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# EPITAXIAL GROWTH OF SILICON ON $CoSi_2(001)/Si(001)$

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## Abstract

Epitaxial Si layers have been grown under a variety of growth conditions on $CoSi_2(001)$ by molecular beam epitaxy (MBE). The structural properties of the Si overgrowth were studied by *in-situ* Reflection High Energy Electron Diffraction (RHEED), as well as *ex-situ* MeV $^4He^+$ ion channeling and High Resolution Transmission Electron Microscopy (HRTEM). Strong influences of the $CoSi_2$ surface reconstruction on the Si overgrowth have been observed. RHEED studies show islanding growth of Si on the $CoSi_2(001)$ $(3\sqrt{2}\times\sqrt{2})R45$ reconstructed surface, but smooth growth of Si on the $CoSi_2(001)$ $(\sqrt{2}\times\sqrt{2})R45$ reconstructed surface, under the same growth conditions. The growth of Si on thin layers of $CoSi_2$ (2nm-6nm) with $(\sqrt{2}\times\sqrt{2})R45$ reconstructed surface at $460^\circ C$ results in high crystalline quality for the Si top layer, as indicated by good channeling minimum yield ($\chi_{min} < 6\%$), but cross-sectional TEM shows that the $CoSi_2$ layers are discontinuous. We also report preliminary results on Si grown on a $2\times2$ reconstructed $CoSi_2(001)$ surface.

## Introduction

Buried epitaxial metal silicide layers in Si have attracted great attention because of their potential application in high speed devices like the metal base transistor and the permeable base transistor, and also as buried epitaxial metal layers in three dimensional integrated circuits. The advantages of $CoSi_2$ are its excellent conductivity, its flourite crystal structure (which is similar to the diamond structure of Si), and its small lattice mismatch with Si (1.2% at room temperature), which increases the possibility of growing high quality heteroepitaxial $Si/CoSi_2/Si$ structures. Despite great success in fabricating high quality $CoSi_2$ and $Si/CoSi_2$ multilayers on Si(111) [1-4], a metal base transistor has been difficult to develop. This may be due to the absence of states in the silicide with the correct transverse momentum (near the Si conduction band minimum) for electron injection along the (111) direction [5]. Such states do exist in the silicide for electrons injection along (001) direction [5], so that the growth of epitaxial $Si/CoSi_2/Si(001)$ structures would have greater technological importance. Monocrystalline $CoSi_2(001)$ has been successfully grown on Si(001) in recent years [6,7], which makes the studies of Si growth on $CoSi_2(001)/Si(001)$ possible.

## Sample growth

In these experiments, four-inch p-type Si(001) wafers with resistivity of 15-25 Ω·cm were used. The wafers were given a modified RCA clean before loading into the MBE system (VG Semicon, model V90S), which had a base pressure of $5\times10^{-11}$ mbar.

Pressures during growth were in the middle of the $10^{-10}$ mbar range. Inside the MBE system, the wafers were heated to high temperature ($750°C - 820°C$) for 15 minutes in order to remove the protective oxide film. This annealing temperature was determined by obtaining a sharp RHEED $2 \times 1$ reconstructed streak pattern. RHEED, with 14 keV electrons, was used at every stage of deposition to monitor the surface. The cobalt and silicon were evaporated from two separate Temescal electron-beam evaporators. Evaporation rates were separately monitored by electron-impact emission spectroscopy and feedback controlled to within 5% by an Inficon Sentinel III deposition controller. The calibration of the evaporation rates was done by RBS. The temperature was measured by a thermocouple and calibrated by an optical pyrometer.

