Moiré Patterns in a bilayer: electronic structure

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What is a Moiré pattern?

A beat between periods
Electronic effects in scanning tunneling microscopy: Moiré pattern on a graphite surface

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We observed by scanning tunneling microscopy (STM) a hexagonal superlattice on graphite with a period of 66 Å. Direct measurement of the angle between lattice vectors confirmed that the superlattice is a Moiré pattern caused by a 2.1° rotation of the topmost (0001) plane with respect to the bulk. The STM corrugation of 2.6 Å is not due to physical buckling, but to differences in electronic structure between AA-stacked, normal AB-stacked, and rhombohedral CAB-stacked graphite. The high tunneling current of AA-stacked regions is in agreement with the high density of states at the Fermi level calculated for AA graphite. The Moiré pattern changes, both the amplitude and the shape, with bias voltage. The observation provides a basis for a comparative study of surface electronic structures with different subsurface layer configuration, which is a vital test of our understanding of STM.

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FIG. 2. (a) A closeup view of the superlattice on which graphite atoms are resolved. The image is taken with set current 5.6 nA, tip bias 72 mV, and scan size 202 × 202 Å². The image is low pass filtered. (b) A cross section along the direction indicated by the line in (a).

Rong and Kuiper, PRB 1993
Plan

- Commensurability conditions
- Continuum modeling: quasi-free Dirac fermions
- Calculation of inter-layer hopping
- Electronic structure.
\[ \cos(\theta_i) = \frac{1 + 1/i + 1/(6i^2)}{1 + 1/i + 1/(3i^2)} \] (1)

\[ i = 15 \Rightarrow \theta = 2.13^\circ, \quad L = 66 \text{ Å} \]
Superlattice basis

\[ t_1 = (i + 1)a_1 + ia_2 \]
\[ t_2 = (2i + 1)a_1 - (i + 1)a_2. \]
Continuum modeling

- Single Layer

\[ \mathcal{H}_1 = -t \sum_i a_1^\dagger (r_i) [b_1 (r_i - s_0) + b_1 (r_i - s_0 + a_1) + b_1 (r_i - s_0 + a_2)] + \hbar c \]

\[
\begin{align*}
  a_1 (r) & \rightarrow v_c^{1/2} \psi_a (r) \exp(iK \cdot r) \\
  b_1 (r) & \rightarrow v_c^{1/2} \psi_b (r) \exp(iK \cdot r)
\end{align*}
\]

\[
\hbar v_F \sum_k \psi_k' \dagger (k) \begin{bmatrix}
  0 & (k_x - i k_y) \\
  (k_x + i k_y) & 0
\end{bmatrix} \psi' (k).
\]
Rotated Layer

\[ H_2 = -t \sum_j b_2^\dagger(r_j) \left[ a_2(r_j + s'_0) + a_2(r_j + s'_0 - a'_1) + a_2(r_j + s'_0 - a'_2) \right] + h.c. \]

\[ a_2(r) \rightarrow v_c^{1/2} \psi_{a'}(r) \exp(iK^\theta \cdot r) \]

\[ b_2(r) \rightarrow v_c^{1/2} \psi_{b'}(r) \exp(iK^\theta \cdot r) \]

\[ \hbar v_F \sum_k \psi'^\dagger(k) \left[ \begin{array}{cc} 0 & e^{i\theta} (k_x - ik_y) \\ e^{-i\theta} (k_x + ik_y) & 0 \end{array} \right] \psi'(k). \]
For each site in unrotated layer (layer 1) there is at most one site in the rotated layer (2) for which there is significant hopping:

\[ r'(r) = r + \delta(r) \quad \text{(in-plane positions)} \]

\[ t_\perp \rightarrow t_\perp^{\alpha\beta} [\delta^{\alpha\beta}(r)] \equiv t_\perp^{\alpha\beta}(r) \quad \alpha(\beta) = A, B(A', B') \]

\[ \mathcal{H}_\perp^{(K)} = \sum_{\alpha,\beta} \sum_k \sum_G \tilde{t}_\perp^{\alpha\beta}(G) \psi_\alpha, k+\Delta K/2 + G \psi_\beta', k-\Delta K/2 \quad (\Delta K = K^\theta - K) \]

\[ \tilde{t}_\perp^{\alpha\beta}(G) = \frac{1}{V_c} \int_{uc} d^2 r \, t_\perp^{\alpha\beta}(r) e^{iK^\theta \cdot \delta_{AB}(r)} e^{-iG \cdot r} \]
Choose \( \mathbf{k} \) origin at mid-point between Dirac points of the two layers.

\[
\begin{align*}
\phi_{\alpha,k} &= \psi_{\alpha,k+\Delta K/2} \quad \text{in layer 1}; \\
\phi_{\alpha',k} &= \psi_{\alpha',k-\Delta K/2} \quad \text{in layer 2};
\end{align*}
\]

\[
\mathcal{H} = \hbar \sum_k \phi_{\alpha,k}^\dagger \mathbf{v}_F \tau \cdot \left(\mathbf{k} + \frac{\Delta K}{2}\right) \phi_{\beta,k} \\
+ \hbar \sum_k \phi_{\alpha',k}^\dagger \mathbf{v}_F \tau^\theta \cdot \left(\mathbf{k} - \frac{\Delta K}{2}\right) \phi_{\beta',k} \\
+ \sum_{\alpha,\beta} \sum_{\mathbf{k},\mathbf{G}} \tilde{t}_{\perp}^{\alpha\beta} (\mathbf{G}) \phi_{\alpha,k\mathbf{G}}^\dagger \phi_{\beta',k\mathbf{G}}.
\]
Calculation of $t_{\perp}(r)$

- $V_{pp\sigma}(r)$ and $V_{pp\pi}(r)$ can be estimated from values of $t \approx 2.78 \text{ eV}$, $t' \approx -0.12 \text{ eV}$ and $t_{\perp} \approx 0.27 \text{ eV}$. 

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Calculation of $\delta^{\alpha\beta}(r)$
Values in eV. Absolute values, for $G \neq 0$.

- **Exact symmetries** relate $\delta^{AB} \leftrightarrow \delta^{BA}$ and $\delta^{AA}, \delta^{AA} \leftrightarrow \delta^{BB}$.
Keeping $\tilde{t}_{\alpha\beta}^{\perp}(G = 0)$

- New energy scale: $\hbar v_F \Delta K \approx 370 \text{meV}$

$$H(q) = \hbar v_F |\Delta K| \begin{pmatrix}
0 & q^* - \frac{1}{2} & Q_\perp & Q_\perp \\
q - \frac{1}{2} & 0 & Q_\perp & Q_\perp \\
Q_\perp & Q_\perp & 0 & e^{i\theta} (q^* + \frac{1}{2}) \\
Q_\perp & Q_\perp & e^{-i\theta} (q + \frac{1}{2}) & 0
\end{pmatrix}$$
Summary

- Full geometrical description of rotated layers (commensurability)
- Workable continuum description for slightly rotated layers: “quasi-free” Dirac electrons
- Preliminary results on electronic structure.