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REDISTRIBUTION OF $CrSi_2$ NANOCRYSTALLITES IN SILICON CAP LAYERS DURING MBE GROWTH ON Si(111) SUBSTRATES

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Semiconducting $CrSi_2$ nanocrystallites (NCs) were grown by reactive deposition epitaxy (RDE) of 0.6 nm Cr at 500, 550 and 600 °C. The NCs were covered by epitaxial silicon at 700 °C with different thickness. It was observed that $CrSi_2$ is localized near the surface in the form of 20 nm 2D nanoislands and 40-80 nm 3D NCs. The 2D nanoisland concentration is found to be reduced by the Si cap growth, while the large 3D NCs appear at the depth of Cr deposition and they also appear at the surface.

1. Introduction

It was shown that chromium disilicide ($CrSi_2$, $E_g = 0.35$ eV) nanocrystallites are embedded in monocrystalline lattice by reactive deposition epitaxy (RDE of Cr) and Si molecular beam epitaxy (MBE) [1]. Redistribution of $CrSi_2$ NCs has been observed in silicon–silicide-silicon heterostructures with one embedded layer by HR XTEM data [2].

This work is devoted to study the influence of substrate temperature on $CrSi_2$ island size distribution on Si substrate and the effect of Si layer thickness at MBE process on the formation of Si(111)/$CrSi_2$ NCs/Si(111) heterostructures and $CrSi_2$ NC moving in it.

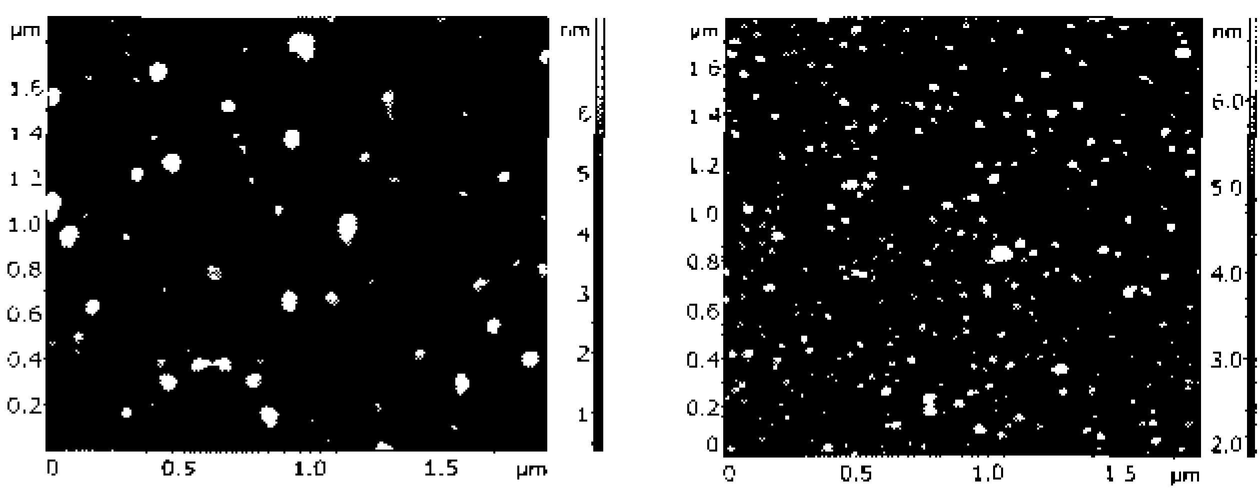
2. Experimental

The structures were grown in an ultra high vacuum (UHV) chamber "VARIAN" with a base pressure of $2\cdot10^{-10}$ Torr equipped with differential reflectance spectroscopy (DRS) [3] for a study of optical properties of the samples. Samples were cut from n-type 0.3 Ω·cm Si(111) substrates. The silicon was cleaned by flashes at 1250 °C (7 times). Surface purity was controlled by AES. RDE was carried out at 500 °C, 550 °C, and 600 °C. The Cr deposition rate was about 0.04 nm/min controlled by a quartz sensor. An additional annealing during 2 min at 700 °C was done for all samples before the growth of silicon epitaxial cap layer.

