. The quantitative information can be obtained by recording the intensity of the diffraction pattern.

Of particular interest are the data on strains in the growing layer which are exactly the main driving force for the observed morphological rearrangements. The strains can be estimated from variations in the lattice constant in the growing Ge film. The variations can be established during heteroepitaxy from the reflection positions in the RHEED patterns. This approach was used to determine the relaxation points in systems Ge/Si [3] and InAs/GaAs [4]. The assumption of the island deformation in the course of 2D growth was supported by observations of periodical changes in the size of the surface 2D cell for A_3B_5 and metals [5,6]. One can also expect periodical variations in the lattice constant resulting from deformation of 2D islands during 2D growth of Ge film on Si.

The present work was aimed at studying the behaviour of the constant of the growing Ge lattice at the Si(1 0 0) surface under the conditions of 2D growth.

2. Results and discussion

A molecular beam epitaxy (MBE) installation Katun-C equipped with two electron beam evaporators for Si and Ge was used for synthesis. Analytical equipment of the chamber included a quadrupole mass spectrometer, a quartz thickness monitor and a high-energy electron (20 kV) diffractometer. Diffraction patterns were monitored during the growth using a CCD camera on line with a PC. The software allowed both the whole images and chosen fragments of the diffraction patterns to be monitored at the rate of 10 frames/s. Ge was grown at

* Corresponding author. Tel.: +7-3832-333286; fax: +7-3832+333502.

E-mail address: nikif@isp.nsc.ru (A.I. Nikiforov).

0921-5107/01/$ - see front matter © 2001 Published by Elsevier Science B.V.
PII: S0921-5107(01)00840-6

the rate of 10 ML/min, temperature was varied from 250 to 600 °C. Silicon wafers misoriented by less than 0.5° were used as substrates. Before a Ge film started growing, the substrate was annealed and a buffer Si layer was grown to reconstruct the original surface.

Growth of Ge films on Si follows the Stranski-Krastanow mechanism. The 2D mechanism is observed with initial three to five monolayers which form a continuous film (the so-called wetting layer). At the further growth, 3D islands appear on the wetting layer due to transition to the 3D growth mode. Elastic relaxation of 2D islands formed during the 2D growth results in distortion of the unit cell of the heteroepitaxial film. RHEED technique allows the deformation to be in situ registered as a variation in the size ($a_{\|}$) of the in-plane surface 2D atomic cell. To do that, variations in the intensity of the diffraction pattern was recorded along the line going across the streaks and bulk spots. The distance between the spots assigned to $0\bar{1}$ and 01 reflections oscillates during the growth that indicates changes in the $a_{\|}$ value at the (1 0 0) plane of the Ge film.

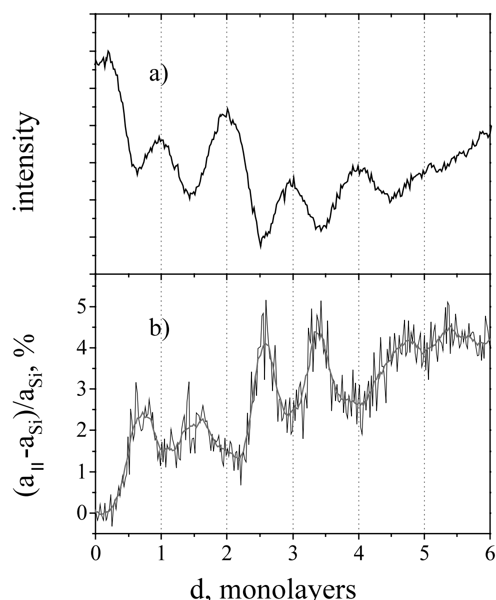

Fig. 1. Variations in specular beam intensity (a), and surface 2D cell constant (b) during growth of Ge film on Si(1 0 0) at 250 °C.

