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Growth temperature dependent strain in relaxed Ge microcrystals

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ABSTRACT

Epitaxial growth of dissimilar materials on patterned substrates is a promising technique for defect-free, monolithic integration of various optoelectronic devices on a single chip. In this work we investigate the structural quality of Ge microcrystal arrays monolithically grown at temperatures ranging from 450 to 575 °C on patterned Si substrates. Using high resolution X-ray diffraction with reciprocal space mapping, we obtain the lattice parameters, strain and degree of relaxation. This structural analysis gives us insight in dislocation formation together with quantitative information about thermal relaxation and lattice bending.

1. Introduction

The heterepitaxial growth of various semiconductor materials on Si has been of great interest for many years, since a successful realization of monolithic defect-free growth of lattice mismatched materials can open a way for the integration of superior optoelectronic devices with the well established Si technology. This follows the trend towards functional scaling according to the so called “More than Moore's law” [1]. Ge and Si have a lattice mismatch of 4.2% and a thermal expansion coefficient mismatch of 120.4% at 300 K. This, unfortunately causes formation of misfit dislocations (MDs) accompanied by threading dislocations (TDs) for layer thicknesses larger than a few nanometers [2]. Dislocations have a detrimental impact on opto-electronic devices [3]. Moreover, thermal mismatch may induce cracks in continuous hetero-epitaxial layers hindering any device fabrication [4].

In order to overcome these obstacles, the heteroepitaxial growth can be performed on substrates patterned into a regular array of pillars with high aspect ratios [5] under out-of-equilibrium deposition conditions (large growth rate and reduced temperature). This unusual epitaxial growth results in a dense network of micron-sized three-dimensional (3D) epitaxial crystals where MDs and TDs are confined close to the heterointerface and the crystal tops remain defect free [6]. This approach was demonstrated for several types of materials deposited by various methods on Si substrates, such as GaAs by metal organic vapor phase epitaxy (MOVPE) [7,8,9], GaN by plasma-assisted molecular beam epitaxy (MBE) [10], SiC by chemical vapor deposition (CVD) [11,12] or compositionally graded SiGe microcrystals by low energy plasma enhanced chemical vapor deposition (LEPECVD) [13,14,15,16].

In this paper we analyze the lattice relaxation and dislocation formation mechanism of Ge microcrystals deposited at various temperatures (450 to 575 °C) on a Si substrate patterned in the form of regular arrays of pillars.

2. Samples

The Ge/Si crystals were grown by the LEPECVD technique [17] on 4-in. Si(001) substrates patterned into arrays of square pillars with a base size L of 2 μm and a height of 8 μm. Two types of patterns were investigated: pattern A with Si pillars separated by 1 μm wide gaps, and pattern E with 2 μm gaps. As illustrated in Fig. 1, the arrays of patterns A and E are grouped into patches of 10 × 10 pillars separated by 2.5 μm trenches, and 8 × 8 pillars separated by 3.5 μm trenches, respectively. More information about substrate preparation, cleaning and Ge growth by LEPECVD are reported in reference [6].

In total 12 Ge/Si samples deposited at different temperature were investigated, 6 samples for each pattern. Growth temperatures of 450, 475, 500, 525, 550 and 575 °C were used, with a Ge growth rate of approximately 4 nm/s, using germane (GeH_4) as a reactive gas. The

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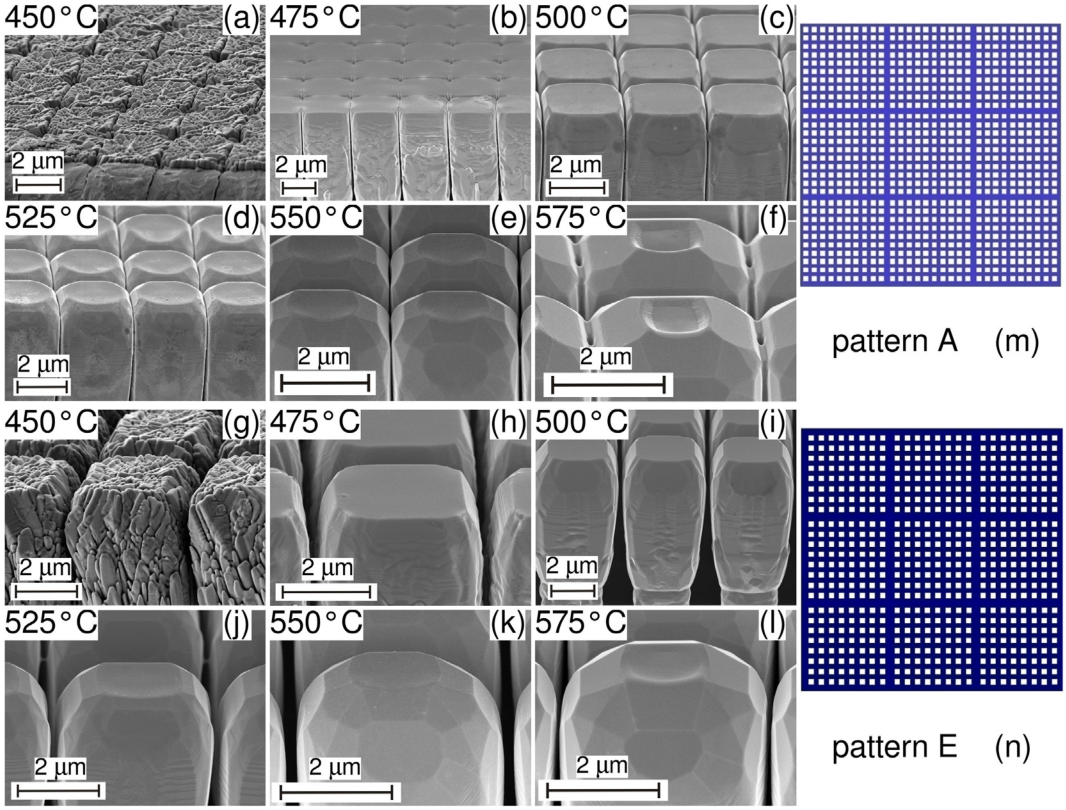