Morphology was studied by AFM (Solver P47) in semicontact mode using a 10 nm radius tip. Philips CM 20 transmission electron microscope operating at 200 keV was used to analyze the surface and cross-section of the samples thinned by our standard ion beam milling procedure [4].

3. Results

The samples prepared at 500 °C, 550 °C and at 600 °C by RDE of 0.6 nm Cr without Si cap layer were analyzed by AFM to characterize the $CrSi_2$ nanoislands. Cr deposition at 500 °C silicide islands have bimodal size distribution (10-20 nm and 40-80 nm) as it is shown in Fig. 1a. The bimodal size distribution indicates that significant secondary nucleation occurs during Cr deposition at 500 °C in parallel to the growth of the islands. At 550 °C a narrow $CrSi_2$ island size distribution was observed as it is shown in Fig. 1b. Islands had the maximal density ($4\cdot10^{10}$ cm^{-2}), minimal sizes (15-20 nm) and heights (2-4 nm). The silicon surface is 30-50% covered by nanoislands.



a) b)

Figure 1. AFM images of the samples prepared by RDE of 0.6 nm Cr onto Si(111)7×7 substrate at: (a) – 500 °C, (b) – 550 °C. In both cases an additional annealing at 700 °C (t=2 min) was done. Right axes show colour scale of height in nm.

Initial stages of silicon growth (up to 4.4 nm) atop $CrSi_2$ islands were studied by DRS. The silicon overgrowth results in an increase of Si contribution and conservation of $CrSi_2$ in the differential spectra with increasing Si thickness as it is shown in Fig. 2. The increased Si component corresponds mainly to silicon growth between the $CrSi_2$ islands. At 9 nm Si cap the sample surface has both pinholes and uncovered $CrSi_2$ islands. Smoothing of the silicon cap was observed starting from 50 nm thickness. Three layer sample exhibited rough surface, but the reflectance spectra indicated monocrystalline Si growth in this sample.

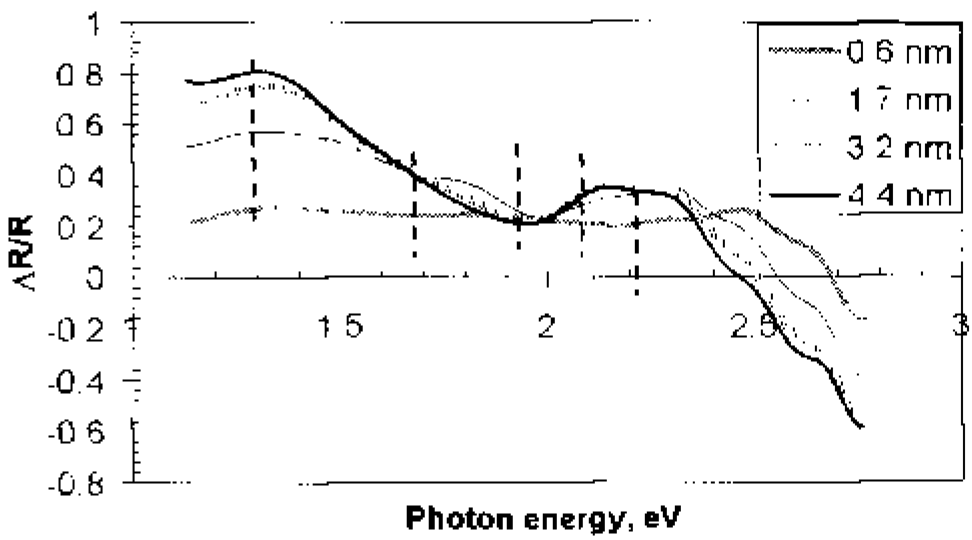


Figure 2. Differential reflectance spectra at different Si thickness (0-4.4 nm) registered during MBE Si growth.

