

Growth of strained-layer semiconductor-metal-semiconductor heterostructures

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Single crystal epitaxial strained-layer semiconductor-metal-semiconductor heterostructures have been grown for the first time. Silicon layers were grown by molecular beam epitaxy over thin ($< 100 \text{ \AA}$) NiSi_2 layers on $\text{Si}(111)$. The presence of $\sim 20 \text{ \AA}$ Si template layers formed at low temperature ($< 500 \text{ }^\circ\text{C}$) on the silicide was shown to have a dramatic effect on subsequent Si growth. The overgrown Si layers were rotated 180° with respect to the NiSi_2 and had a channeling minimum yield of $\sim 3\%$. Epitaxial strained-layer semiconductor-metal-semiconductor heterostructures represent a new class of material system with potential for high-speed device applications.

Molecular beam epitaxially (MBE) grown silicon-silicide heterostructures represent a new materials system which is important for technological as well as fundamental physical reasons. For example, it has been shown that single crystal, epitaxial, NiSi_2 metal grows in one of two orientations on $\text{Si}(111)$ substrates giving rise to two different Schottky barrier heights (SBH).¹ This observation has important consequences for theories of SBH formation. Silicon-silicide heterostructures also show promise for future devices. Recently, attempts have been made to fabricate transistors from epitaxial $\text{Si-CoSi}_2\text{-Si}$ heterostructures in which the CoSi_2 forms the transistor base.² However, the observed transistor action arises from electron transport through "pinholes" in the silicide layer³ and, as such, classifies the device as a permeable base transistor (PBT). Unlike CoSi_2 , thin films of NiSi_2 can be grown essentially pinhole-free on Si and, because of a better lattice match to Si, NiSi_2 can be grown pseudomorphically and, hence, is a potentially better choice as a buried metal layer. An exciting prospect is the use of pinhole-free $\text{Si/NiSi}_2\text{/Si}$ structures to fabricate a high-speed metal base transistor (MBT) in which the electrons transit the base ballistically. In this letter we show for the first time how to solve the problems associated with the MBE growth of such structures. We report new techniques which have enabled us to fabricate near-perfect $\text{Si-NiSi}_2\text{-Si}$ heteroepitaxial structures on $\text{Si}(111)$. Results of growth on $\text{Si}(100)$ are also presented.

Earlier attempts to grow $\text{Si-NiSi}_2\text{-Si}$ structures⁴ have been hampered by the instability of NiSi_2 which tends to diffuse to the surface as Si is deposited. For thick NiSi_2 layers ($\sim 1000 \text{ \AA}$) with misfit dislocations at the interface, this problem seemed to be averted⁵ although the quality of the Si overlayers and the stability of the interfaces were not carefully studied. For high-speed device applications such as the MBT, a metal thickness of less than $\sim 100 \text{ \AA}$ is desirable. The growth of uniform, strained heterostructures of such thin layers represents an entirely new and more difficult task.

The formation of a thin epitaxial layer at a low temperature before subsequent epitaxial growth at a higher temperature is known in a few cases to improve the uniformity and crystallinity of the epitaxially grown films. This improvement was first demonstrated in NiSi_2 growth over Si where it was also discovered that the orientation can be controlled by

the thickness of such a template.⁶ Epitaxial growth of Ge and Si films on fluorides has also been achieved with template layers.⁷ In this letter we show that Si epitaxy on thin ($\leq 100 \text{ \AA}$) NiSi_2 layers is greatly improved by proper choice of a Si template resulting in near-perfect epitaxial $\text{Si-NiSi}_2\text{-Si}$ structures.

Silicon substrates were degreased and chemically cleaned before a final oxide layer was grown on the surface.⁸ Substrates were then introduced into a ultrahigh vacuum (UHV) chamber with a base pressure of $\sim 1 \times 10^{-10}$ Torr. After a brief anneal at $800\text{--}850 \text{ }^\circ\text{C}$ removed the oxide from the surface, no impurities were detected by Auger electron spectroscopy (AES). Sharp 7×7 and 2×1 patterns were observed by low-energy electron-diffraction (LEED) for (111) and (100), respectively. Nickel or silicon was electron beam evaporated from separate crucibles at rates of $\sim 0.4\text{--}2 \text{ \AA/s}$. During evaporation, the pressure in the chamber remained below 4×10^{-10} Torr.

