Modeling dislocations and grain boundaries in graphene

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Graphene
Outstanding properties of graphene

Thinnest imaginable material (first 2D material ever made)
Largest surface area (~1,400 m² per gram)
Strongest material ‘ever measured’ (theoretical limit)
Stiffest known material (stiffer than diamond)
Most stretchable crystal (up to 20% elastically)
Record thermal conductivity (outperforming diamond)
Highest current density at room T (1,000s times of Cu)
Highest intrinsic mobility (100 times more than in Si)
Conducts electricity in the limit of no electrons
Lightest charge carriers (zero rest mass)
Longest mean free path at room T (micron range)
And if we look more carefully?

Point defects

Edges

Meyer et al., 2008

Girit et al., Nature 2009
... and also topological defects

Heckl& Binnig 1992

Simonis et al., 2002

Coraux et al., 2008

Cervenka et al., 2009

Hashimoto et al., 2004

Huang et al., 2010
Basic definitions

\[ \vec{b} \quad \text{Burgers vector} \]

In 2D only edge dislocations \((\vec{b} \perp \vec{\xi})\) are possible

\[ \theta = \theta_1 + \theta_2 \quad \text{misorientation angle; } \]
\[ \psi = |\theta_1 - \theta_2| \quad \text{tilt angle} \]

In 2D only tilt grain boundaries are possible. More specifically, in graphene
\[ \theta \in [0, 60^\circ], \psi \in [0, \theta] \]
Non-locality of topological disorder

Dislocations vs. point defects
Disclinations in graphene

positive disclination $s = 60^\circ$

ideal graphene

negative disclination $s = -60^\circ$

Seung & Nelson, 1988
Dislocations in graphene

(1,0) dislocation
$|\vec{b}| = \sqrt{3}d_{cc} = 2.46\,\text{Å}$

(1,1) dislocation
$|\vec{b}| = 3d_{cc} = 4.23\,\text{Å}$

(1,0)+(0,1) dislocation
$|\vec{b}| = 3d_{cc} = 4.23\,\text{Å}$

Large-angle symmetric grain boundaries in graphene

Frank’s equations:

GB’s along armchair direction:

\[ \theta = 2 \arcsin \frac{|\mathbf{b}_{(1,0)}|}{2d_{(1,0)}} \]

\[ 0^\circ < \theta < 21.7^\circ \]

GB’s along zigzag direction:

\[ \theta = 60^\circ - 2 \arcsin \frac{|\mathbf{b}_{(1,1)}|}{2d_{(1,1)}} \]

\[ 21.7^\circ < \theta < 60^\circ \]

Experimental image of a large-angle GB

Huang et al., 2010
Computational methodology

\[ d_y \text{ – translational vector on graphene lattice} \]

DFT-GGA calculations (SIESTA)
**Grain boundary energetics (flat regime)**

Flat regime (bulk-like):
Read-Shockley equation

\[
\gamma(\theta) = \frac{\mu |\vec{b}|}{4\pi(1-\nu)} \theta (A - \ln \theta)
\]

\[
A = 1 + \ln\left(\frac{|\vec{b}|}{2\pi r_0}\right) \quad r_0 = 1.2 \, \text{Å}
\]

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**Grain boundary energetics (buckled regime)**

Flat regime (bulk-like):
Read-Shockley equation

\[ \gamma(\theta) = \frac{\mu |\vec{b}|}{4\pi(1-v)} \theta(A - \ln \theta) \]

\[ A = 1 + \ln\left(\frac{|\vec{b}|}{2\pi r_0}\right) \quad r_0 = 1.2 \text{ Å} \]

Buckled regime (membrane):
Finite dislocation energy

\[ \gamma(\theta) = \frac{E_f \theta}{|\vec{b}|} \quad E_f = 7.5 \text{ eV} \]

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Buckled (1,0) dislocation

Theory:

Experiment:

Coraux *et al.*, Nano Lett. 2008
Electronic structure – large-angle GBs

Simulated STM images
(LDOS $E \in [-0.6\text{eV}, 0.6\text{eV}]$)

Electronic structure – small-angle GBs

Electronic transport in polycrystalline graphene

Yazyev & Louie, Nature Mater. 9, 806 (2010)
Zone-folding approach

\[ k_\parallel d = \]

\[
\begin{array}{cccc}
4\pi & 3\pi \\
2\pi & \pi \\
0 & -\pi \\
-2\pi & -3\pi \\
-4\pi & \ldots
\end{array}
\]

\[ n - m = 3q \]

\[ n - m \neq 3q \]

Yazyev & Louie, Nature Mater. 9, 806 (2010)
Two distinct transport behaviors

Class Ia

\[ n_L - m_L = 3q \]
\[ n_R - m_R = 3q' \]

Class Ib

\[ n_L - m_L \neq 3q \]
\[ n_R - m_R \neq 3q' \]

Class II

\[ n_L - m_L = 3q \text{ or } n_L - m_L \neq 3q \]
\[ n_R - m_R = 3q' \]

\[ E_g = \frac{\hbar \nu_F}{3d} \approx \frac{1.38}{d[nm]} \text{ [eV]} \]

Yazyev & Louie, Nature Mater. 9, 806 (2010)
Green’s function approach to transport

\[
T(k_{||}, E) = \text{Tr} \left[ \Gamma_L(k_{||}, E) G_S^\dagger(k_{||}, E) \Gamma_R(k_{||}, E) G_S(k_{||}, E) \right]
\]

\[
G_S(k_{||}, E) = \left[ E^+ I - \mathcal{H}_S - \Sigma_L(k_{||}, E) - \Sigma_R(k_{||}, E) \right]^{-1}
\]

\[
\Gamma_{L(R)}(k_{||}, E) = i \left( \Sigma_{L(R)}(k_{||}, E) - \Sigma_{L(R)}^\dagger(k_{||}, E) \right)
\]

Hamiltonians:

- first-principles (TranSIESTA)
- tight-binding

\[
\mathcal{H} = -t \sum_{\langle i, j \rangle} [c_i^\dagger c_j + \text{h.c.}]
\]

Example of circuit construction:

\[
d_x \perp d_y - \text{both translational vectors on graphene lattice}
\]
Ab initio Green’s function results

Class I

(2, 1)(2, 1)-class Ia

(2, 1)

Class II

(5, 0)(3, 3)-class II

(5, 0)

Yazyev & Louie, Nature Mater. 9, 806 (2010)
Challenges

Graphene is an outstanding electronic material, BUT:

• no intrinsic electronic band gap; difficult to induce one
• Klein tunneling

Katsnelson, Novoselov, Geim, Nature Phys. 2006

леж Диффілт то коントроль транспорт бай тейлоринг електростатычны потэнциал (“традицыйны” праход)
леж Low on/off current ratios of graphene FET (~5)
леж Graphene is not suitable to digital electronics
Practical implications

Controlling transport by means of momentum-mismatch at the grain boundary defects for device applications

\[ |E| < E_g/2 \quad T = 0 \]
\[ |E| > E_g/2 \quad T > 0 \]

Challenges:
- engineering grain boundaries in graphene
- well-ordered grain boundaries are instrumental
  (short-ranged charge impurities are not critical though)

*Yazyev & Louie, Nature Mater. 9, 806 (2010)*
Conclusions

• A systematic approach for constructing dislocations and grain boundaries in graphene

• Low formation energies of topological defects

• 2D nature of graphene plays central role

• Pronounced effects on the electronic structure

• Extraordinary transport behavior with implication for technological applications
Thank you!

Questions?

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