Si nanoribbons on Ag(110):
Si-induced substrate reconstruction and optical response.

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Si nanoribbons on Ag(110)

Outline

- Structural investigation of Si growth on Ag(110)
  - Real-time STM during growth at RT
  - X-ray diffraction for Si layer grown at 190 °C

- Surface Differential Reflectance Spectroscopy at 180°C
  - comparison to silicene
  - Analysis of the optical data

- Conclusion
Si nanoribbons on Ag(110)

Complete Self-Assembled Nano-Ribbons (SANR) obtained at 190°C for $0.8 \pm 0.2$ ML of Si

*(checked by Rutherford Back-Scattering in INSP)*


SPA-LEED in INSP:

c(10x2)

$\theta = 0.8$ ML
Si nanoribbons on Ag(110)

Real-time STM during Si deposition at room temperature

Tip retracted by 1 μm for each evaporation for avoiding shade effect

Real-time monitoring of growth by STM + SDRS

Si evaporation

UV-vis light
Real-time monitoring of growth by STM + SDRS
Si nanoribbons on Ag(110): real-time STM

clean Ag(110)  
frizzy step edges

0.1 ML Si  
meandering of the step edges

0.2 ML Si  
serrated step edges

formation of fingers

0.3 ML Si

Room temperature

Bernard, Prévot, Massson, YB et al, PRB 88, 121411(R) (2013)
Si nanoribbons on Ag(110): real-time STM

Room temperature

bare Ag(110) to 0.3 ML Si

234 nm x 234 nm

bare Ag(110) 0.1 ML Si

0.2 ML Si

0.3 ML Si

234 nm x 234 nm

SNR

fingers

elongated island

Bernard, Prévot, Massson, YB et al, PRB 88, 121411(R) (2013)
Si nanoribbons on Ag(110): real-time STM

Room temperature

bare Ag(110) to 0.3 ML Si

234 nm x 234 nm

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Si nanoribbons on Ag(110): real-time STM

Room temperature

Bernard, Prévot, Massson, YB et al, PRB 88, 121411(R) (2013)

0.2 ML Si

Ag fingers

0.3 ML Si

Si NR

2ML Ag fingers

75 x 82 nm²

0.145 nm

= 1 single Ag(110) step

Bernard, Prévot, Massson, YB et al, PRB 88, 121411(R) (2013)
For 2 Si atoms arriving on the surface, 1 Ag atom is released from the substrate and moves to a step edge or to a new island.

Extrapolation to high temperature:

4 Ag atoms per 5x2 cell
(10 Ag atoms and 8 Si atoms)

Bernard, Prévot, Massson, YB et al, PRB 88, 121411(R) (2013)
Higher temperature:

- STM not possible because of the fast motion of steps
- use of X-ray diffraction
Si nanoribbons on Ag(110): X-ray diffraction

T=190°C

nominal surface

\[ \vec{Q}_i \quad \vec{Q} \quad \vec{Q}_d \]

GIXD (ID3 Beam line in ESRF)

Bragg spot

diffraction rods with 1/5 order

Crystal Truncation Rod

Bernard, Prévot, Massson, YB et al, PRB 88, 121411(R) (2013)
Si nanoribbons on Ag(110): X-ray diffraction

$T=190^\circ C$

$\theta_{Si} = 0.8 \text{ ML}$

substrate anti-Bragg reflection

superstructure reflection

Bragg spot

diffraction rods with 1/5 order

Crystal Truncation Rod

Bernard, Prévot, Massson, YB et al, PRB 88, 121411(R) (2013)
Si nanoribbons on Ag(110): X-ray diffraction

**T = 190°C**

- **Bragg spot**
- **Crystal Truncation Rod**
- **Bragg spot**
- **diffraction rods with 1/5 order**

Structure factor:

\[
F(\mathbf{q}) = A_o \left| A_{Ag}(\mathbf{q}) + A_{Si}(\mathbf{q}) \right| = A_o \sum_{Ag} f_{Ag}(q)e^{i\mathbf{q}.\mathbf{r}_n - \alpha z_n} + \sum_{Si} f_{Si}(q)e^{i\mathbf{q}.\mathbf{r}_n}
\]

Bernard, Prévot, Massson, YB et al, PRB 88, 121411(R) (2013)
Si nanoribbons on Ag(110): X-ray diffraction

$T=190^\circ C$

**Structure factor**

Bare Ag surface: $F(1,0,0) = f_{Ag} \left( \frac{1}{2} - \theta_{Ag} \right)$

![Graph showing structure factor](image)

Structure factor:

$$F(\vec{q}) = A_o \left| A_{Ag}(\vec{q}) + A_{Si}(\vec{q}) \right| = A_o \sum_{Ag} f_{Ag}(q)e^{i\vec{q} \cdot \vec{r}_n - \alpha z_n} + \sum_{Si} f_{Si}(q)e^{i\vec{q} \cdot \vec{r}_n}$$

Bernard, Prévot, Massson, YB et al, PRB 88, 121411(R) (2013)
Intermediate conclusion

The Ag(110) substrate is 2x1 missing-row reconstructed below the Si NRs

- two Ag atom rows out of five are removed on the complete SANR structure
- the released Ag atoms diffuse toward edge steps and form fingers or new Ag islands
Si nanoribbons on Ag(110)

When Epioptics-13 meets Silicene-1

How can silicene can be identified? Optical response!