## Results and Discussion

Epitaxial $CoSi_2$ layers of different thickness were grown using the direct codeposition [7], the template I [6,7], and what we call the template II, methods. For the direct codeposition method, the epitaxial $CoSi_2$ was grown at $550°C$, at a Co:Si ratio of 1:1.8. The deposition rates for Co and Si were 0.021nm/s and 0.07nm/s, respectively. The $CoSi_2$ in this case displayed a $(\sqrt{2} \times \sqrt{2})R45$ reconstructed RHEED pattern. The template I growth of $CoSi_2$ involved depositing an initial 0.2nm of Co, then codepositing 0.2nm Co and 0.72nm Si, all at room temperature, followed by annealing at $460°C$ to form a 1.4nm $CoSi_2$ layer. Codepositing Co and Si in 1:2 ratio at $460°C$ was used to thicken the template to the desired $CoSi_2$ thickness. We have only observed the $(3\sqrt{2} \times \sqrt{2})R45$ reconstructed RHEED patterns for $CoSi_2$ grown by the template I method, although Yalisove et al. [8] reported observing both the $(\sqrt{2} \times \sqrt{2})R45$ and the $(3\sqrt{2} \times \sqrt{2})R45$ reconstructed $CoSi_2$ surfaces with this growth procedure. RBS channeling measurements on the $CoSi_2$ layers grown by both the direct codeposition and template I methods show good epitaxial quality ($\chi_{min} < 5\%$). This is also confirmed by the sharp RHEED patterns for both growth procedures. A second template technique (template II) for growth of $CoSi_2$ was used which involved sequential room temperature deposition of 0.26nm Co and 0.7nm Si, followed by annealing at $460°C$ to form 0.9nm $CoSi_2$. The $CoSi_2$ layer grown by the template II method displays a $2 \times 2$ reconstructed RHEED pattern.

The RBS channeling studies of Si overgrowth on $CoSi_2$ layers of different thickness and at different temperatures, are shown in Figure 1. A deposition rate of 0.05nm/s was used for all Si overgrowth reported in this paper. RBS shows that Co diffuses to the surface when Si is deposited at $550°C$. Room temperature deposition of a thin Si buffer layer (1nm and 2nm) before further Si growth at $550°C$ does not stop the diffusion of Co. The crystalline quality of the Si top layer, indicated by channeling minimum yield, improves at higher growth temperatures. Figure 1 also shows the dramatic improvement of Si crystalline quality for Si grown on thinner $CoSi_2$ layers. A growth temperature of $460°C$ was used for Si overgrowth on $CoSi_2$ with different surface reconstructions. The results are summarized in Table 1.

During Si growth on the $(3\sqrt{2} \times \sqrt{2})R45$ reconstructed surface, RHEED observations show that islanding takes place immediately after the start of Si deposition, and continues throughout the Si overgrowth. This is shown in Figure 2. Faceting of the overgrown Si layer can be seen in the RHEED pattern (Figure 2(b)). The crystalline quality of the $CoSi_2$ and the top Si layer is very poor, as indicated by the very high channeling minimum yields for both Si and Co. In contrast to the faceted growth of Si on the $CoSi_2$ $(3\sqrt{2} \times \sqrt{2})R45$ reconstructed surface, Si growth on the $CoSi_2$ $(\sqrt{2} \times \sqrt{2})R45$

