The interface structure of few layer epitaxial graphene grown on 4H_SiC(0001)

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Why graphene?

Why graphene?

MOORE’S LAW

YEAR

TRANSISTORS

YEARS


1,000 10,000 100,000 1,000,000 10,000,000 100,000,000 1,000,000,000

8080 8086 8088 4004

Intel® Pentium® II Processor
Intel® Pentium® Processor
Intel486™ Processor
Intel® Pentium® IV Processor
Intel® Pentium® III Processor
Intel® Pentium® II Processor
Intel® Pentium® Processor
Intel® Itanium® Processor
Intel® Itanium® Processor
Dual-Core Intel® Itanium® Processor
Intel® Pentium® Processor
Intel® 8088 Processor
Why graphene?

- Is a single layer of graphite
- Electrical properties as good as Carbon Nano Tubes and is without the helicity problem
- Flat graphene sheets have zero energy gap so a viable candidate for post CMOS electronics
- Demonstrates 2D properties
Single layer graphene

- Ballistic transport ⇒ highest mobilities ever observed
  
  \[
  \text{GRAPHENE: 250,000 cm}^2/\text{V}\cdot\text{s}, \ \text{Si: 1360 cm}^2/\text{V}\cdot\text{s}
  \]

- Micron scale electron coherence lengths

- Essentially no electron-phonon coupling

**ITRS 2007 “emerging research devices”**
Graphene in GaTech..

- Grown by UHV method
- Si Face - slow growth, 1-5 layers thick, periodicity is $6\sqrt{3} \times 6 \sqrt{3}$
- Electron mobility and coherence length are a magnitude smaller than C face graphene
- Using furnace C Face – fast growth, more than 5 layers of thickness, has high concentration of nanocaps and defects
Research Goal

- To study the structure of interface graphene layer grown on SiC
- Learn about the charge transfer between substrate and the graphene film
- My role is to see whether small changes in the parameters of the model will provide a better fit for the reflectivity data
X ray diffraction

- Crystallography software used to model diffraction patterns based on assumed structure
- Model compared to experiment to characterize the interface structure
Surface X-ray Diffraction

X-ray reflectivity measures vertical density gradients
FIG. 1: A schematic model of multi-layer graphene grown on the 4H-SiC(0001) substrate. Dashed lines are the bulk SiC lattice planes before interface relaxation (¢'s). The 5th plane of atoms (adatom) is displaced \( d_{ad} \) from the topmost atom plane in the interface. \( (\ddagger) \) are carbon atoms and \( (\pm) \) are silicon atoms. The shaded circles in the interface ("layer-0") can be either carbon or silicon atoms. The graphene layers above the interface layer are referred to as "layer-1", -2, -3,
Graphene/SiC Interface

F. Varchon, et al., condmat (2008). **Si-face**

Dangling bond states

**Dirac cone**

**Gap**

2.3Å

Si-Face

0.12nm

“buffer layer”

0.17nm

Bulk SiC
Graphene modulation

Si-face

Si-adatom model, \( \sigma_G = 0.16\,\text{Å} \)

4H-SiC (001) rod

\( \sigma_G = 0.16\,\text{Å} \)

\( \sigma_G = 0.00\,\text{Å} \)

C-face

\( \sigma_G = 0.25\,\text{Å} \)

\( \sigma_G = 0.00\,\text{Å} \)

Integrated Intensity (arb. units)

\( l \) (r.l.u.)

\( \sigma_G = 0.16\,\text{Å} \)

\( \sigma_G < 0.05\,\text{Å} \)
Proposed model

FIG. 3: Three graphene/SiC interface ball models for graphene grown on the Si-face of SiC determined by surface x-ray reflectivity; (b) Si-up model, (c) Si-down model and (d) C-adatom model. Open circles are silicon atoms and shaded circles are carbon atoms. The densities $\rho$ are relative to the densities of bulk SiC shown in (a).
My part

- Created an excel file for data and computed all the delta’s
- Modified the C code to accommodate the corrugated graphene layer contribution to the intensity of the scattered electron
- Do various fits on the reflectivity data by changing a few parameters
Fits for Reflectivity data...

Si Face INTFINAL

Integrated intensity (arb. units)

\(1.0 \times 10^{-2} \) \(1.0 \times 10^{0} \) \(1.0 \times 10^{2} \) \(1.0 \times 10^{4} \) \(1.0 \times 10^{6} \) \(1.0 \times 10^{8} \) \(1.0 \times 10^{10} \) \(1.0 \times 10^{12} \)

\( l \) (r.l.u.)

- intfinaldat
- ck582_a
- ck582_b
- CK582_c
- CK582_d
Fits for Reflectivity data…
Results

- The purple line is the best fit so far.
- Assuming that there is some corrugation present in graphene layers seems valid.
- The interface is not composed of a simple graphene-like layer above a relaxed SiC bilayer instead, the interface reconstruction is more complicated and extends deeper into the bulk.
Future Research

• Studying the properties of interface layers of C – face graphene grown by UHV method

• Properties of interface layers of furnace grown Si – face
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