Surface Differential Reflectance Spectroscopy at 180°C

- comparison to silicene
- Analysis of the optical data
Si nanoribbons on Ag(110): Optical properties

Dirac cone

Optical absorption in $\pi\alpha$ ($=0.023$) unit

$\pi\alpha = 0.023$
Optical absorption in $\pi\alpha$ ($=0.023$) unit

$\pi\alpha = 0.023$
Graphene: Optical properties


Fine Structure Constant Defines Visual Transparency of Graphene

R. R. Nair, P. Blake, A. N. Grigorenko, K. S. Novoselov, T. J. Booth, T. Stauber, N. M. R. Peres, A. K. Geim

There are few phenomena in condensed matter physics that are defined only by the fundamental constants and do not depend on material parameters. Examples are the resistivity quantum, $\hbar/e^2$, that appears in a variety of transport experiments, including the quantum Hall effect and universal conductance fluctuations, and the magnetic flux quantum, $\hbar/2e$, playing an important role in the physics of superconductivity ($\hbar$ is Planck's constant and $e$ the electron charge).

By and large, it requires sophisticated facilities and special measurement conditions to observe any of these phenomena. In contrast, we show that the opacity of suspended graphene ($I$) is defined solely by the fine structure constant, $\alpha = \frac{e^2}{\hbar c} = 1/137$ (where $c$ is the speed of light), the parameter that describes coupling between light and relativistic electrons and that is traditionally associated with quantum electrodynamics rather than materials science. Despite being only one atom thick, graphene is found to absorb a significant ($\alpha \approx 2.3\%$) fraction of incident white light, a consequence of graphene's unique electronic structure.

We have studied specially prepared graphene crystals ($\mathcal{G}$) such that they covered submillimeter apertures in a metal scaffold (Fig. 1A inset). Such large one-atom-thick membranes suitable for use on graphene become strongly warped and nonlinear and the approximation of Dirac fermions breaks down. However, our calculations (5) show that finite-$\mathcal{G}$ corrections are surprisingly small (a few %) even for visible light. Because of these corrections, a metrological accuracy for $\alpha$ would be difficult to achieve, but it is remarkable that the fine structure constant can so directly be assessed practically by the naked eye.

References and Notes

Fig. 1. Looking through one-atom-thick crystals. (A) Photograph of a 50-μm aperture partially covered by graphene and its bilayer. The line scan profile shows the intensity of transmitted white light along the yellow line. (Inset) Our sample design: A 20-μm-thick metal support structure has several apertures of 20, 30, and 50 μm in diameter with graphene crystallites placed over them. (B) Transmittance spectrum of single-layer graphene (open circles). Slightly lower transmittance for $\lambda < 500$ nm is probably due to hydrocarbon contamination. The red line is the transmittance $T = (1 + 0.5\alpha)^{-2}$ expected for two-dimensional Dirac fermions, whereas the green curve takes into account a nonlinearity and triangular warping of graphene’s electronic spectrum. The gray area indicates the standard error for our measurements (5). Inset) Transmittance of white light as a function of the number of graphene layers (squares). The dashed lines correspond to an intensity reduction by $\alpha x$ with each added layer.
**SDRS for a monolayer of graphene on SiO$_2$**

![Graph showing SDRS for graphene on SiO$_2$](image)

**Mak, Shak, Heinz, PRL 2008**

**FIG. 1** (color online). Experimental data for the reflection from a graphene monolayer on the SiO$_2$ substrate for photon energies in the range of 0.5–1.2 eV. The curves associated with the left vertical axis are the measured reflection spectra of the substrate alone (lower curve) and of the graphene monolayer on the substrate (upper curve). The curve associated with the right vertical axis represents the fractional change in reflectance from the graphene monolayer.

\[
\frac{R_{g+s} - R_s}{R_s} = \frac{4}{n_s^2 - 1} A,
\]
Graphene: Optical properties

SDRS for a monolayer of graphene on $\text{SiO}_2$

\[ \frac{R_{g+s} - R_s}{R_s} = \frac{4}{n_s^2 - 1} A, \]

FIG. 1 (color online). Experimental optical conductivity (solid line) and the universal optical conductivity (dashed line) of monolayer graphene in the spectral range of 0.2–5.5 eV. The experimental peak energy is 4.62 eV. Note the deviation of the optical conductivity from the universal value at low energies is attributed to spontaneous doping [16].

