Ground state of Si(111)-(4x1)/(8x2)-In nanowires from mid-infrared response

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In/Si(111)-(4×1) surface: RT Structure

- Strong interest in quasi-1D structures: Fascinating physical properties & large technological potential
- Highly anisotropic surface superstructures such as the In/Si(111)-(4×1) surface are suitable model systems
- By now exp. & theor. establ. struct. model for room temp. phase

In/Si(111)-(4×1) surface: LT Structure

- Reversible $(4\times1)\rightarrow(8\times2)$ phase transition @ 120K
- Seen in STM images, sharp conductance drop in transport measurements, peak splitting in reflectance anisotropy meas.
- Interpretation of STM images in terms of structure difficult

(2) T. Uchihashi, et al., APL 80, 22 (2002)
(3) Fleischer et al., PRB 67 235318 (2003)
**In/Si(111)-(4×1) surface: LT Structure II**

- LT structure unclear, *trimer & hexagon models* suggested
- Density functional theory (DFT) calculations problematic, ground state depends on approximation

⇒ try optical spectroscopy

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(4) A. A. Stekolnikov et al., *PRL* **98** 026105 (2007)
(5) C. Gonzalez et al., *PRL* **96** 136101(2006)
Reflectance anisotropy spectroscopy (RAS)

- **Experiment:** Strong peak around 2 eV
  - Splits upon \((4\times1)\rightarrow(8\times2)\) phase transition

- **Theory:** Splitting observed for both trimer & hexagon model
  \[ \Rightarrow \text{Usual RAS spectral region not helpful in this case} \]

\[
\frac{\Delta R(\omega)}{R_0(\omega)} = \frac{16\pi d \omega}{c} \Im \left[ \frac{\alpha_{xx}(\omega) - \alpha_{yy}(\omega)}{\epsilon_b(\omega) - 1} \right]
\]

(3) Fleischer et al., PRB 67 235318 (2003)

Recent RAS Results

- New experiment measures RAS in mid-infrared regime

⇒ Look at calculated RAS data again
Recent RAS Results

- New experiment measures RAS in mid-infrared regime
- *Ab initio* calculation for RT phase reproduces experiment well, if *intraband* contributions are accounted for
Recent RAS Results

- Anisotropic Drude-tail is replaced by 2 strong peaks after cooling
Recent RAS Results

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- Trimer model does not match experiment
Recent RAS Results

- Anisotropic Drude-tail is replaced by 2 strong peaks after cooling
- Trimer model does not match experiment
- Hexagon model exhibits experimentally observed peaks!
- Strong evidence for hexagon formation
(8x2) hexagon: RAS Transitions I

- Anisotropic transitions responsible for peaks originate from close to XM high symmetry line
- High joint density of states due to nearly parallel val/cond. bands
- Also some transitions from inside of the Brillouin zone
Ground state of Si(111)-\(\text{(4x1)(8x2)}\)-In nanowires from mid-infrared response

\((8x2)\) hexagon: RAS Transitions II

\[ \text{Energy [eV]} \]
Ground state of Si(111)-(4x1)(8x2)-In nanowires from mid-infrared response

(8x2) hexagon: RAS Transitions II
(8x2) hexagon: RAS Transitions II

Ground state of Si(111)-(4x1)(8x2)-In nanowires from mid-infrared response
Summary & Conclusion

- Measured RAS shows 2 low energy anisotropic peaks for low temperature phase

- *Ab initio* calculations reproduce peaks for hexagon model, but not for the trimer model

- These results provide strong evidence for the hexagon model
Structure of Si(111)-In Nanowires Determined from the Midinfrared Optical Response

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(Received 3 March 2009; published 5 June 2009)

Thank you for your attention!

Questions?