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STM studies of silicon growth on rare earth silicide surfaces

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Introduction

Epitaxial films of rare earth (RE) silicides grown on silicon surfaces have been the subject of a number of studies in recent years.[1] This has been motivated in part by the good lattice match of the silicide to the Si(111) surface and the useful electrical and electronic properties of these silicides (e.g. unusually low Schottky barriers[2,3] with *n*-type Si). In the low-coverage regime, a scanning tunnelling microscopy (STM) study of the growth of Ho on Si(111) has been previously reported.[4]

At a metal coverage of 1 ML a two-dimensional (2D) silicide may be grown[5] on Si(111) in which a single monolayer of RE is located sub-surface beneath a buckled surface Si bilayer, as seen in Fig. 1(a). This surface Si layer resembles one of the Si bilayers that form bulk Si, and it shows a 1×1 reconstruction. Upon exposure to atomic hydrogen, the 2D RE silicide surface is modified such that the buckling direction of the surface Si bilayer is changed[6] as seen in Fig. 1(b).

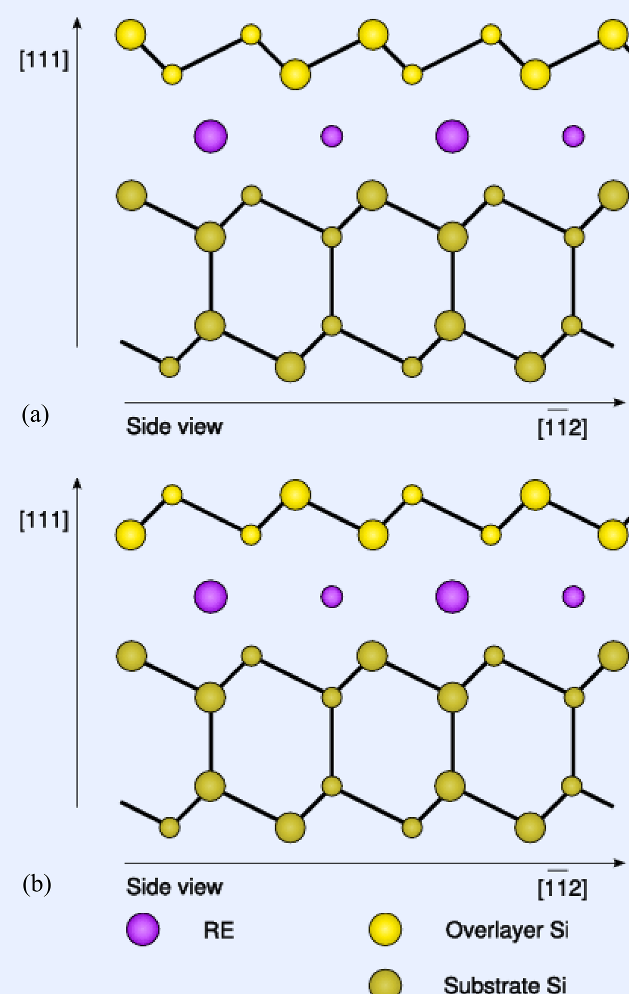


Fig. 1. Schematic of the 2D rare earth silicide (a) before and (b) after hydrogen termination.

The silicon-like exposed surface of the 2D RE silicides opens up the possibility of growing further layers of Si on top so as to form a buried Si layer in a silicon/silicide/silicon structure. In this work we present STM images of Si growth on the 2D Ho silicide surface, and also images from the H-terminated 2D silicide surface both before and after Si growth.

Experiment

Samples were prepared and characterised in-situ in an ultra-high vacuum (UHV) chamber with base pressure < 2×10^{-10} mbar. At various stages during the preparation, surface order was assessed by low-energy electron diffraction. STM measurements were obtained using an Omicron Nanotechnology GmbH. instrument.