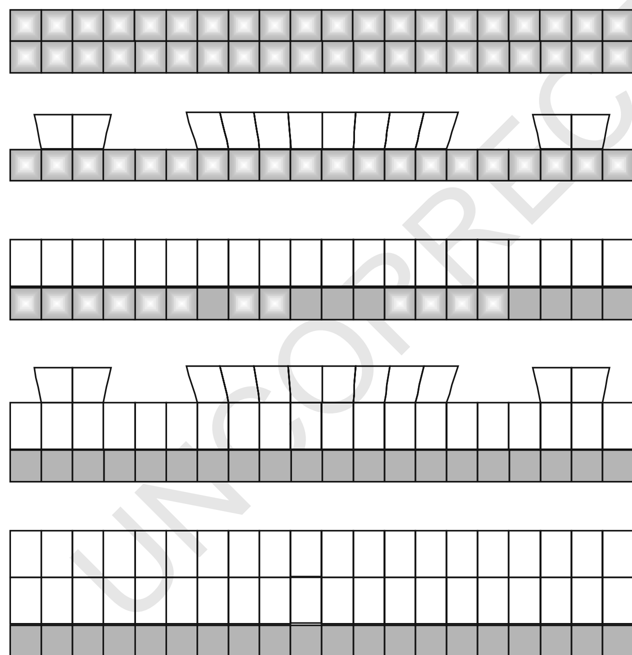

Fig. 2. Schematic representation of variations in the lattice constant. Solid squares are for the unit cell, and open squares for Ge.

Fig. 1 shows variations in the 2D surface cell constant (as percentage with respect to the $a_{\|}$ value of the pure silicon surface) during growth of a Ge film at the Si(1 0 0) surface at 250 °C. The corresponding intensity variations of the RHEED specular beam reflected by the substrate surface is also shown in Fig. 1. The $a_{\|}$ value is seen to change, in periodical manner, during the growth, while the oscillation range reaches 2%. The periodic variations in the lattice constant of the 2D Ge cell in (1 0 0) plane is of the same nature as the specular beam intensity oscillations. Hence, there is the same reason for variations both in $a_{\|}$ and in the specula beam intensity, viz. the periodical changes in the surface roughness of the growing film. It is common knowledge that these changes observed for 2D growth mode are caused by nucleation and coalescence of 2D islands. However, 2D lattice constant oscillations are half-period shifted with respect to the corresponding specular electron beam oscillations. The maximum of the lattice constant oscillations coincides with the minimum of the intensity oscillations at half monolayer coverage. Such behaviour means that the elastic deformation of 2D islands is maximal at the maximal surface roughness, and the atomic cell has the maximal lattice constant. When each monolayer is completed, the islands coalesce to form a smooth surface and the 2D surface cell of the film reaches its minimum. A decrease in $a_{\|}$ of the smooth surface indicates the maximal increase in the surface cell to occur at the edge of the islands; the island coalescence results in a decrease in the in-plane elastic deformation. The mean constant of the 2D cell during growth of the wetting Ge layer increases progressively. The whole pattern of $a_{\|}$ variations for various stages of Ge growth on the Si(1 0 0) surface is given elsewhere [7].

A scheme of the lattice constant variations in the Ge layer growing according to the 2D growth mode is shown in Fig. 2. Solid and open squares stand for silicon and germanium unit cells, respectively. The cyclic nature of the roughness variations causes oscillations of the observed constants. The smooth surface of the continuous layer corresponds to the maximum in oscillations of the specular beam and to the minimum in oscillations of the 2D cell lattice constant. The presence of 2D islands at the growth surface results in

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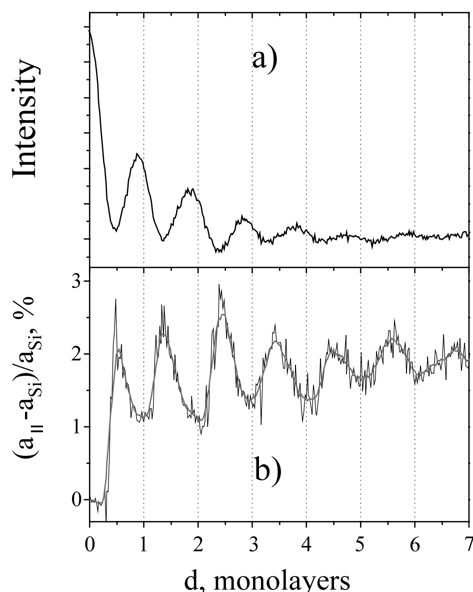

Fig. 3. Variations in specular beam intensity (a), and surface 2D cell constant (b) during growth of Ge film on Si(1 1 1) at 50 °C.

