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**THE ROLE OF SURFACE ACTIVE SPECIES IN HETEROEPITAXIAL GROWTH OF Ge THIN FILMS AND NANOSTRUCTURES ON Si(113) SUBSTRATES**

The paper deals with the investigation of the formation of Ge thin films and nanostructures on clean surface of Si(113) by in-situ ultra-high vacuum (UHV) scanning tunneling microscope (STM) and low energy electron diffraction (LEED), and the role of surface active species (surfactant) in heteroepitaxial growth. Ge layers were grown on the Si(113) surface by Ge deposition at elevated substrate temperatures and different duration of Ge deposition. For a detailed structural characterization during the growth in-situ STM and LEED studies were used to achieve information regarding the growth modes and the nucleation of Ge on Si(113) surface.

**Keywords:** surfactant, heteroepitaxial growth, thin film, surfactant mediated growth.

The Si(113) surface has received much attention because of its high stability and technological importance. In general, high-index Si surfaces tend to be unstable and to facet into lower-index planes upon annealing [1]. However, the Si(113) surface is an exception. It has an energy that is comparable to that of the low-index surfaces and therefore it has potential as a substrate for growth [2]. Recently, a lot of efforts have been devoted to improve epitaxial growth of such materials as Ge on Si. Although one can hardly understand initial stages of epitaxial growth without knowing the atomic structure of the substrate, there is at least one silicon surface which is of potential interest for epitaxy [3], but which has an unknown microscopic structure [4]. Experimental and theoretical issues have been previously carried out to study the atomic structure of the Si(113) surface. The first STM determination of the Si(113) structure was carried out by Knall and his co-workers [5]. In LEED pattern a 3x1 reconstruction is observed. The second STM study on Si(113) supported the 3x1 reconstruction [6]. At the moment there are a majority of studies [1, 2, 5] supporting a 3x2 structure at 300 K, while others [6] argue for a 3x1 structure. Jacobi and his co-workers [7] have found that at 300K Si(113) surface has a 3x2 reconstruction that is transformed into a 3x1 structure. Despite all these studies, the atomic structures and relative stability of these reconstructed surfaces are still not completely solved. For the Si(113) 3x1 surface, several structural models have been suggested, such as Runke's "dimmer and adatom" model [8], Dabrowski's model with interstitial Si [9], and the packing model [10]. However, the detailed atomic structure of the Si(113)-3x1 surface is not solved completely.

A substantial modification of the growth of thin films and nanostructures may be obtained by introducing a third element which lowers the surface free energy of both Ge and Si. Surface active species (surfactant) mediated epitaxy [11] of semiconductor surfaces has attracted considerable interest recently because it enables the growth of nanostructures, which are not achievable by conventional molecular beam epitaxy (MBE) or chemical vapour deposition (CVD). So far Bi [12] has been reported to successfully act as surfactants for growth of Ge on Si (111). Both lattice strain and surface free energy help determine whether a film

undergoes layer-by-layer growth (Frank-van der Merwe), islanding (Volmer-Weber), and layer-by-layer growth followed by islanding (Stranski-Krastanov).

The experiments are carried out in an UHV STM system. Nominally undoped Si(113) samples with a resistance of  $10\text{ ohm}\cdot\text{cm}$  and a size of  $2\text{ mm} \times 5\text{ mm}$  are used for substrates. The samples are cut from highly oriented Si(113) wafers with a remaining miscut of less than 0.02 degrees. After cleaning in methanol, the samples are inserted into UHV system through a load lock and degassed at about  $600^\circ\text{C}$  for more than 24 hours. The substrates are flashed by short annealing cycles up to  $1200^\circ\text{C}$  for nearly 15 seconds in order to remove any contamination. The samples are resistively heated directly by DC current and the sample temperature is measured using an infrared pyrometer. This procedure reliably resulted in the removal of the native oxide layer and in the formation of a well ordered Si(113)- $3\times 2$  surface reconstruction which is checked by LEED and STM. For the growth of Ge thin films and nanostructures atomic Ge is evaporated from Ge Knudsen cell. The Ge growth deposition is set between  $300^\circ\text{C}$  and  $430^\circ\text{C}$ . Subsequently LEED and STM measurements are performed at room temperature. The base pressure in the UHV system is below  $5\times 10^{-11}\text{ mbar}$ , and do not exceed  $1 \times 10^{-10}\text{ mbar}$  during Ge deposition.