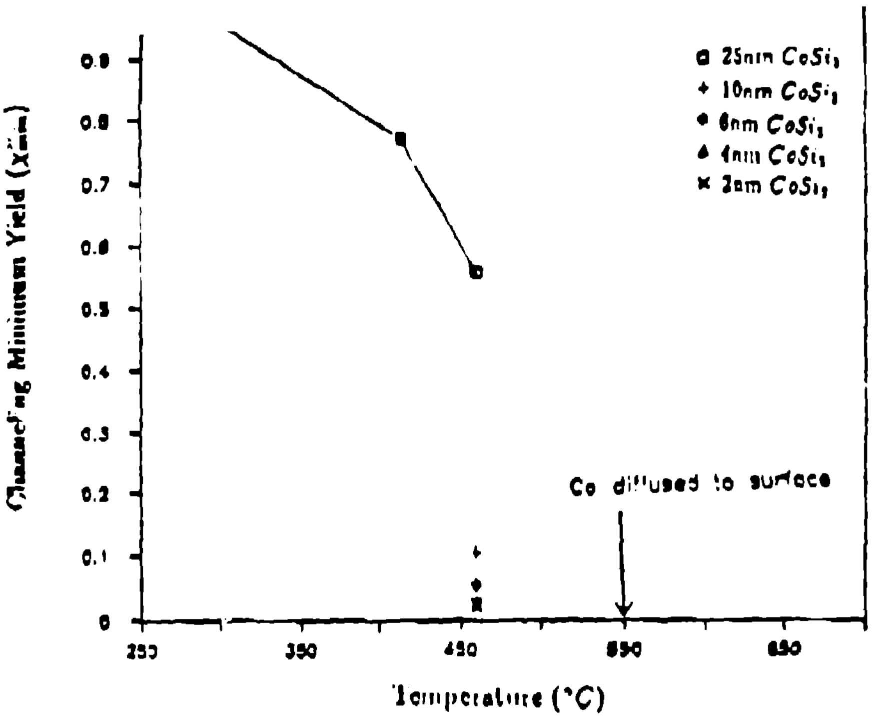
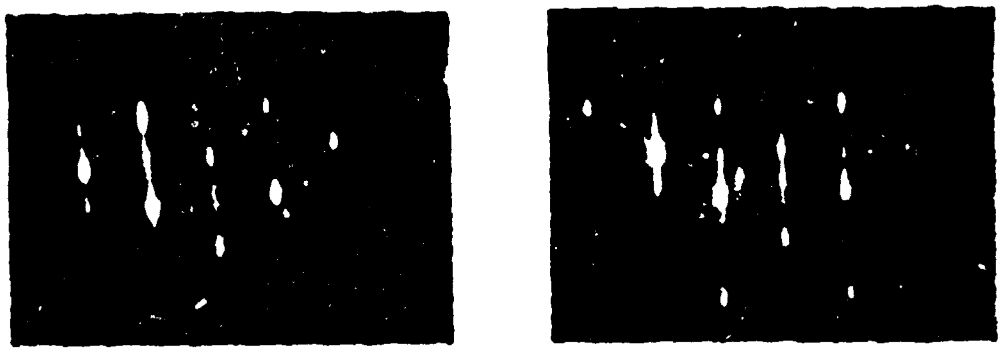



Figure 1. RBS channeling results of silicon overgrowth on $CoSi_2$ layers of different thicknesses at different temperatures.

Table 1 Summary of silicon overgrowth on $CoSi_2(001)$ at 400°C. The silicon deposition rate is 0.05nm/s for all the samples.

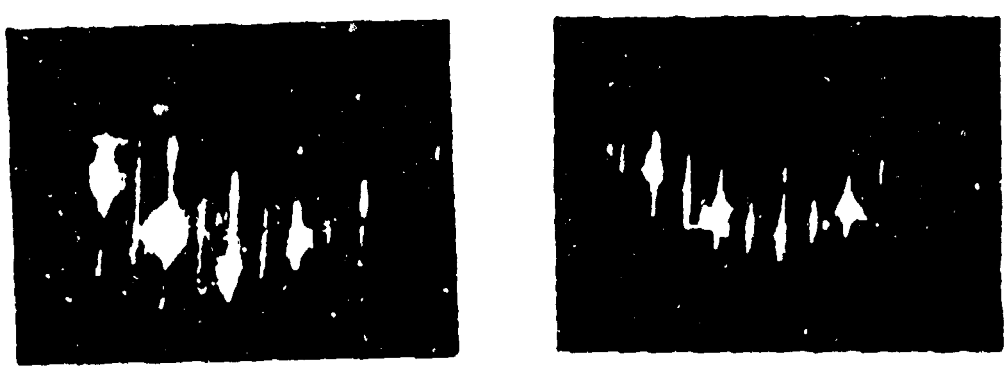
| $CoSi_2/Si(001)$ | | | $Si/CoSi_2/Si(001)$ | | |
|---|---|---|---|---|---|
| growth method | RHEED | thickness (nm) | $\chi_{min}$(Si) (%) | $\chi_{min}$(Co) (%) | RHEED |
| codeposition | $(\sqrt{2}\times\sqrt{2})R45$ | 10 | 10.6 | 31.8 | smooth growth |
| codeposition | $(\sqrt{2}\times\sqrt{2})R45$ | 6 | 5.6 | 36 | smooth growth |
| codeposition | $(\sqrt{2}\times\sqrt{2})R45$ | 4 | 2.8 | 30 | smooth growth |
| codeposition | $(\sqrt{2}\times\sqrt{2})R45$ | 2 | 2.4 | 28 | smooth growth |
| template I | $(3\sqrt{2}\times\sqrt{2})R45$ | 6 | 62 | 77 | faceted growth |
| template I | $(3\sqrt{2}\times\sqrt{2})R45$ | 2 | 62 | 73 | faceted growth |
| template II | $2\times2$ | 0.0 | 2.2 | 4.7 | smooth growth |