Si growth on 2D holmium silicide

- Effect of Si deposition at room temperature onto the 2D Ho silicide surface shown in Fig. 2.
  - Si clusters of diameter 3 – 8 nm and height 0.5 – 0.8 nm seen.
  - Between clusters, undisrupted Ho silicide film seen.
  - Silicide surface relatively passive; Si diffuses across surface forming clusters which are pinned by defects in film or when they reach critical size.
  - High density of clusters seen near step edges (Fig. 2) or around defects (Fig. 3).
- Post-deposition annealing results in a fairly rough surface (Fig. 4) featuring island growth.
  - Lowest level of Si islands 0.4 – 0.6 nm above the silicide substrate.
  - Again, the undisrupted 2D silicide surface is still visible in gaps in the Si film.
  - Uppermost levels of Si islands can be seen to have formed fragments of 7×7 and 2×1 reconstructions characteristic of Si(111) as seen in Fig. 5.
- Si deposition onto the heated 2D Ho silicide surface held at 400 °C followed by 30 min annealing leads to the surface shown in Fig. 6.
  - Island size much larger due to increased diffusion during early stages of growth.
  - The exposed Ho silicide surface is still visible in-between the Si islands.
  - Lower levels of the Si island show a “1×1”-like reconstruction; higher levels have reconstructed into mixture of 2×1 and DAS structures (Fig. 7).
  - As the coverage is increased to 8 ML, the nature of the growth remains largely unchanged, with an overall increase in island heights commensurate with the higher coverage. The 7×7 and 2×1 reconstructions on top of these islands can still be clearly seen (Fig. 8).

Fig. 2. STM image of surface after deposition of 1 ML Si at room temperature on the 2D silicide surface; no annealing (200 nm × 200 nm).

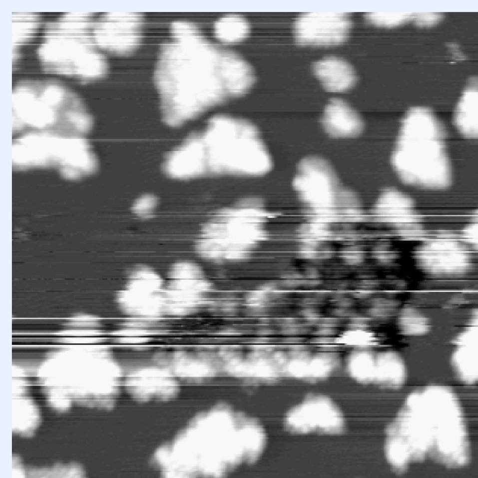


Fig. 3. STM image of surface after deposition of 1 ML Si at room temperature on the 2D silicide surface, showing defect in the silicide film; no annealing (33.5 nm × 33.5 nm).

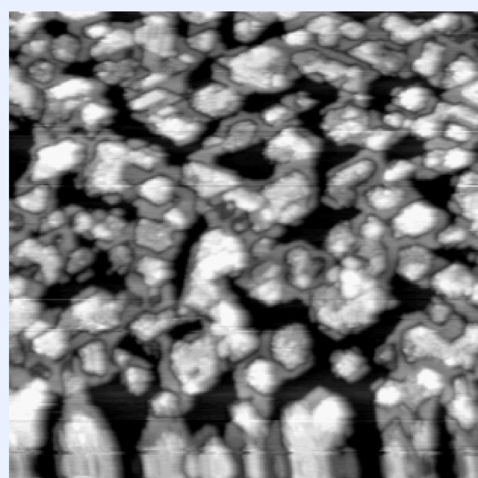


Fig. 4. STM image of the 2D Ho silicide surface after growth of 2 ML Si at room temperature followed by 15 min annealing at 400 °C (100 nm × 100 nm).

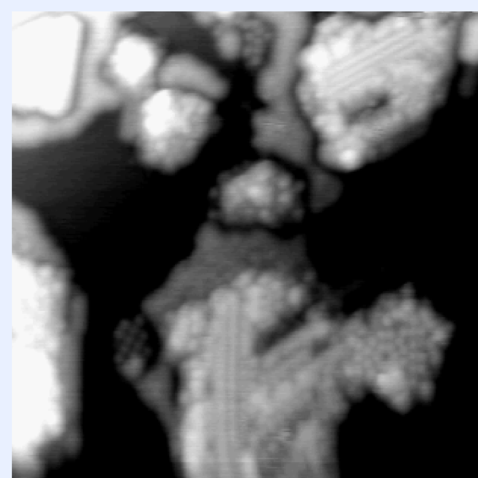
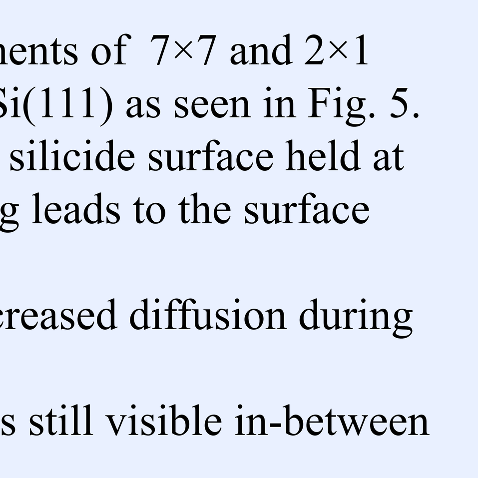


Fig. 5. STM image of the 2D Ho silicide surface after growth of 2 ML Si at room temperature followed by 15 min annealing at 400 °C (30 nm × 30 nm).