The research is carried out at the University of Bremen, Germany. The STM images and the LEED patterns are used for the analysis of the atomic structure, morphology and reconstruction of Si(113) clean surface, as well as the formation of Ge thin films and nanostructures on Si(113) surface. The STM images of the clean surface of Si(113) at different scales are shown in Fig. 1. The scan areas are  $1000\text{ nm} \times 1000\text{ nm}$  (a),  $250\text{ nm} \times 250\text{ nm}$  (b) and  $56\text{ nm} \times 13\text{ nm}$  (c), using sample voltage - 2 V and tunnelling current 0.3 nA.

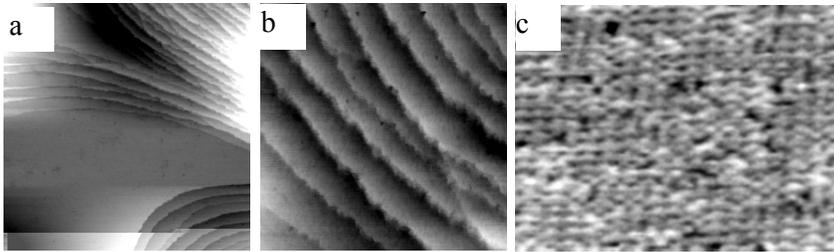


Fig. 1

The LEED pattern of the clean surface of Si(113) is shown in Fig. 2. Electron energy is  $75\text{ eV}$ .

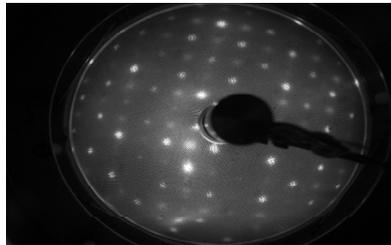


Fig.2

For large area scans individual steps are found for the clean Si(113) surface according to the remaining miscut of the sample (Fig. 1 a and b). No indication for facet formation was found. The LEED images were taken at various energies of electrons. Both the STM images and the LEED patterns of the Si(113) clean surface show a 3x2 reconstruction.

The STM images of clean surface of Si(113) (a), Ge/Si(113) interface after 2 *min* (b), 30 *min* (c) and 10 *min* using surfactant of Bi (d) at a substrate temperature of 430°C are shown in Fig.3. The scan areas are 500 *nm* x 500 *nm*, using sample voltage of - 2 *V* and tunnelling current of 0.3 *nA*.

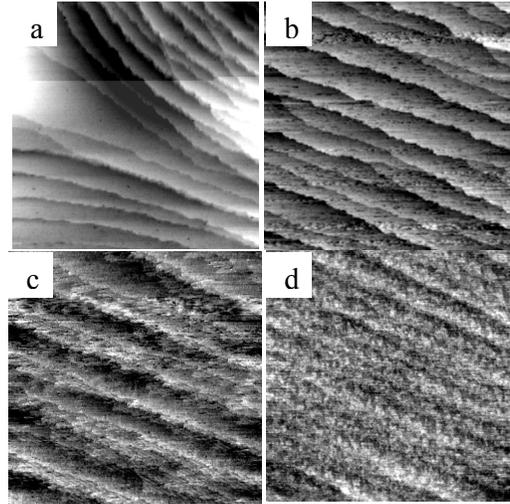


Fig. 3

After 2 minutes' deposition of Ge atoms only very few patches of Ge atoms are observed on the clean Si(113) surface (Fig. 3 b). After increasing the duration of the deposition of Ge atoms on the clean Si(113) surface up to 15 minutes at the same temperature of substrate we find a sub-bilayer coverage of Ge at step edges of the Si(113) surface. Ge growth is layer-by-layer and there are no Ge islands on the surface. Preferential nucleation of Ge at step edges can be attributed to a larger number of dangling bonds available at the steps. After 30 minutes' deposition of Ge at the same growth temperature, in contrast with previous cases of 2 and 15 minutes' deposition, a continuous Ge layer is formed on parts of the Si(113) terraces (Fig. 3 c). The STM and the LEED investigation at atomic scale show a mixture of 3x2 and 3x1 surface reconstruction, which can be attributed to remaining by open Si(113) and Ge/Si(113) 3x1 areas, respectively.

During 30 minutes' deposition of Ge atoms on the clean Si(113) surface at 300°C substrate temperature a sub-bilayer coverage of Ge on the Si(113) surface arises. Scattering Ge islands are formed on the Si(113) surface with single atomic steps. At a growth temperature of 300°C the mobility of Ge atoms is less than that of 430°C and deposited Ge atoms cannot reach the step edges and bind. Hence, by decreasing substrate temperature from 430°C to 300°C Ge islands are formed on Si(113) surface and layer by layer growth arises by islanding. The STM is used to gain information regarding the surface morphology of the formation of Ge films at a

sub-nanometer scale on Si(113) surface (Fig. 3). By increasing the growth temperature from 300°C to 430°C Ge atoms become sufficiently mobile to reach step edges. Thus, based on STM observations, and by optimizing the growth conditions (growth temperature, rate of the deposition, etc.) considerable smooth Ge films on Si(113) are obtained. To obtain more smooth Ge thin films, we used the third element (Bi) during the growth by surfactant mediated epitaxy (Fig. 3 d). We succeed as well as in obtaining Ge nanostructures on Si(113) substrates.