reconstructed surface is smooth, according to RHEED observations (Figure 2). Small modulations in the intensity along the main streak disappear as the Si grows thicker, giving way to a sharp Si $2\times1$ reconstructed pattern. RBS channeling measurements show high crystalline quality for Si grown on thin $CoSi_2$ layers with the $(\sqrt{2}\times\sqrt{2})R45$ reconstructed surface, but relatively poor crystalline quality for the buried $CoSi_2$ layer ($\chi_{min}$ about 30% for the Co including the interfaces peaks).



(a) (b)

Figure 2. RHEED patterns (along the [001] azimuth) taken during Si growth on the 5 nm thick $CoSi_2$ film with a $(3\sqrt{2} \times \sqrt{2})R45$ reconstructed surface (a) at 6.5nm, and (b) at 100nm.



(a) (b)

Figure 3. RHEED patterns (along the [001] azimuth) taken during Si growth on the 2 nm thick $CoSi_2$ film with a $(\sqrt{2} \times \sqrt{2})R45$ reconstructed surface (a) at 1.5nm, and (b) at 40nm.

*HRTEM* was used to study 100nm Si films grown on 6nm and 2nm $CoSi_2$ layers with the $(\sqrt{2} \times \sqrt{2})R45$ reconstructed surface. TEM shows that the $CoSi_2$ layers are not continuous in both samples (Figure 4). Increased $CoSi_2$ coverage and grain size were observed for the sample with the thicker $CoSi_2$ layer. The epitaxial Si layer on 6nm $CoSi_2$ contains a higher density of microtwins and stacking faults near the $CoSi_2$ layer. The tendency of $CoSi_2$ to facet along (111) planes is also observed, again indicating the relatively low Si(111)/$CoSi_2$(111) interface energy. The overall quality of the Si(111)/$CoSi_2$(111) and Si(001)/$CoSi_2$(001) interfaces is good.

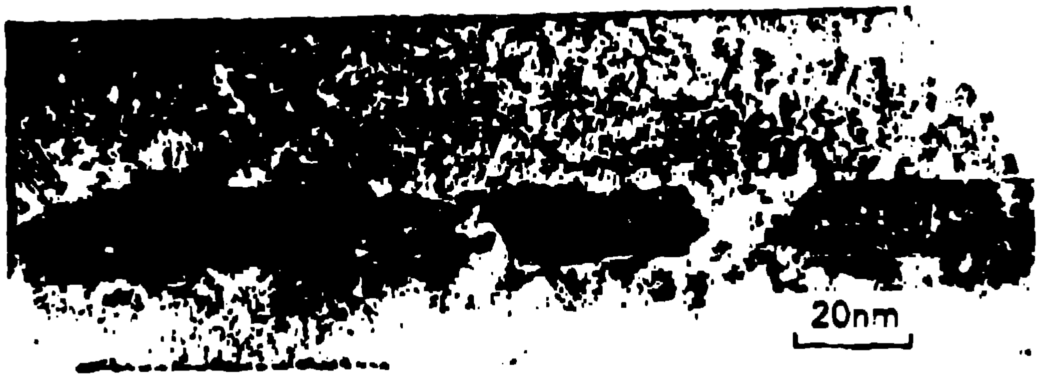



Figure 4. A cross-sectional high-resolution TEM image of 100 nm Si grown on a 6 nm $CoSi_2$(001) layer, imaged along the [001] direction.

Figure 5 shows RBS channeling spectra of 40nm of Si grown on a 0.9nm 2 × 2 surface reconstructed $CoSi_2$ layer grown by the template II method. It shows high crystalline quality for both the Si top layer and the buried $CoSi_2$ layer. The RHEED observations shows the smooth growth of Si on this 2 × 2 surface reconstructed $CoSi_2$ layer. The disordering of $CoSi_2$ layers, observed after Si growth on the previous two types of reconstructed $CoSi_2$ surfaces, was not observed for Si growth on the 2 × 2 surface reconstructed $CoSi_2$ layer. These results indicate a promising method of obtaining high quality epitaxial structures of Si/$CoSi_2$/Si(001), by depositing Si on a 2 × 2 surface reconstructed $CoSi_2$ layer.