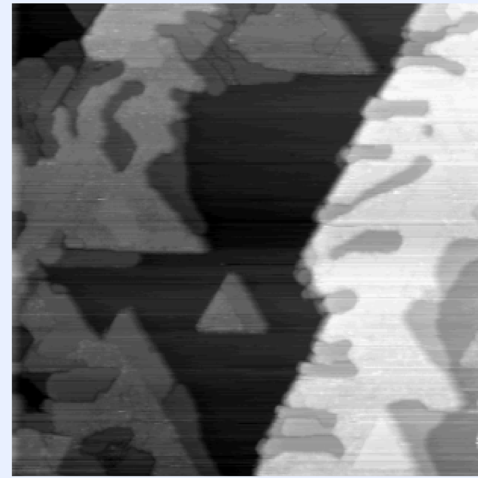
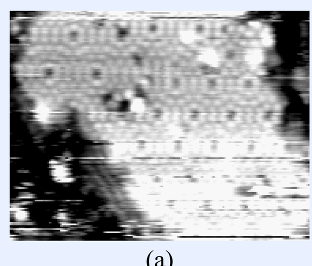


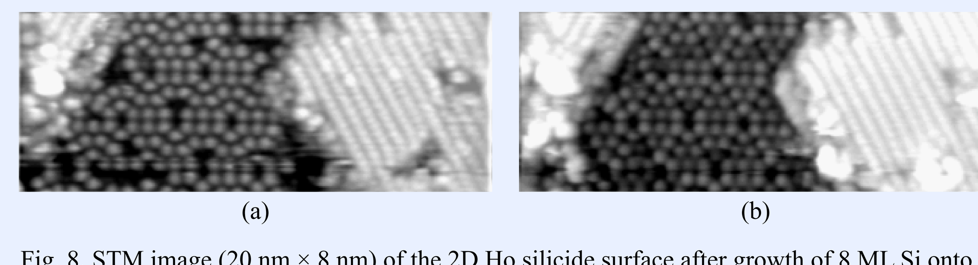
Fig. 6. STM image of the 2D Ho silicide surface after growth of 4 ML Si at room temperature followed by 30 min annealing at 400 °C (200 nm × 200 nm).



(a) (b)

Fig. 7. STM image of the 2D Ho silicide surface after growth of 4 ML Si at room temperature followed by 30 min annealing at 400 °C showing (a) 7×7 reconstruction (19.0 nm × 14.6 nm) and (b) 2×1 reconstruction (15.0 nm × 6.9 nm).

- Growth process illustrated in Fig. 9 where (a) initial Si deposition is followed by (b) 1×1 and (c) 7×7 island formation and (d) 2×1 regions form on cooling.



(a) (b)

Fig. 8. STM image (20 nm × 8 nm) of the 2D Ho silicide surface after growth of 8 ML Si onto the heated surface at 400 °C followed by 30 min anneal, showing co-existence of the 7×7 and 2×1. (a) Empty and (b) filled states.

