Patterned Atomic Layer Epitaxy of Si / Si(001):H

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The growth of few-monolayer (ML) structures of epitaxial Si within an atomic-scale pattern on the technologically relevant Si(001) substrate is a critical step towards the development of Atomically Precise Manufacturing (APM) technology. We utilise Scanning Tunnelling Microscopy (STM lithography)[1] to pattern a hydrogen-passivated substrate, and then deposit disilane to perform gas-source Atomic Layer Epitaxy (ALE) of silicon. While, these are both well-known processes, their combination raises new challenges, particularly in the area of substrate temperature.

Epitaxial growth requires that the temperature is high enough for the deposited atoms to diffuse and form well-ordered layers. Any disorder in the islands of one layer will adversely affect the growth of islands on the second layer, leading eventually to rough, amorphous growth. Furthermore, during Chemical Vapour Deposition (CVD), high temperatures are typically used to thermally desorb H. However, in patterned epitaxy, the temperature must be kept low enough so that diffusion or desorption of H does not destroy the pattern and passivating H layer. Yet there is still the need for high rates of diffusion of Si, so as to form well-ordered layers. We have therefore identified the critical step for success as the growth of the second ML, i.e. the first to be grown on top of epitaxial islands instead of the clean substrate.

Additional challenges lie in the patterning process. STM lithography becomes more difficult at higher temperatures, with the depassivation yield dropping, and the rate of sample drift increasing. Furthermore, as the disilane adsorption is self-limiting, saturating the patterned area with at best 0.5 ML of Si per cycle, the patterning process must be performed multiple times, each with atomically precise registration.

We present results from Patterned ALE experiments between 200-300°C and a range of disilane fluxes, which proceed by a series of steps, as shown in Figure 1: drift stabilisation, initial patterning, and then cycles of disilane dosing and depassivation of the disilane fragments to form islands and eventually new layers of silicon. We discuss the effect of substrate temperature and disilane flux on the average island size, and characterise the types of defect found in the first ML of growth, for example APBs between islands or preexisting surface defects. In light of our results, we will discuss the optimisation of this process given the critical step that we have identified, and the ultimate feasibility of this process for APM.

[1] M. A. Walsh and M. C. Hersam. Atomic-scale templates patterned by ultrahigh vacuum scanning tunneling microscopy on silicon. *Annu. Rev. Phys. Chem.*, **60,** 193–216 (2009).

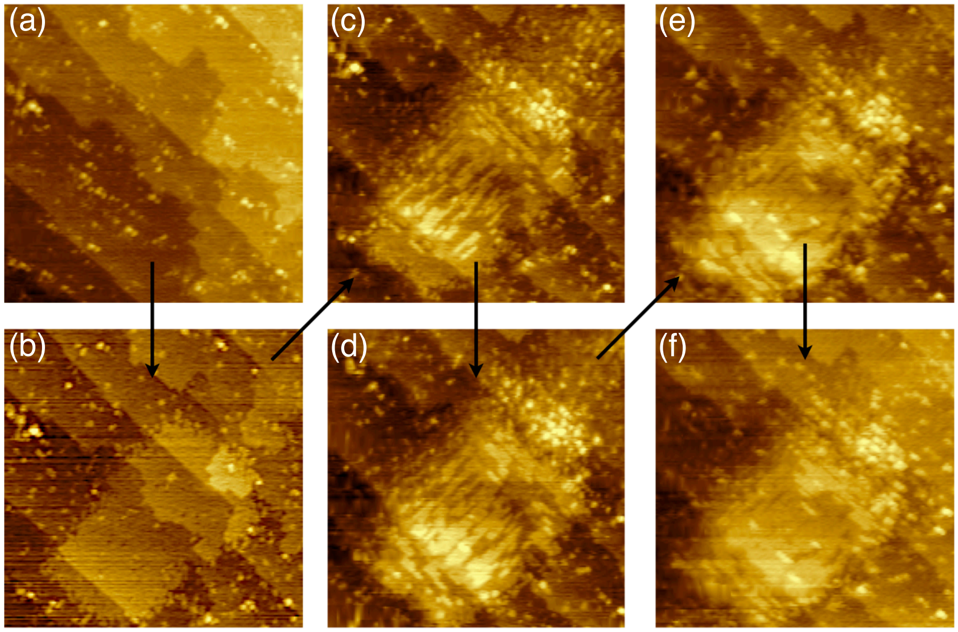

Fig.1 : A sequence of six STM images,showing growth of a single ML of Si by Patterned ALE at 290°C. A disilane dose of 3 x 10^{-6} mbar for 10s is used. Three cycles of disilane deposition and depassivation are required to form a single ML of silicon. (a, b): The clean surface before and after initial patterning. (c,d,e) The surface after growth cycles 1,2,3 respectively.) (f): Some rearrangement has taken place during an anneal of the surface in (e).