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Thin Solid Films 508 (2006) 6 – 9
thin solid films
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Surfactant-mediated epitaxy of high-quality low-doped relaxed germanium films on silicon (001)

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Available online 2 December 2005

Abstract

Direct growth of relaxed Ge layers on Si(001) substrates was achieved using Sb as a surfactant. Deposition of Ge at substrate temperatures around 670 °C under large Sb flux resulted in complete compensation of lattice mismatch via a regular array of 90° dislocations at the interface. A residual 0.20% tensile strain is found caused by thermal mismatch between Ge and Si. The density of defects threading through the Ge films is as low as 5×10^7 cm^{-2}. This is ascribed to an abrupt strain release during the initial micro-rough growth phase, which occurs only under the selected growth conditions. We also observed n-type Sb background doping levels in the Ge layers well below 10^{17} cm^{-3} presumably related to an enhanced Sb surface segregation due to the high growth temperature. Such relaxed Ge films grown by surfactant-mediated epitaxy on Si(001) open attractive perspectives for integration of novel Ge devices into mainstream Si technology.

Keywords: Germanium; Silicon; Molecular beam epitaxy (MBE); Growth mechanism

1. Introduction

High-mobility epitaxial Ge layers on Si substrates offer attractive possibilities for the integration of high-performance Ge-channel MOSFETs into sub-100 nm Si-CMOS technology [1–3].

It has been demonstrated that by surfactant-mediated epitaxy (SME), relaxed Ge films with low defect densities can directly be grown on Si(111) substrates without buffer layers [4]. 3D islanding is suppressed, and smooth, relaxed Ge (or SiGe) films can be realized as the surfactant (e.g. Sb), changes the diffusion length of adatoms and alters the surface free energy of the involved materials [5,6]. The utilization of the surfactant leads to the formation of an interfacial dislocation network compensating the lattice mismatch, and, after a few monolayers (ML), results in the growth of fully relaxed and, in principle, defect-free Ge films [7]. This growth mechanism is presumed to occur only for the Ge/Si(111) system [8]. Low-doped, relaxed high electron and hole mobility Ge films on Si(111) were subsequently achieved [9–11], leading to the first demonstration of Ge-MOSFETs on Si wafers, with record high hole inversion channel mobilities [12,13]. Until now, however, such a surfactant-mediated growth of device quality Ge films could not be achieved on (001)-oriented Si substrates, which is the standard orientation of mainstream CMOS technology. While on Si(001) the surfactant also promotes layer-by-layer growth at temperatures around 500 °C [14], it was found that strain is released gradually by introduction of dislocations, resulting in a high density of defects reaching through the growing film [15–17]. A very high background doping concentration caused by incorporation of the surfactant was an additional obstacle for device applications [18].

Here, we report on the Sb-surfactant assisted MBE of relaxed Ge layers with low defect densities directly on Si(001). Full relaxation of the epilayers was found by a residual strain analysis using reciprocal space maps (RSM). We propose a relaxation mechanism involving the abrupt formation of a dense misfit dislocation network confined to the Ge/Si interface instead of the gradual strain relief observed so far. Furthermore, we achieved a low surfactant incorporation into the Ge films indicating the device application potential of this material.

2. Sample preparation

The Ge films were grown on four inch p-type (B, 1.4–2.6 Ω cm) Si(001) substrates under a constant Sb-flux of ~3×10^{13}

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doi:10.1016/j.tsf.2005.08.410

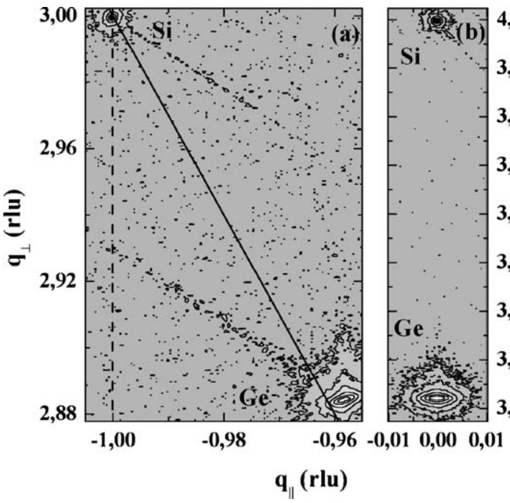

Fig. 1. Strain analysis of a 1-μm-thick Ge layer on Si(001) grown by SME showing the reciprocal space maps (RSM) of the ($\bar{1}\bar{1}3$) and (004) peaks, (a) and (b), respectively. $q_{\|}$ is in the (110) in-plane direction and $q_{\perp}$ is in the (001) vertical direction, both given in the corresponding reciprocal lattice units (rlu) 1 rlu$=2\pi|h,k,l|/a_{Si}$. In (a), the calculated solid and dotted lines represent the relaxed and the pseudomorphic state, respectively. From the position of the Ge reflex, a residual tensile in-plane strain of 0.20% is obtained. This is in good agreement with the assumption of a fully relaxed Ge layer on a Si substrate cooled down from growth temperature to room temperature yielding a value of 0.21% tensile strain induced by different thermal expansion coefficients.

cm^{-2} s^{-1} up to a thickness of 1.0 μm at 670 °C in a VG 80S MBE system. An electron beam source was used for Ge, whereas Sb was evaporated from a Knudsen cell. Substrate cleaning included an ex situ UV/ozone treatment followed by in situ thermal processing until a clear 2×1 superstructure was observed by reflection high energy electron diffraction (RHEED). One monolayer of Sb was deposited prior to the evaporation of Ge.

