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Epitaxy relationships between Ge-islands and SiC(0 0 0 1)

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Abstract

Reflection high-energy electron diffraction (RHEED) has been used to determine epitaxy relationships and in-plane orientations between Ge and SiC(0 0 0 1). Three monolayers of Ge have been deposited at 500 °C on a graphitized SiC $(6\sqrt{3} \times 6\sqrt{3})R30^\circ$ reconstructed surface, this surface supporting epitaxial Ge island growth in a Volmer–Weber mode. Nucleation of relaxed Ge-islands gives rise to transmission electron diffraction patterns allowing to deduce that pure Ge grows according to only one epitaxy relationship Ge{1 1 1}//SiC(0 0 0 1). These {1 1 1}-Ge-islands have two in-plane orientations, a preferential one, Ge⟨-1-12⟩//SiC⟨1-100⟩ and a minority one, Ge⟨-1-12⟩//SiC⟨10-10⟩, deduced one from the other by a 30° rotation around the ⟨1 1 1⟩-Ge (or [0 0 0 1]-SiC) growth axis. Due to the three-fold symmetry of the {1 1 1}-Ge plane, each in-plane orientation is degenerated into two twin orientations, differing by a 180° angle around Ge⟨111⟩.

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1. Introduction

In order to design new electronic devices, the elaboration of low-dimensional structures with IV-IV compound and alloy semiconductors has been the subject of many studies in surface physics and materials science. The experience gained in Ge nanostructure growth on standard or modified Si substrates – a prototypical quantum system – has motivated similar works on silicon carbide (SiC) ones. Thus, Ge growth on on- and off-axis SiC surfaces has been investigated [1–7] with an increasing interest justified by the desire to develop optoelectronics in SiC technology.

Very recently, it has been demonstrated that Ge nanocrystals embedded in a wide-band gap (~3 eV) SiC matrix – by ion implantation with subsequent annealing – allow strong carrier confinement. Electro-

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luminescence applications have therefore been predicted [8]. To obtain confinement effects even at room temperature, the dimensions required for these islands must be of a few nanometers. The understanding of how the structure and the composition of SiC surfaces influence the Ge growth process is therefore a prerequisite.

Over the past years, numerous investigations have been devoted to the basic Si-rich (3 × 3) and ($\sqrt{3} \times \sqrt{3}$)R30° (or $\sqrt{3}$), and C-rich ($6\sqrt{3} \times 6\sqrt{3}$)R30° (or $6\sqrt{3}$) reconstructions of the crystallographically equivalent 4H and 6H (0 0 0 1) and 3C (1 1 1) surfaces [9–15]. Concerning the $6\sqrt{3}$ reconstruction, a precursor study has been made by Van Bommel et al. [9] during SiC graphitization. The authors proposed that three successive C layers of SiC, after evaporation of Si by annealing up to about 1200 °C, collapse into one single layer of C atoms with a surface density of 3.66×10^{15} ($3 \times 1.22 \times 10^{15}$) atoms/cm^2, very close to the C density of one graphite layer (3.80×10^{15} atoms/cm^2). The low energy electron diffraction (LEED) $6\sqrt{3}$ pattern is interpreted as a multiple diffraction of the SiC and a graphite monolayer (ML), rotated by 30° with respect to the SiC lattice. The $6\sqrt{3}$ parameter is related to $6\sqrt{3} \times a_{\text{SiC}} = 6\sqrt{3}$ x 3.07 = 31.9 Å which fits very well $13 \times a_{\text{Graphite}} = 13 \times$ 2.46 Å = 32.0 Å. The model proposed for the $6\sqrt{3}$ by Van Bommel et al. [9] consists therefore of a graphite monocrystalline layer on top of the (0 0 0 1) Si surface. Posterior results agreed [10,15] with this model and also demonstrated that the $6\sqrt{3}$ LEED corresponds to a (6 × 6) scanning tunneling microscopy geometry; the discrepancy between the two observed reconstructions can be explained by an incommensurate character of the graphite monolayer [10]. $k_{\|}$-resolved inverse photoemission spectroscopy studies performed on the $6\sqrt{3}$ reconstruction by Forbeaux et al. [13], showing unshifted π^* states, have allowed the authors to conclude that the interaction between the graphite and the substrate is very weak, i.e. of Van der Waals type.

Nevertheless, a slightly different $6\sqrt{3}$ superstructure was proposed by Northrup and Neugebauer [11]. Their calculations explained the $\sqrt{3}$ reconstruction as a Si-T$_4$ adatom array on a Si-terminated SiC(0 0 0 1) plane, a surface much more stable than an ideal one. Based on this result, the authors proposed that the $6\sqrt{3}$ structure arises from a graphite ML above such a $\sqrt{3}$ surface with weak interactions between them. This finding has also been approved by other authors [13,14].

In previous studies, we have shown that Ge growth on the Si-rich (3 × 3) and $\sqrt{3}$ surfaces follows a Stranski–Krastanov mode with a wetting-layer formation of about 1 ML, that forms a new (4 × 4) superstructure, before island nucleation [5–7]. Reflection high-energy electron diffraction (RHEED) oscillation measurements have led us to propose a model for this interesting Ge-induced reconstruction [7]. Furthermore, we have recently systematically compared a same room temperature Ge deposit (1 ML) on the different ((3 × 3), $\sqrt{3}$ and $6\sqrt{3}$) reconstructions during isochronal annealings [5]. We have thus shown that (i) Ge wets the Si-rich (3 × 3) and $\sqrt{3}$ reconstructions and grows in a Volmer–Weber mode on the C-rich $6\sqrt{3}$ one, (ii) Ge starts to desorb on the three reconstructions above 800 °C and (iii) the $6\sqrt{3}$ superstructure allows a better observation of epitaxial Ge-islands between 400 and 800 °C than the other two.

The present study focuses on Ge growth on the C-rich surface reconstructed $6\sqrt{3}$. This superstructure has been chosen because it best induces epitaxial Ge-islands. Three ML Ge have been deposited on such a prepared surface at 500 °C, a temperature allowing a sufficient sticking rate. The main aim is to explore possible epitaxy relationships between Ge and SiC(0 0 0 1), a highly mismatched system (30%), and, more precisely, Ge-island in-plane orientations, i.e. Ge and SiC azimuthal coincidences in the (0 0 0 1)-SiC plane.

2. Experiment

The growth experiments are carried out in an ultra-high vacuum (UHV) chamber with solid-source molecular beam epitaxy (MBE) system using an electron gun evaporator and a Knudsen effusion cell for Si and Ge, respectively. The residual base pressure of the UHV system is lower than 5×10^{-11} mbar. The Si and Ge deposition rates are measured by water-cooled quartz crystal oscillators. The MBE chamber is equipped with the RHEED technique operating at an accelerating voltage of 30 kV ($\lambda = 0.07$ Å). This tool allows real-time crystallographic characterization of