

1D nanolines and single atom chains on Si(001)

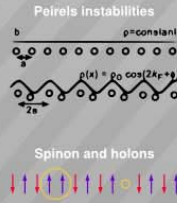
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UCL and LCN, London

Motivations

Why 1D chains on Si(001)?

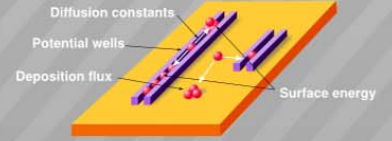
- Explore 1D experimentally
- Probe the Tomonaga-Luttinger liquid theory
- More versatile than systems on vicinal surfaces
- Implement the infinite length limit condition addressed by theory
- Interconnects for novel electronics



Nanolines templating

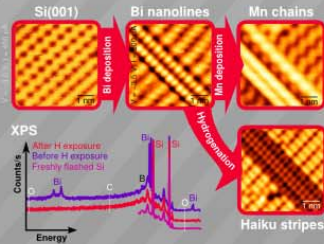
Possible metallic chains on Si(001) and Bi-nanolines:

- Au, Ag atomic chains
J. Phys. Cond. Mat. 19, 226219 (2007)
Mater. Sci. and Eng. 140, 180 (2007)
- Fe interstitial atomic chains
Appl. Phys. Lett. 86, 09315 (2005)
Appl. Surf. Sci. 254, 99 (2007)
- Nearly Mn atomic chains
Surf. Sci. 602, 598 (2008)



Synthesis

- Bi nanolines grow on Si(001) at 570 °C
- Mn chains form between Bi nanolines
- Haiku stripes form by exposing Bi nanolines to hydrogen:
 - Bi dimers are stripped by H, exact mechanism not yet understood
 - No trace of contaminations after hydrogenation in XPS



Properties & Interests

- Straight, no kinks
- Nearly defect free
- Tunable line density
- Length limited by defects and terraces
- Si dimers
- Self-assembled
- No vicinal surface
- Independent of step edges
- Gapped substrate
- Industrially relevant surface

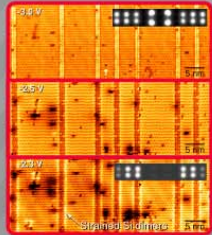


Bismuth nanolines

J. Owen, et al. *J. Mater. Sci.* 41, 4568 (2006)

Haiku structure

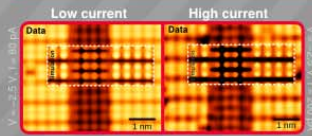
- 4 Si dimers wide, 1.54 nm
- Double chain of Bi dimers
- Si reconstruction (Haiku structure) below the Bi nanolines
- Composed of 5- and 7-fold rings of Si extending 5 layers below the surface
- Bias dependant contrast in filled state reproduced by STM simulation



Haiku stripes

F. Bianco, *Phys. Rev. B*, 84, 035328 (2011)

Filled state



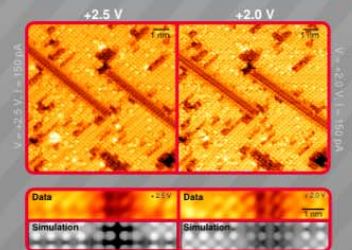
- Very good matching between STM simulation (integrated DFT) and experimental data
- Electronic effects: both central atoms are raised at high current

Model

Hydrogen covered Haiku structure, no Bi

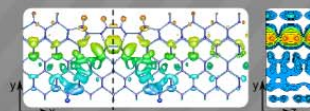


Empty state



- 1D delocalized state close to the Si band gap
- Purely electronic effect
- Run along the nanolines
- Does not correspond to any atom position in the structure

Charge densities simulations



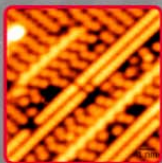
- Reproduce the 1D central state...
- ... and predict it as delocalized along the nanoline

Perfect 1D electronic model system?

Manganese chains

S. A. Köster, in prep. (2012)

Mn chains near Bi nanolines

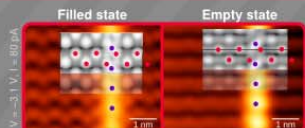
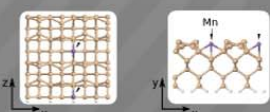


- Up to 40 atoms chains (self-assembled)
- Unusual zig-zag chain structure
- Structure still under investigation together with DFT modelling
- Bi nanolines promote growth of long Mn chains



Proposed model

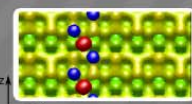
- C-type chains
- Mn between Si dimers in first layer



- Fairly good matching between STM simulation (integrated DFT) and experimental data

Spin densities simulations

- Interesting magnetic structure predicted by spin polarized DFT



Sena, Bowler, *J. Phys.: Cond. Mat.* 23 (2011) 305003
Liu et al. *Surf. Sci.* 602 (2008) 988

Perfect 1D spin chain model system?

Interests for 1D

Haiku stripes

- Stable up to 400 °C in UHV
- Inert in air
- Stable in real life's lab!



- Huge aspect ratio (length/width) achievable
- Promising 1D templates for atom chain assembly
- Mn chains are good candidate for 1D spin system
- Look for metallic properties...
- ... and contacting for transport measurements
- Optical measurements

Outlook