Thin ($< 70 \text{ \AA}$) and uniform NiSi_2 layers were grown on $\text{Si}(111)$ by deposition of $\sim 18\text{--}20 \text{ \AA}$ Ni at room temperature for the type A orientation and deposition of 18 and 50 \AA Si for the type B orientation.⁶ A short anneal at $\sim 500 \text{ }^\circ\text{C}$ allowed the epitaxial silicide layers to form. The orientation of the silicide was determined by LEED.⁶ For thicker NiSi_2 layers, nickel was deposited on the NiSi_2 surface at $\sim 600 \text{ }^\circ\text{C}$ until the desired silicide thickness was reached. A thin ($\leq 50 \text{ \AA}$) Si layer was then deposited at room temperature and

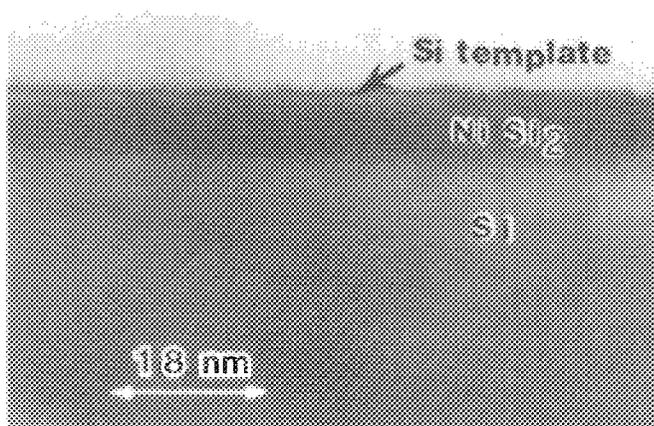


FIG. 1. Cross-section TEM picture of a NiSi_2 layer on $\text{Si}(111)$ on which a thin (20 \AA) Si template layer has been grown at $\sim 480 \text{ }^\circ\text{C}$.

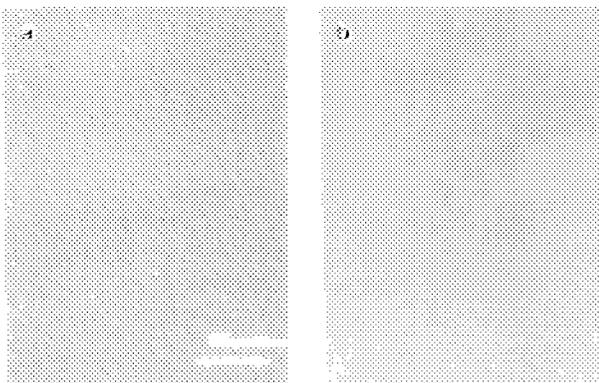


FIG. 2. Nomarski micrographs of the surface of heteroepitaxial Si(111)-65 Å NiSi₂-1500 Å Si structures grown at 520 °C: (a) no Si template was used, and (b) a 20 Å Si template was grown before the Si MBE growth.

annealed at 400–500 °C for a short period of time. The Ni to Si ratio of AES remained unchanged before and after the anneal, indicating little diffusion had taken place. The LEED pattern changed to a 7×7 with the integer order beams carrying much more intensity than the reconstructed beams. For Si thickness of ~15–30 Å, the integer spots showed strong 3-fold symmetry; the pattern, however, was similar to the original NiSi₂ pattern with a 180° rotation. Because a shift in intensity between (1,0) and (0,1) type beams usually comes from a change in the position of the second atomic layer relative to the surface Si layer, the obser-

vation of a rotated pattern suggests that the Si layer was rotated by 180° with respect to the NiSi₂. The morphology of the Si template layer, as revealed by transmission electron microscopy, is shown in Fig. 1. Although the Si layer is somewhat rough, it appears to cover the majority of the NiSi₂ surface.