3. Strain analysis

High-resolution X-ray diffraction (HRXRD) measurements were performed with a BRUKER D8 DISCOVER diffractometer using Cu_{K_α} radiation, a Ge(220) Bartels-monochromator, and a channel cut analyser. Strain analysis was carried out measuring reciprocal space maps of symmetrical and asymmetrical reflexes of a 1-μm-thick Ge film grown on a Si(001) substrate by SME. Fig. 1(a) and (b) show the RSM of the ($\bar{1}\bar{1}3$)- and (004)-reflexes, respectively. Incomplete compensation of the lattice mismatch between Si and Ge would leave the epitaxial film under compressive stress resulting in a reflex position between the dashed and the solid lines, that represent the pseudomorphic and the relaxed state in Fig. 1(a). In fact, only a minute deviation from the bulk Ge lattice constant is found indicating small tensile stress. A value of 0.20% tensile in-plane strain is obtained. This can be explained considering the different thermal expansion coefficients of Ge and Si. Assuming complete relaxation of the Ge layer at growth temperature, the cooling process to room temperature would induce a tensile thermal stress of 0.21%. The excellent agreement with the measured residual strain shows that the entire thermal stress is compensated elastically by the Ge film. Thus, no additional dislocation generation is necessary in the cooling process. This is in contrast to the case of relaxed 1.2-μm-thick $Ge_{0.9}Si_{0.1}$ films grown on Si(111) by liquid phase epitaxy at 820 °C, where plastic relaxation of thermal stress was observed [19].

4. Microstructure

The crystalline quality of 1-μm-thick Ge films was evaluated by X-ray rocking curve analysis yielding dislocation densities of $\sim 5\times10^7$ cm^{-2}, which is in good agreement with the results obtained from plan view and cross-sectional transmission electron microscopy (TEM) measurements performed with a JEOL JEM-2010 microscope operating at 200 kV. The cross-sectional dark-field TEM micrograph shown in Fig. 2 demonstrates the high crystalline quality of the Ge films. Dislocation strain fields are visible in the vicinity of the Ge/Si interface, while no crystal defects are observed in the epilayer. The weak-beam dark-field TEM micrograph shown in Fig. 3 reveals a set of parallel lines oriented along $\langle\bar{1}10\rangle$ directions in the interface. Recently, an extensive TEM analysis could show that the array consists of two rectangular sets of 90° dislocations [20]. Only one set is visible in Fig. 3 due to the $\vec{g}\cdot\vec{b}=0$ criterion considering the $\vec{g}=[220]$ imaging conditions. The dislocation spacing of 9.5 nm found in Fig. 3 is consistent with complete relaxation of the 4.2% lattice mismatch assuming two rectangular sets of misfit dislocations with $\langle\bar{1}10\rangle$ line directions and Burgers vectors $\vec{b}=\frac{1}{2}\langle110\rangle$ lying in the plane of the interface.

5. Relaxation mechanism

The generation of the dislocation network can be explained similarly to the case of SME of Ge on Si(111), where misfit

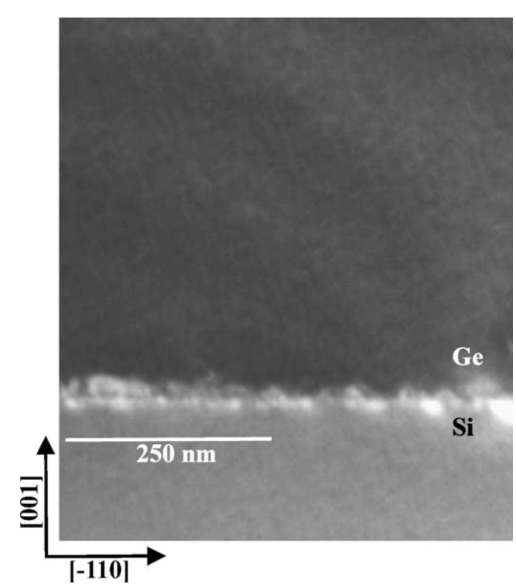

Fig. 2. Cross-sectional dark-field TEM image of the near-interface region of a 1.0-μm-thick Ge film grown by SME on Si(001). In the micrograph, strain fields due to the misfit dislocation network are visible in the vicinity of the Ge/Si interface, whereas no crystal defects are present throughout the epilayer.