## Summary

Our results show that the $CoSi_2$(001) surface reconstructions have strong influences on Si overgrowth at 460°C. Depositing Si on the $(3\sqrt{2} \times \sqrt{2})R45$ reconstructed $CoSi_2$ surface results in islanding growth, and the crystal quality of both the Si overlayer and the buried $CoSi_2$ layer is very poor. Si growth on the $(\sqrt{2} \times \sqrt{2})R45$ reconstructed $CoSi_2$ surface is smooth, and results in a high quality Si overlayer, but the buried $CoSi_2$ layer is disordered. TEM also shows that the $CoSi_2$ layer is discontinuous. High crystalline quality is observed for both the buried $CoSi_2$ layer and the epitaxial Si overlayer grown by depositing Si on the 2 × 2 surface reconstructed $CoSi_2$ layer.

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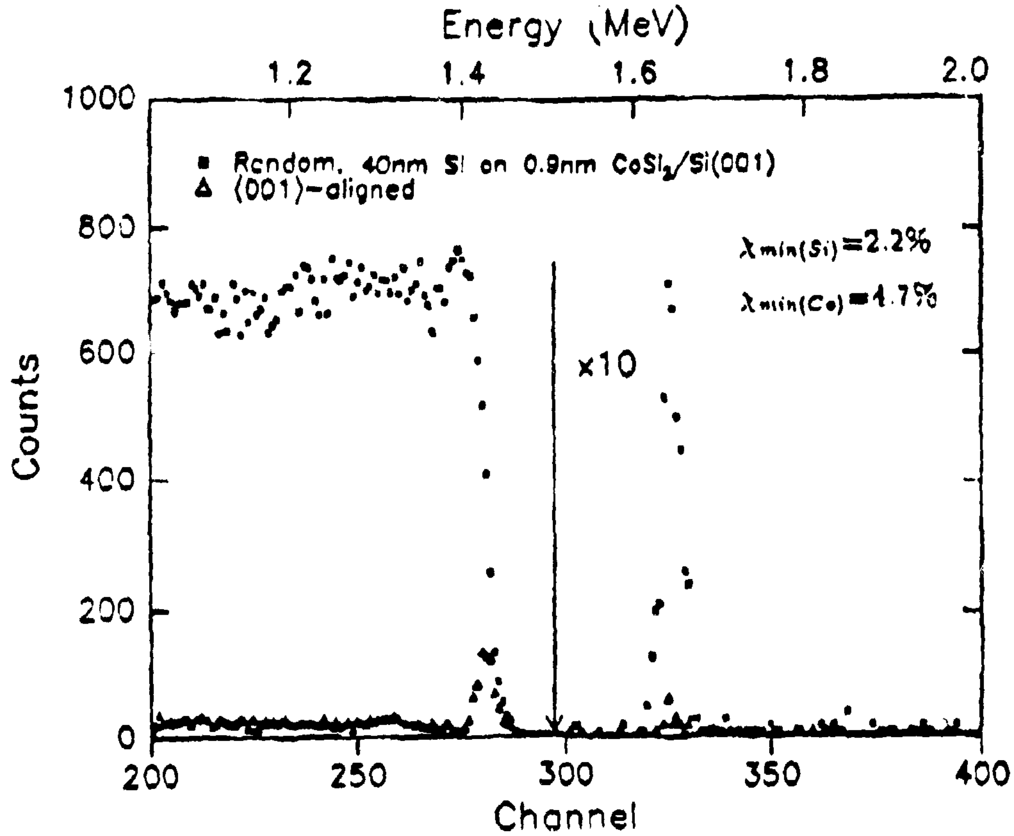


Figure 5. Random and channeling spectra of 40nm Si grown on 0.9nm $CoSi_2$ (grown by template II) with a 2×2 reconstructed surface.

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