Engineered Si wafers: Global integration of 100 % Ge layers on Si(111) via complex oxide heterostructures

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I Motivation

The integration of Germanium (Ge) on the Silicon (Si) material platform is important for a number of future technologies. For example, in the field of highly integrated Si based microelectronics, the integration of Ge as high mobility channel material in combination with high-k gate oxides is intensively pursued to manufacture sub-50 nm CMOS technologies. Furthermore, Ge is accepted in Si technology as a CMOS compatible material and therefore considered as a promising mediator material to achieve the manufacturing of III-V/Si hybrid devices. Another example is given by wafer supplier companies which study the integration of single crystalline Ge layers on the mature Si material platform via oxide heterostructures as an approach to develop a cheap Ge substrate platform, for example for high performance GaAs solar cells or infrared camera devices. It must however be pointed out that, to the best of our knowledge, the quality of the up to nowadays available Ge – oxide heterostructure systems on Si, prepared by two simple subsequent oxide & Ge epi-steps, did not yet achieve the level of technological relevance. This is mainly due to the fact that the fundamental physics of the interaction between Ge and oxide heterostructures (i.e. transition & rare earth (RE) oxide) is poorly understood at present. Typical unsolved solid state physics issues, governing the structural and in consequence electrical properties, concern for example the thermodynamic stability of Ge in contact with transition & RE dielectrics, the control of the growth mode to achieve closed film structures, the mechanisms at work in the creation of defects in the films and at the interfaces etc. In this talk, a materials science study is presented to evaluate the feasibility of the global integration of single crystalline Ge layers on the Si(111) material platform via oxide heterostructures.

II Interaction of Ge with the PrO2(111) / Si(111) support

Fig. 1: Complex growth scenario of single crystalline Ge(111) layers on PrO2 / Si(111) support systems
The oxide buffer heterostructure of our choice are PrO$_2$(111) films on Si(111). Details of the recipe to achieve the preparation of single crystalline, type B oriented PrO$_2$ layers which match the Si(111) surfaces on the basis of a (1x1) coincidence lattice, were recently reported [1]. Fig. 1 summarizes the complex Ge growth mode on the PrO$_2$ / Si(111) support: Ex-situ X-ray diffraction (XRD) techniques indicate that the interaction between Ge and PrO$_2$(111) results in a complete reduction of the buffer oxide to a cubic Pr$_2$O$_3$(111) film [2]. In-situ reflection high energy electron diffraction (RHEED), X-ray and Ultraviolet Photoelectron spectroscopy (XPS & UPS) studies demonstrate that this chemical reduction of the oxide support occurs during the initial Ge growth stage. The interaction of PrO$_2$ with Ge results in the formation of an amorphous Ge oxide layer by the diffusion of lattice oxygen from the dielectric to the semiconductor deposit. After the complete conversion of PrO$_2$ to cubic Pr$_2$O$_3$, the supply of lattice oxygen is exhausted and the Ge deposition reduces the initially formed amorphous GeO$_2$-like film to GeO. The sublimation of volatile GeO uncovers the cubic Pr$_2$O$_3$(111) film which is a thermodynamically stable template for Ge heteroepitaxy.

III Growth Mode Study of Ge on the Pr$_2$O$_3$(111) / Si(111) support

![Fig. 2: GI-SAXS study on the Ge nanocrystals on Pr$_2$O$_3$ / Si(111) support resulting from initial V.– W. growth.](image)

A Volmer–Weber (V.W.) growth mode is initially observed and Synchrotron based XRD, including small angle & anomalous scattering, were applied to determine the Ge island shape, size and distance (Fig. 2) [3]. The Ge islands were found to grow single crystalline in (111) orientation and the shape closely approaches the equilibrium crystal shape expected by theory. Furthermore, no real ordering of the Ge island was found, pointing to the absence of periodic nucleation patterns on the cubic Pr$_2$O$_3$ (111) surface (e.g. decoration of regular dislocation networks).