The thin Si template layers had a very dramatic effect on subsequent Si growth. Deposition of 1000–3000 Å Si at 520–570 °C on NiSi₂ without the use of a Si template resulted in an uneven surface (see Fig. 2) on which Ni was detected by AES. Rutherford backscattering showed that the NiSi₂ layer had become discontinuous and broadened to the surface. However, with the proper choice of Si template, the surface was smooth and impurity-free under the same Si growth conditions. RBS and channeling spectra of typical heterostructures grown with the use of a Si template are shown in Fig. 3. The buried NiSi₂ layers remained uniform. A χ_{min} of ~3% was measured for the Si overlayers, indicating near-perfect crystallinity for the epitaxial structure. Channeling along the inclined <110> and <114> axes showed the top Si layer occupied the same orientation as the original Si template, namely, rotated 180° with respect to NiSi₂. Considerable dechanneling in NiSi₂ indicated that these layers were strained. Taking advantage of the NiSi₂ template technique,⁶ we have been able to grow strained epitaxial Si_{sub}-NiSi₂-Si_{over} structures with A/B/A and A/A/B orientations.

Figure 4 shows cross-section TEM images of (a) AAB

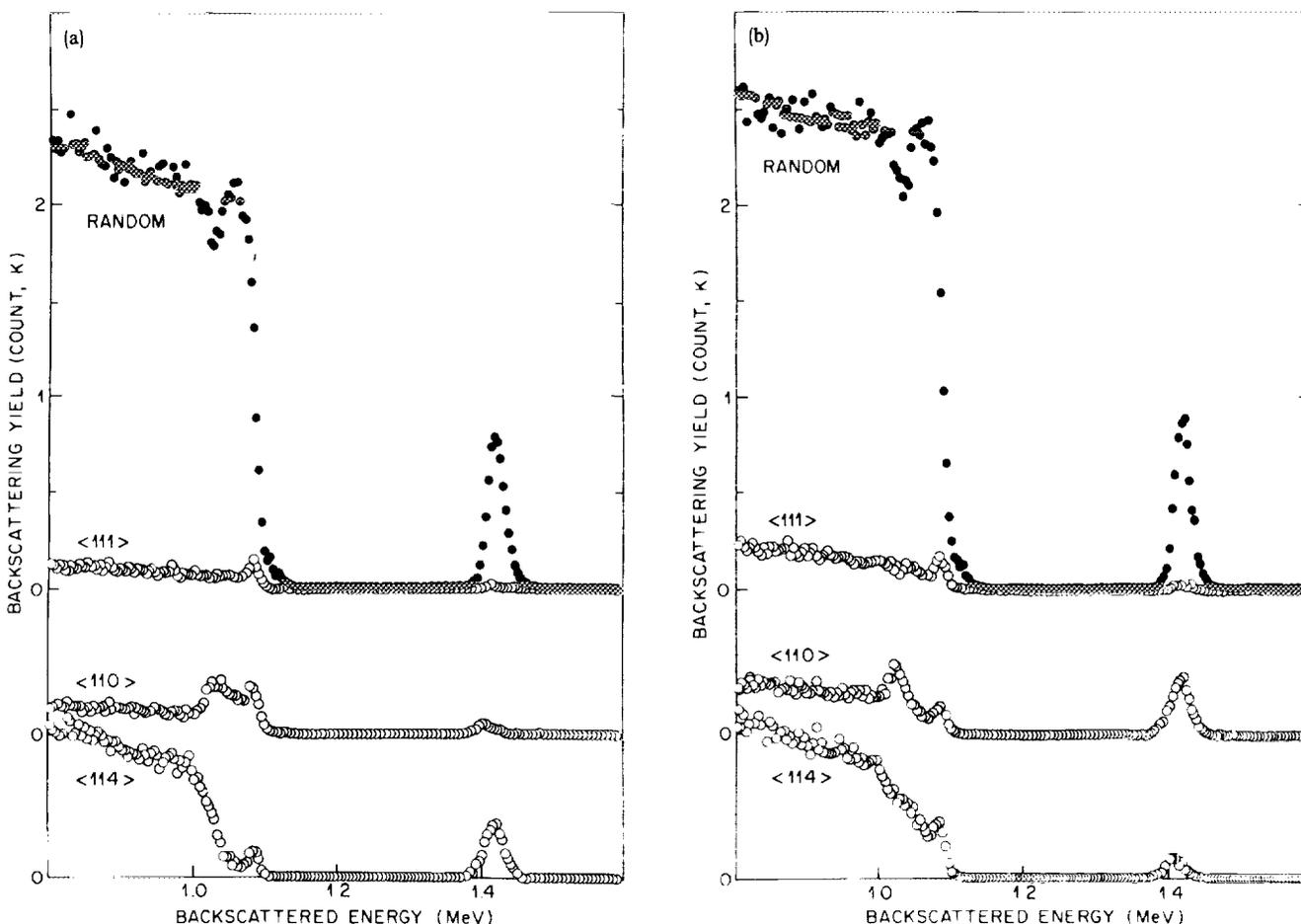


FIG. 3. Channeling and random RBS spectra of epitaxial Si(111)-90 Å NiSi₂-1500 Å Si structures: (a) of the A/A/B orientation and (b) of the A/B/A orientation.

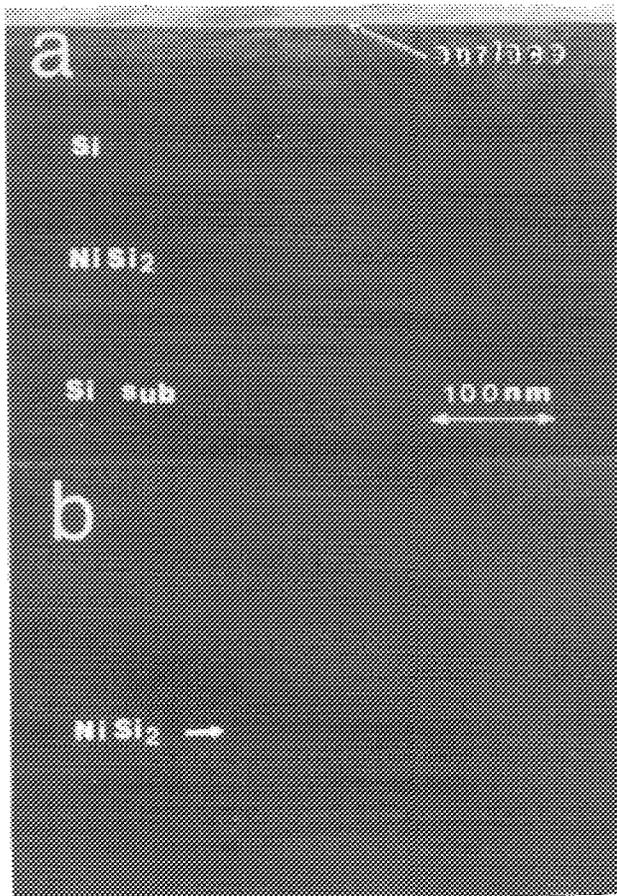


FIG. 4. Cross-section TEM images of NiSi₂ double heteroepitaxial structures on Si(111) of (a) A/A/B and (b) A/B/A orientation.

and (b) ABA Si-NiSi₂-Si heterostructures. These images were taken near the $\langle 112 \rangle$ zone axis in bright field at 200 kV accelerating voltage. NiSi₂ template layers are uniform and pseudomorphic; that is, they are strained so that their in-plane lattice parameters are essentially equal to that of the substrate and overlayer. Thin strained type A NiSi₂ layers are essentially free of misfit dislocations ($< 10^4 \text{ cm}^{-2}$). Some thin type B NiSi₂ layers contain higher densities of dislocations but almost an order of magnitude less than observed in thick ($\sim 1000 \text{ \AA}$) films.⁹ In comparison with CoSi₂ layers,³ pinhole densities are negligible. Furthermore, Si overlayer quality is also better than for Si-CoSi₂-Si heterostructures.

