

Properties of Intrinsic Ripples on Suspended/Free-Standing Graphene

Graphene-based Energy Harvesting
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Presenter : Vinit Doke
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Causes of Ripples

- ▶ Mermin-Wagner Theorem
- ▶ Stretching (in-plane displacement) and Bending (out of plane displacement)
- ▶ Dynamic flexing due to acoustic phonons
- ▶ Static Corrugation due to configuration energy
- ▶ Asymmetric Distribution of single/double bonds at room temperature

Causes of Ripples

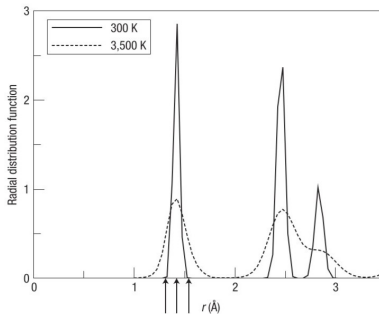


Figure 4 Radial distribution function for the $N = 8,640$ sample at $T = 300 \text{ K}$ and $T = 3,500 \text{ K}$ as a function of interatomic distance. The arrows indicate the length of double ($r = 1.31 \text{ \AA}$), conjugated ($r = 1.42 \text{ \AA}$) and single ($r = 1.54 \text{ \AA}$) bonds.

Simulation

- ▶ *ab-initio* DFT-based simulation was considered prohibitive due to length scale
- ▶ Monte-Carlo based atomistic simulation with LCBOPII Bond-Order Potential

Ripple Properties

- ▶ \vec{u} (in-plane) ; h (out of plane)
- ▶ Case where bending and stretching are decoupled (under Harmonic Approximation) :

$$\langle h^2 \rangle \propto \frac{T}{\kappa} L^2$$

- ▶ κ : Bending Rigidity (1.44 eV)
 T : Temperature
 L : Linear Sample Size
- ▶ Tension dictates Shape and Rate of Curvature Inversion

From the Patent

- ▶ Membrane with supports:
 - ▶ STM Tip forming a Capacitive Region
 - ▶ Voltage Source for a set-point current
- ▶ Graphene Membrane with a Metal contact in the substrate
- ▶ Fixed Charges added to an insulating layer (membrane) and another capacitor plate
- ▶ 1 pW/ripple (*approx* 1000 atoms)

From Other Papers

- ▶ Bending Rigidity (1.44 eV) calculated using DFT and configuration energy of the membrane determined by Helfrich Hamiltonian

$$E = \int_S [\gamma + 2B_M(C_M - C_0/2)^2 + B_G C_G] dS$$

- ▶ γ : Energy of Flat Surface
 B_M : Bending Rigidity
 C_x : Curvature Properties