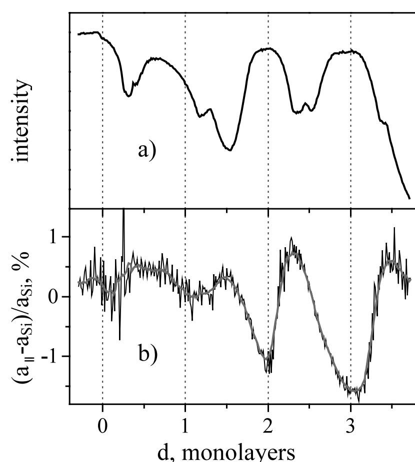

Fig. 4. Variations in specular beam intensity (a), and surface 2D cell constant (b) during growth of Ge film on Si(1 1 1) at 370 °C.

a decrease in the specular beam intensity, and the lattice distortion at the island edges gives rise to the observed enlargement of the surface cell of the Ge film. Oscillations of the $a_{\parallel}$ parameter are detected over all ranges of temperature and growth rate when oscillations of the RHEED specular beam are observed. The fashion of the surface cell constant variations at the growth temperature range between 250 and 500 °C remains the same as that shown in Fig. 1. As the temperature is elevated, the oscillation range decreases gradually to become comparable with the noise level at 500 °C. At the temperature below 250 °C, the oscillation range also must be gradually narrowed and then disappear due to the transition to the 3D growth mode. However, steady oscillations of both specular beam and $a_{\parallel}$ are observed at the growth temperature as low as 50 °C. Fig. 3 shows oscillations of the specular beam and surface cell constant at the growth temperature equal to 50 °C. The amplitude of $a_{\parallel}$ oscillations is the same as that at 250 °C but almost 3% increase happens at the growth onset and the centre line is always at the 2% level. Seemingly, the heteroepitaxial Ge layer is, in average, relaxed to this value and does not change during growth of the whole wetting layer. The growth of Ge on the Si(1 1 1) surface also is accompanied by oscillations of in-plane lattice constant of the 2D atomic cell. Oscillations of the intensity and parameter $a_{\parallel}$ during Ge growth on Si(1 1 1) at the substrate temperature 370 °C are shown in Fig. 4.

A characteristic feature of the growth on this surface is variations in the in-plane constant of the surface atomic cell of the Ge film around zero value, i.e. the $a_{\parallel}$ value of silicon. Parameter $a_{\parallel}$ is $\approx 1\%$ increased at the maximal roughness and $\approx 1\%$ decreased at the minimal roughness. Another distinctive feature is a slight variation in $a_{\parallel}$ at the thickness range corresponding to one monolayer. This behaviour is characteristic of a wide temperature range and independent of the presence or absence of intensity oscillations at this thickness. It is known that the intensity variations corresponding to the first monolayer is observed at not all growth temperatures that is accounted for by the double-level growth mode at the given stage. Islands varied in size are thought to occur on the growth surface at this stage. A wide island size range results in averaging parameter $a_{\parallel}$ and changes in the lattice constant of the surface atomic cell are not observable.

3. Conclusions

Variations in the lattice constant of Ge film were determined in the course of the MBE film growth on silicon (1 0 0) and (1 1 1) surfaces. Oscillations of the in-plane atomic cell constant were observed for the Ge film growing according to the 2D mechanism. The in-plane constant oscillates in the same manner as the specular beam intensity but is half-period shifted. Variations in the 2D lattice constant at the stage of 2D growth are caused by elastic deformation of edges of 2D islands.

Acknowledgements

The study was supported by the Russian Foundation for Basic Research (Projects 00-02-18012, 01-02-06437 and 00-02-17638).

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