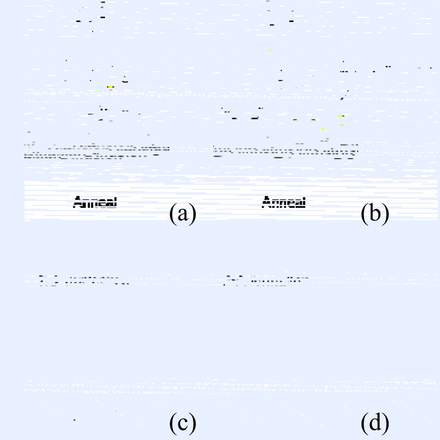
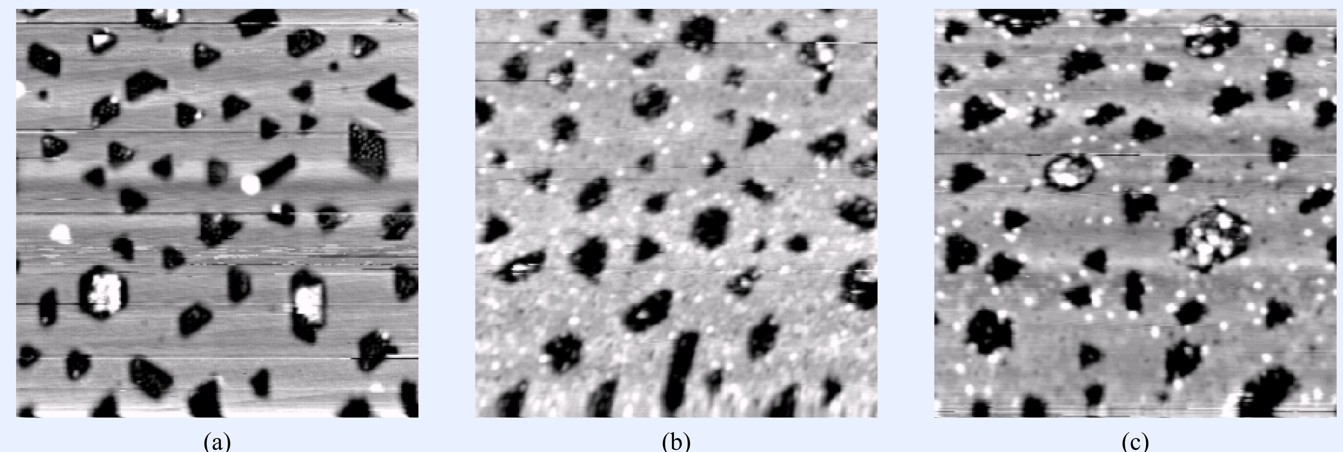


Fig. 9. Proposed model for the growth of Si on 2D holmium silicide.

H-terminated 2D holmium silicide

- Hydrogen termination achieved by exposing 2D silicide to atomic hydrogen.
- Atomic hydrogen produced by admitting H_2 gas to the UHV chamber and cracking it on white-hot W filaments; dose controlled by varying exposure time — effect of changing dose seen in Fig. 10.
- After a 10 min H exposure, the 2D Ho silicide surface is seen to roughen; further H exposure yields a smoother surface. This can be understood as partial hydrogenation of the surface resulting in a surface composed of a mixture of B-type and A-type structures [Fig. 1(a) and (b) respectively]. Such mixtures have been reported previously for the Ge(111)1×1-Dy-H surface[7] but these STM data indicate a unexpectedly small domain size.



(a) (b) (c)

Fig. 10. STM image (50 nm × 50 nm) of the 2D Ho silicide surface prepared by room temperature deposition of Ho followed by annealing to 400 °C. (a) Before H exposure, (b) after 10 min H exposure and (c) after 20 min H exposure.

Si growth on the H-terminated 2D silicide

- The greater degree of passivation of the top-most Si dangling bond after H-termination of the 2D Ho silicide is expected to result in a surface which is even less reactive.
- Growth of Si on the H-terminated 2D silicide surface can be seen in Fig. 11. Overall, order seems better with the edges of Si islands following 6-fold directions of the substrate rather than being ragged as found on the non-hydrogenated surface. This is in constrast to the effect of H on Si homoepitaxy where the presence of H results in poorer growth.
- The exposed 2D silicide surface in-between the Si islands once again appears smooth [in comparison to Fig. 10(c)] suggesting that the H has desorbed during the post-annealing step to leave the plain 2D silicide surface. Thus the presence of H is believed to play a role in influencing the growth process.
- In the filled-states image of Fig. 12 the presence of adatoms atop the Si islands can be seen.
- The higher resolution image of the Si island surface in Fig. 13 shows a 1×1 termination. This suggests that growth of Si on the H-terminated 2D Ho silicide surface may proceed by substitution of the top-most H atom by Si, with the displaced H atom subsequently available to saturate the exposed dangling bonds of the growing Si layer.