Fig. 1. Perspective SEM views of arrays of Ge microcrystals showing the evolution of crystal morphology with growth temperature. The substrate of pattern A (a)-(f) consists of 2 × 2 μm pillars separated by 1 μm gaps and grouped into patches of 10 × 10, separated by 2.5 μm trenches; the substrate of pattern E (g)-(l) consists of 2 × 2 μm pillars separated by 2 μm gaps and grouped into patches of 8 × 8, separated by 3.5 μm trenches.

observed shape of Ge microcrystals is the result of self limited lateral growth by flux shielding of neighboring crystals. It depends on the growth kinetics [5,18,7], which keeps the crystals separated by spacing of only a few tens of nanometers. The height of Ge microcrystals in Fig. 1 is 8 μm. Some Ge is also deposited on the pillar sidewalls and in the trenches. The morphology of the Ge microcrystals deposited at different temperatures is shown in the perspective scanning electron microscopy (SEM) micrographs in Fig. 1(a)–(f) and Fig. 1(g)–(l) for pattern A and pattern E, respectively. The images were taken with a Zeiss ULTRA 55 digital field emission microscope.

3. Experimental techniques

The structural quality averaged over thousands of Ge microcrystals was studied by reciprocal space maps (RSMs) measured by high resolution X-ray diffraction (HRXRD) [19,20,21]. The X-ray diffraction measurements were performed with a Rigaku Cu based rotating anode diffractometer (45 kV, 180 mA), with a high resolution setup using a parabolic multilayer mirror and an additional monochromator. The parallel and monochromatic beam was defined by the Bartels-type monochromator Ge (220) placed behind the mirror. The scattered X-rays were collected with a point detector after passing the Ge channel-cut (220) analyzer placed behind the sample. The typical beam size, defined by the slit opening was 5 × 1 mm^2. In order to gain insight in the strain status and the tilt of crystal lattice planes, we recorded the RSMs around the symmetrical (004) and the asymmetrical (224) reciprocal lattice points.

As sketched in Fig.2, the incident X-ray beam is represented by the wavevector K_0 and the scattered radiation by the wavevector $\mathbf{K}_s$, where $\mathbf{Q} = \mathbf{K}_s - \mathbf{K}_0$ defines the scattering vector and $|\mathbf{K}_s| = |\mathbf{K}_0|$ since the scattering is considered to be perfectly elastic. The scattered intensity is then represented in reciprocal space as a function of the momentum

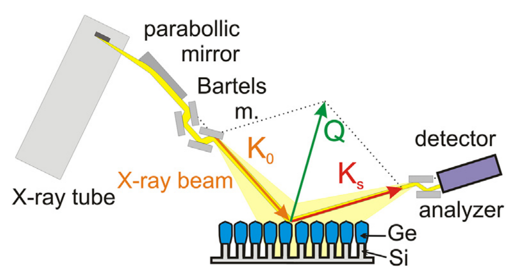

Fig. 2. Schematics of the experimental setup used for the HRXRD measurements on arrays of Ge microcrystals.

vector coordinates $\mathbf{Q} = (Q_x, Q_y, Q_z)$, where in the standard laboratory conditions we integrate the intensity along the Q_y direction because of the use of linear slits, resulting in a decreased resolution out of the scattering plane. The RSMs are typically represented in 2D (Q_x, Q_z) coordinates, as shown in Fig.3.

An example of the symmetrical (004) and asymmetrical (224) RSMs recorded around reciprocal lattice point of the Si substrate and of Ge microcrystals grown at 575°C is shown in Fig.3 for pattern E. In addition to the narrow Si substrate peak with some surrounding diffuse scattering, we detect two broader peaks originating from Ge material exhibiting different strain status. Thus, peak I is responsible for the strained Ge deposited inside the trenches between Si pillars and peak II originates from the relaxed Ge microcrystals on top of the Si pillars. In this paper we will study the evolution of these peaks as a function of growth temperature.

According to the basic definition of reciprocal space, and assuming a kinematical approach to be valid, the positions of diffraction peaks are determined by the lattice parameters and by the orientation of crystal lattice, while the shape of diffraction peaks results from the shape of