Good quality heterostructures on Si(100) have proved more difficult to fabricate. The MBE growth temperature for Si on NiSi₂(100) is lower than with (111). Using a Si template, good quality Si layers ($\chi_{\text{min}} = 6\%$) can be grown at 400–470 °C. No nickel was found on the surface after Si deposition. RBS and channeling spectra of a Si(100)-NiSi₂-Si epitaxial structure is shown in Fig. 5. However, TEM studies of such samples in cross section revealed that the interface between NiSi₂ and Si overlayer had become faceted along $\langle 111 \rangle$ planes. There were also pinholes in the NiSi₂ layer allowing the Si overlayer to be connected with the substrate Si. However, the likelihood of improving (100) heterostructures by the use of suitable template layers has not been fully explored.

In summary, we have demonstrated for the first time the growth of single crystal Si over thin ($\leq 100 \text{ \AA}$) strained

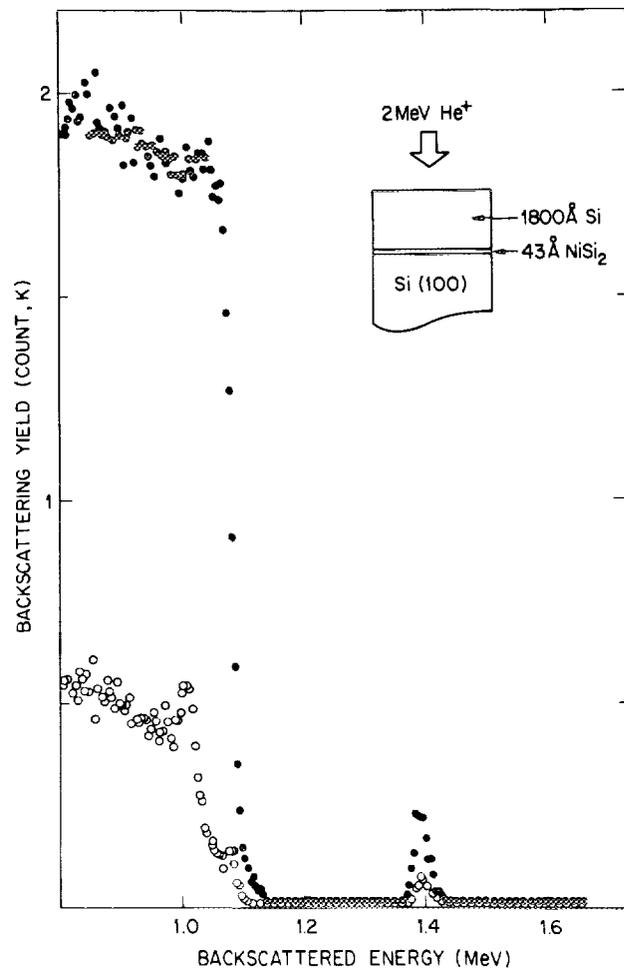


FIG. 5. Channeling and random RBS spectra of a Si(100)-40 Å NiSi₂-1500 Å Si structure.

NiSi₂ layers on Si. The formation of Si template layers on NiSi₂ was instrumental in obtaining uniform and high quality Si overlayers through subsequent MBE growth. The Si overlayers occupied a 180° rotated orientation with respect to the NiSi₂(111) layers. Channeling and TEM observations indicated the near perfection and the strained nature of the epitaxial structure. The silicon-silicide-silicon strained-layer heterostructure was shown to be uniform and continuous. The striking perfection of these metal-semiconductor heterostructures allows us to envision fabricating devices with novel electrical and optical properties previously unattainable with conventional semiconductor superlattices.

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