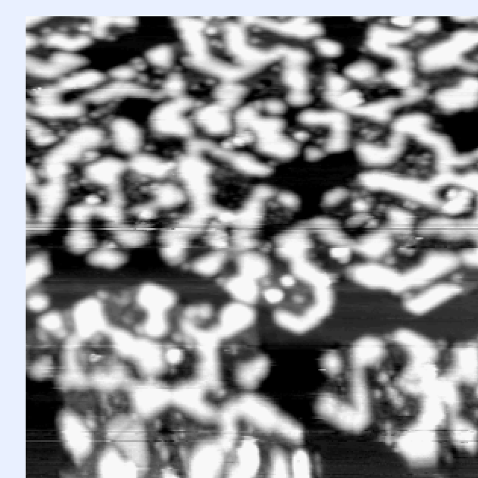


Fig. 11. STM image of surface after growth of 1 ML Si at room temperature on the H-terminated 2D silicide surface; 15 min post-annealing at 400 °C (44 nm × 44 nm).

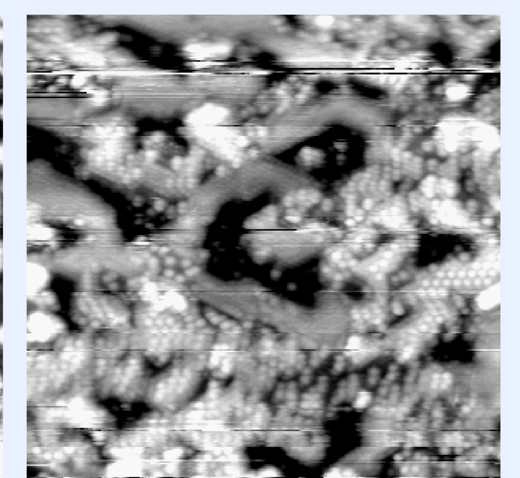


Fig. 12. Filled states STM image of surface after growth of 1.3 ML Si at room temperature on the H-terminated 2D silicide; 15 min anneal at 400 °C (35.0 nm × 35.0 nm).

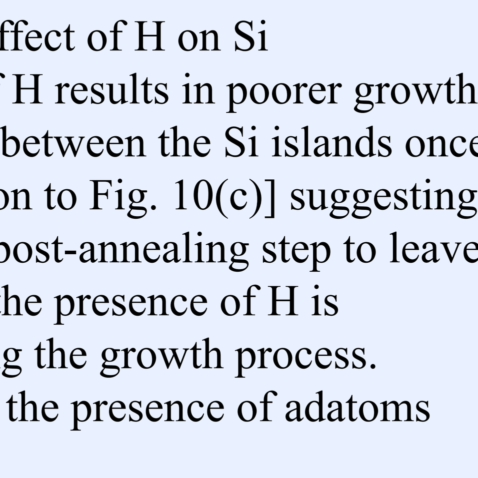


Fig. 13. STM image of surface after growth of 1.5 ML Si at room temperature on the H-terminated 2D silicide surface; 15 min post-annealing at 400 °C (7.8 nm × 7.8 nm).

Conclusions

The growth of Si on the 2D Ho silicide surface has been investigated by STM. Island growth has been observed with the overlays eventually forming 2×1 and 7×7 reconstructions as they become thicker. Si growth on the H-terminated surface is strikingly different with a tendency for more ordered growth with less islanding; further work is however needed to establish whether H remains in the resulting surface.

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References

[1] F. P. Netzer, J. Phys.: Condens. Matter 7, 991-1022 (1995).
[2] K. N. Tu, R. D. Thompson and B. Y. Tsaur, Appl. Phys. Lett. 38(8), 626-628 (1981).
[3] H. Norde, J. de Sousa Pires, F. d'Heurle, F. Pesavento, S. Petersson and P. A. Tove, Appl. Phys. Lett. 38(11), 865-867 (1981).
[4] E. W. Perkins, I. M. Scott and S. P. Tear, Surf. Sci. 578(1-3), 80-87 (2005).
[5] C. Bonet, I. M. Scott, D. J. Spence, T. J. Wood, T. C. Q. Noakes, P. Bailey and S. P. Tear, Phys. Rev. B 72, 165407 (2005) and references therein.
[6] P. Wetzel, C. Pirri and G. Gewinner, Europhys. Lett. 38(5), 359-364 (1997).
[7] D. J. Spence, T. C. Q. Noakes, P. Bailey and S. P. Tear, Phys. Rev. B 62(8), 5016-5020 (2000).

Further details of the work described in this poster may be found in E. W. Perkins, C. Bonet and S. P. Tear, Phys. Rev. B 72, 195406 (2005).

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