Cross sectional TEM (XTEM) investigations were used to determine the distribution of the NCs in Si cap layer. XTEM images for three different Si cap thicknesses are shown in Fig. 3a,b,c). NCs appear near the Cr deposition, and

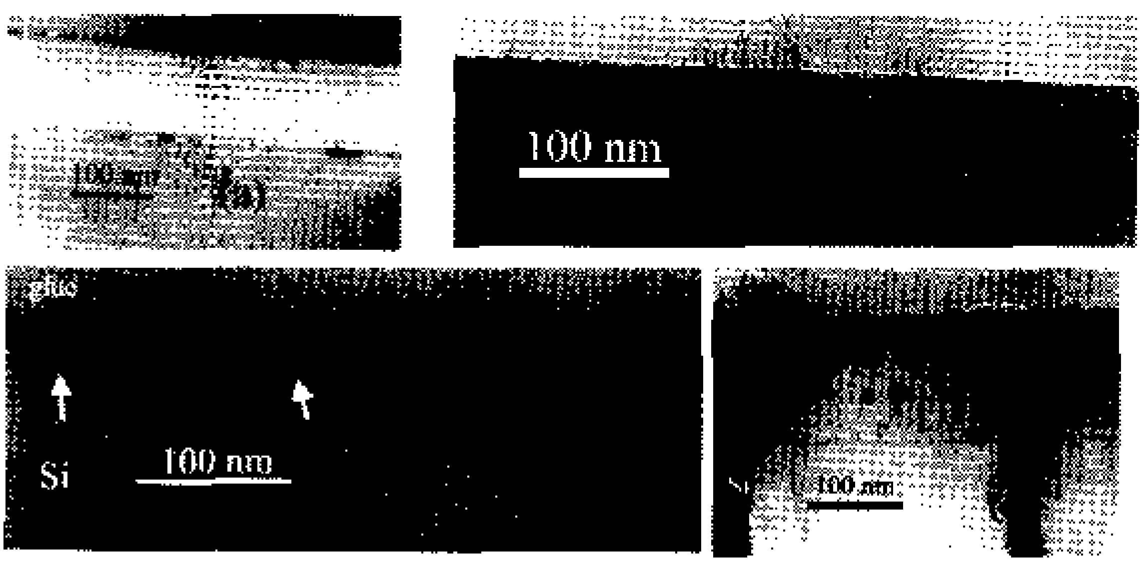


Figure 3. Cross sectional TEM images of samples prepared by RDE of 0.6 nm Cr at 550 °C of different Si cap thickness' (a - 9 nm, b - 20 nm), c - 40 nm and d -3×(0.6 nm Cr RDE+50 nm Si).

near the Si surface. Fig. 3d shows XTEM image of a sample including three 0.6 nm layers of Cr deposited by RDE at 550 °C and 50 nm Si layer deposited at 700 °C. An increased density of the NCs at the Cr depth and at the sample surface is apparent that correlates with AFM data (Fig. 2b) for Cr islands grown at 550 °C. It is remarkable that a dashed-line pattern appears in the XTEM at the Cr depth, indicating that some of the $CrSi_2$ islands are stabilized in 2D form. The cross sectional and surface view TEM show that some of the $CrSi_2$ flat nanoislands are transformed into 3D spherical NCs during the silicon cap growth partly at the deposition depth, partly at the sample surface. Some of the 2D nanoislands are also localized at the deposition depth.

We assume the diffusion of Cr takes place in the form of small size silicide NCs below the surface. Most of small (10-20 nm) NCs are not stabilized at the Cr deposition. During deposition of Si cap at 700 °C the small silicide islands diffuse and they form 3D NCs near the Si surface. Some of the large NCs, both 2D and 3D ones, are stable during the silicon cap growth. It is known that above 700 °C Cr has a tendency to diffuse toward the surface [5]. So, we suppose the silicon has a continuous high Cr concentration ($>10^{21}$ cm^{-3} range) at the growth front during the deposition of the cap layer. It explains the nucleation and growth of $CrSi_2$ NCs far from the original Cr deposition plane as observed by TEM, and also explains the effect of NCs observed by AFM on the surface.

4. Conclusions

Monolithic Si(111)/$CrSi_2$ NCs/Si(111) heterostructures with buried $CrSi_2$ NCs were grown. The large 3D NCs nucleated near the deposition depth, but most of $CrSi_2$ nanoislands diffuse toward the Si cap surface. The observed large redistribution of Cr shows that for improving the distribution of the NCs the growth temperature at the initial stage of the silicon cap growth has to be reduced.

Acknowledgments

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