Based on UHV STM and LEED observations clean surface of Si(113), Ge/Si(113) interface and the reconstruction and morphology of the formation of Ge thin films and nanostructures on Si(113) are investigated. We clarified that clean surface of Si(113) has 3x2 reconstruction and Ge/Si(113) interface - 3x2 and 3x1 reconstructions. Analyzing the morphology of the formation of Ge films on Si(113) clearly shows that it is possible to obtain considerable smooth and homogeneous Ge films on Si(113) at 430°C substrate temperature after 30 minutes' Ge deposition. The use of Bi surfactant allow to obtain more smooth and homogeneous Ge thin films and nanostructures on Si(113).

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## Գ.Ե. ՇՄԱՎՈՆՅԱՆ

### ՄԱԿԵՐԵՎՈՒԹԱՅԻՆ ԱԿՏԻՎ ՏԱՐՐԵՐԻ ԴԵՐՈՇ $\text{Si}(113)$ ՀԱՐԹԱԿՆԵՐԻ ՎՐԱ Ge - Ի ԲԱՐԱԿ ԹԱՂԱՆԹՆԵՐԻ ԵՎ ՆԱՆՈԿԱՌՈՒՑՎԱԾՔՆԵՐԻ ՀԵՏԵՐՈՒՊԻՏԱՔՍԻԱԼԱՅԻՆ ԱՃԵՑՄԱՆ ԴԵՊՔՈՒՄ

Հողվածի նպատակն է՝ ժամանակակից գերբարձր վակուումային փռող թունելային մանրադիտակով և փոքր էներգիայով էլեկտրոնների դիֆրակցիայի եղանակով ուսումնասիրել Ge-ի բարակ թաղանթների և նանոկառուցվածքների աճեցումը  $\text{Si}(113)$ -ի մաքուր մակերևութային վրա, ինչպես նաև մակերևութային ակտիվ տարրերի դերը հետերոէպիտաքսիալային աճեցման դեպքում: Ge-ի շերտերը աճեցվել են Ge նստեցնելով  $\text{Si}(113)$  հարթակի մակերևութի վրա բարձր ջերմաստիճանների և Ge-ի նստեցման տարբեր ջերմաստիճանների դեպքերում: Աճեցման ընթացքում կառուցվածքային մանրակրկիտ բնութագրում կատարելու համար ժամանակակից փռող թունելային մանրադիտակի օգնությամբ հնարավոր դարձավ տեղեկություն ստանալ  $\text{Si}(113)$ -ի վրա Ge-ի աճեցման ձևի և բյուրեղացման կենտրոնների առաջացման մասին:

**Առանցքային բառեր.** մակերևութային ակտիվ տարր, հետերոէպիտաքսիալային աճեցում, բարակ թաղանթ, մակերևութային ակտիվ տարրերի միջոցով ձևափոխման էպիտաքսիա:

## Г.Ш. ШИМАНЯН

### РОЛЬ ПОВЕРХНОСТНО-АКТИВНЫХ ЭЛЕМЕНТОВ ПРИ ГЕТЕРОСТРУКТУРНОМ РОСТЕ ТОНКИХ ПЛЕНОК И НАНОСТРУКТУР Ge НА ПОДЛОЖКАХ $\text{Si}(113)$

Исследуются вопросы формирования тонких пленок и наноструктур Ge на чистой поверхности  $\text{Si}(113)$  с помощью современного сверхвысокого вакуумного сканирующего туннельного микроскопа и метода дифракции электронов с низкой энергией. Показана роль поверхностно-активных элементов при гетероструктурном росте. Слои Ge выращены на поверхности  $\text{Si}(113)$  при осаждении Ge в высоких температурах подложки и разных продолжительностях осаждения Ge. С целью подробной структурной характеристики современный сканирующий туннельный микроскоп позволил получить информацию о формах роста и образованиях центров кристаллизации Ge на поверхности  $\text{Si}(113)$ .

**Ключевые слова:** поверхностно-активное вещество, четырехэпитаксиальный рост, тонкая пленка, рост посредством поверхностно-активного вещества.