*Mak, Shak, Heinz, PRL 2011*
Si nanoribbons on Ag(110): Optical properties

Absorption

\[ \pi \alpha = 0.023 \]

Reflectance

after Matthes, Pulci, Bechstedt (2013)
Si nanoribbons on Ag(110): SDRS

In the infrared, change in reflectance is smaller than 0.002: difficult to measure and doesn't differentiate clearly from other layer.

Absorption

$$\pi\alpha = 0.023$$

$\frac{\Delta R}{R}$

after Matthes, Pulci, Bechstedt (2013)
Si nanoribbons on Ag(110): SDRS

Borensztein, Prevot, Masson, PRB 89, 245410 (2014)
Si nanoribbons on Ag(110): SDRS

Real time SDR evolution

SDRS exp. results at 180°C

full coverage of evaporated Si

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Si nanoribbons on Ag(110): SDRS

Full coverage of evaporated Si

Cristalline silicon

Real time SDR evolution

Borensztein, Prevot, Masson, PRB 89, 245410 (2014)
Si nanoribbons on Ag(110): SDRS

Real time SDR evolution

SDRS exp. results at 180°C

Borensztein, Prevot, Masson, PRB 89, 245410 (2014)
Effect of Ag(110) reconstruction?

\[
\frac{\Delta R}{R} = 8\pi \frac{\lambda}{\Delta \varepsilon_{xx}(\omega)} \Im \left\{ \frac{\Delta \varepsilon_{xx}(\omega)}{\varepsilon_{\text{sub}}(\omega) - 1} \right\}
\]

1. modification of the Drude parameters in the Ag surface region

\[
\varepsilon_{\text{Ag}}(\omega) = \varepsilon_{\text{i.b.}} + 1 - \frac{\Omega_p^2}{\omega(\omega + i\tau^{-1})}
\]

\[\hbar \Omega_p = 9.2 \text{ eV} \quad \hbar \tau^{-1} = 0.021 \text{ eV}\]

1: \[\hbar \tau^{-1} = 0.21 \text{ eV}\]

2: \[\hbar \Omega_p = 10.2 \text{ eV}\]

3: \[\hbar \Omega_p = 8.2 \text{ eV}\]
Effect of Ag(110) reconstruction?

\[ \frac{\Delta R}{R} = 8 \pi \frac{\Delta \varepsilon_{xx}(\omega)}{\lambda} \text{Im} \left\{ \frac{\Delta \varepsilon_{xx}(\omega)}{\varepsilon_{\text{sub}}(\omega) - 1} \right\} \]

1. modification of the Drude parameters in the Ag surface region

\[ \varepsilon_{\text{Ag}}(\omega) = \varepsilon_{i.b.} + 1 - \frac{\Omega_p^2}{\omega(\omega + i\tau^{-1})} \]

\[ \hbar \Omega_p = 9.2 \text{ eV} \quad \hbar \tau^{-1} = 0.021 \text{ eV} \]

2. Ag surface region = grating Ag / vacuum

\[ (1-f) \text{ Ag f.a} \]

\[ t = 0.4 \text{ nm} \]

\[ \varepsilon_{\parallel} = f \varepsilon_{\text{Ag}} + (1-f) \]

4: \[ \varepsilon_{\perp}^{-1} = f \varepsilon_{\text{Ag}}^{-1} + (1-f) \]
Si nanoribbons on Ag(110): SDRS

Calculation with Lorentzian dielectric functions: \( \varepsilon_L(\omega) = 1 - \frac{F_0^2}{\omega^2 - \omega_o^2 + i \omega \tau^{-1}} \)

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<th>( \omega_o )</th>
<th>( \tau^{-1} )</th>
<th>( F_0 )</th>
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<td>3.0 eV</td>
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<td>Si NR ⊥</td>
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Borensztein, Prevot, Masson, PRB 89, 245410 (2014)
Conclusion

1. Strong interaction between Ag and Si (RT and 190°C)

2. Si coverage at completion = 0.8 ± 0.2ML (appears to be not compatible with silicene)

3. 2x1 missing-row reconstruction beneath the Si SANR layer

4. The optical response of the Si layer is different from the one expected from silicene weakly interacting with the substrate

5. If silicene, it seems to lose its optical response because of the interaction with the substrate (rather sp³ hybridized than sp²)

Consider the Ag reconstruction for future structure calculation

Is the Si layer pure silicon, or some kind of Ag-Si alloy?
Acknowledgements

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