The Condensed Matter Theory / Computational Materials Science Seminar $CMT/CMS\ seminar$

Date & Time:Mar 4th (Mon.) 1:30 pm - 2:30 pmPlace:6F seminar room, Sengen main bldg.Speaker:Dr. J. H. G. Owen (Zyvex Labs)

Patterned Epitaxy of Si and Ge on Si(001) using disilane and digermane

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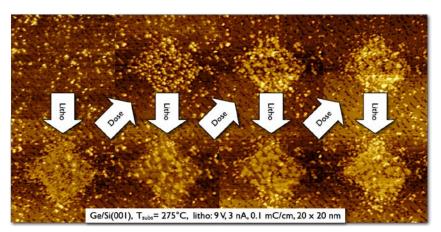
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Working towards our goal of Atomically Precise Manufacturing, we are developing the ability to build nanostructures deterministically on the Si(001) surface by repeated cycling of STM H depassivation in a local patch of the surface, and disilane (and digermane) adsorption into the exposed area.

We have investigated disilane and digermane decomposition pathways using a combination of STM, FT-IR, and DFT modelling. We have identified a pathway which begins with adsorption as Si_2H_5 and H, and continues through an on-row ad-dimer structure. This ad-dimer also provides a low-barrier desorption pathway for surface H, allowing H to desorb from the disilane fragments at lower temperatures than is possible on the flat surface. GGA finds barriers substantially lower than experiment, but the more accurate HSE06 functional gives values for the desorption barriers which are closer to the experimental values.

In the process of low-temperature Patterned Epitaxy, the STM tip is used to remove H from the adsorbed disilane fragments, and enable epitaxial growth within a small defined area. Using this technique, we are able to grow Si layer by layer, depositing about 1/3 ML of Si per cycle. The quality

of the epitaxy is found to be very sensitive not only to the total electron dose, but also to the energy of the electrons used in the STM lithography. This process raises some interesting questions which will be discussed.



Patterned Epitaxial Growth of Ge on Si(001) at 250°C. Contact: MIYAZAKI.Tsuyoshi@nims.go.jp - 理論計算科学ユニット (ext. 2624)