IV Structure & Defects of closed Ge(111) layers on the Pr$_2$O$_3$(111) / Si(111) support

![Fig. 3: Morphology study of the Ge / Pr$_2$O$_3$ / Si(111) heterostructure by RHEED (a), SEM(b) and XRR(c).](image)
After island coalescence and proper tuning of the growth parameters, atomically smooth Ge(111) layers are formed. Fig. 3 reports the Ge layer morphology study. The RHEED image 3a) along the Si <1-10> azimuthal projection exhibits a streaky nature, pointing to the presence of a mostly 2D Ge surface morphology. In addition, the dotted arrows indicate the appearance of a superstructure with respect to the Ge(111) surface unit cell which can probably be attributed to the formation of a c(2 x 8 ) surface reconstruction. The Secondary Electron Micrograph (SEM) in Fig.3b) proves the formation of a closed Ge layer structure. X-ray reflectivity (XRR) was applied in Fig. 3c) to quantify the thickness and roughness of the various layers of the Ge / Pr$_2$O$_3$ / Si(111) heterostructure. In the present case, the Ge and Pr$_2$O$_3$ layer thicknesses amount to 260 and 8 nm, respectively. The fit results furthermore in a root mean square roughness (rms) of the Ge surface of about 1 nm and of the Ge / Pr$_2$O$_3$ interface close to 0.4 nm. Synchrotron – radiation grazing incidence X-ray diffraction was applied to study with high resolution and sensitivity the structure and defect properties of the Ge layer on the cubic Pr$_2$O$_3$(111) / Si(111). The heterostructure is found to be single crystalline and the Transmission Electron Microscopy (TEM) image plus the atomic structure model in Fig. 4 summarize the main structure results: The epitaxy relationship of the Ge(111) / Pr$_2$O$_3$ / Si(111) heterostructure follows a so-called type A / B / A stacking sequence [4]. It is noted that this nomenclature describes fcc-related heterostructures, namely a fcc-layer adopting the stacking sequence of the Si(111) substrate is named type A whereas a fcc-structure which is characterized by a rotation of its stacking vector by 180° around the Si[111] surface normal is labelled type B [1]. In consequence, the epi-Ge layer exhibits the same stacking sequence as the Si(111) substrate but a stacking fault at the Ge / oxide as well as at the oxide / Si interface exists with respect to the type B oriented Pr$_2$O$_3$ layer. To highlight this structure relationship, inclined arrow structures are sketched in Fig.4 to indicate the different orientation of the surface normal of (11-1) lattice planes in the oxide and the semiconductor layers. Ab initio structure calculations were applied to understand the epitaxy mechanisms at work in stabilizing the stacking fault configuration at the oxide / semiconductor interfaces. It was found that mainly the electrostatic interaction across the ionic oxide / covalent semiconductor interface is the driving force for the formation of the type A / B / A stacking sequence in the Ge(111) / Pr$_2$O$_3$ / Si(111) heterostructure [4].

Fig.4: TEM image (left) and atomistic structure model (right) of the Ge(111)/ Pr$_2$O$_3$(111)/Si(111) heterostructure.

Fig.5: RSM of the Si(111) (Q$_y$=0,Q$_z$=0.32) and Ge(111) (Q$_y$=0,Q$_z$=0.307) Bragg diffraction peaks on [00L] rod.
Defect characterization of the epi-Ge layer structure was carried out by (diffuse) XRD studies in combination with high resolution (HR) TEM analysis. As an example, the reciprocal space map (RSM) of the Si(111) ($Q_x=0, Q_y=0.32$) and Ge(111) ($Q_x=0, Q_z=0.307$) Bragg diffraction peaks on [00L] rod is shown in Fig.5. In contrast to the sharp Si(111) Bragg peak, the Ge(111) diffraction signal is accompanied by a broad halo, indicating strain fields as well as lattice defects [5]. The most obvious feature is the streak inclined by about 19.5° with respect to the Si [111] sample normal, running that way parallel to the surface normal of the inclined Ge (11-1) lattice planes. It is well known that the formation of these diffuse streaks in the XRD pattern is due to structural defects in the diamond lattice of the epi-Ge(111) layer, namely in form of stacking faults and/or microtwins [5].

V Outlook

Defect engineering approaches need to be applied to improve the long-range order of the as-deposited single crystalline epitaxial Ge films grown on cubic Pr$_2$O$_3$ / Si(111) support systems. Furthermore, the transfer of MBE based “proof of principle” studies towards mass-production compatible CVD techniques is currently in progress.

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