

Interactions and the minimal conductivity of graphene

Phonon-phonon interactions and the elastic properties of graphene



VietNam 2013

IXth Rencontres du Vietnam
Quy-Nhon
August 4-10, 2013

Nanophysics: from fundamentals to applications (the return)

M. I. Katsnelson

V. Parente

B. Amorim

C. Gomez-Navarro

J. Gomez

G. Lopez-Polin

F. Perez-Murano

also M. M. Fogler,
M. Polini

Outline

- Ballistic graphene
- Tunneling and dissipation
- Phonon-phonon interactions in graphene
- Defects and elastic constants

Graphite. Interactions, transport, and disorder.

A. Castro-Neto (Boston U.)

N. M. R. Peres (U. Minho, Portugal)

E. V. Castro, J. dos Santos (Porto), J. Nilsson (BU), A. Morpurgo (Delft), D. Huertas-Hernando (Trondheim), J. González, F. G., M. P. López-Sancho, T. Stauber, M. A. H. Vozmediano (CSIC, Madrid)

Outline

- The electronic structure of graphite.
- A graphene plane. The Dirac equation.
- The electron-electron interaction.
- Renormalization.
- Related systems and lattice defects.
- Disorder. Localized states.
- Magnetism, cracks and voids.
- Self doping.
- Transport properties. Universal conductance.
- The quantum Hall effect.

Even more interesting references

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Showing results 1 through 25 (of 221 total) for ti:(graphene OR graphite)

1. **cond-mat/0607247** [[abs](#), [ps](#), [pdf](#), [other](#)] :

Title: **Low energy theory of disordered graphene**

Authors: [Alexander Altland](#)

Comments: 4 pages

Subj-class: Mesoscopic Systems and Quantum Hall Effect

80 articles so far in 2006!

Even more interesting references

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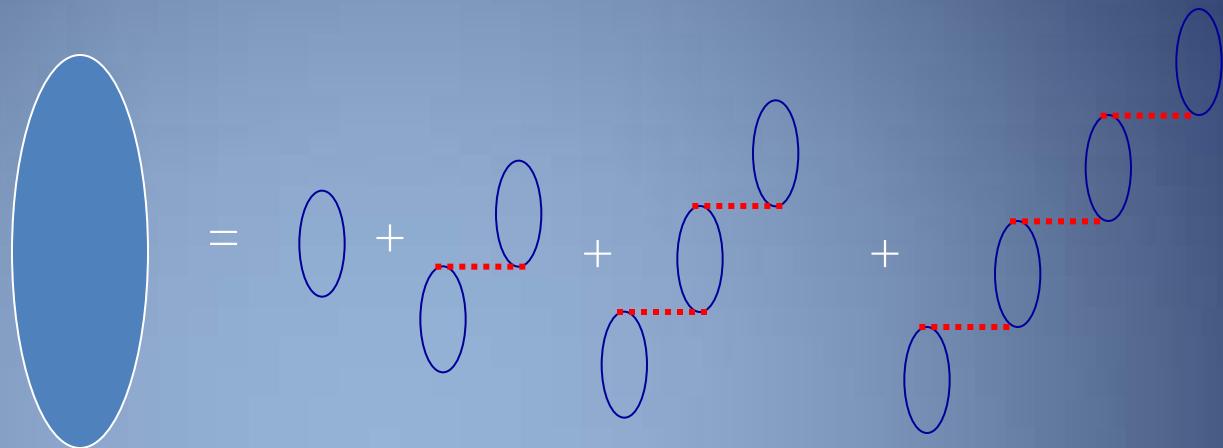
Subj-class: Mesoscopic Systems and Quantum Hall Effect

80 articles so far in 2006!

Renormalization of the Coulomb interaction.

J. González, F. G. and M. A. H. Vozmediano, Phys. Rev. B **59**, R2474 (1999)

RPA summation:



RG flow equation:

(which can be analytically extended to $g > 1$)

$$\Lambda \frac{\partial}{\partial \Lambda} g = \frac{8}{\pi^2} \left(g + \frac{\arccos g}{\sqrt{1 - g^2}} \right) - \frac{4}{\pi}$$

The coupling constant always flows to zero at low energies.

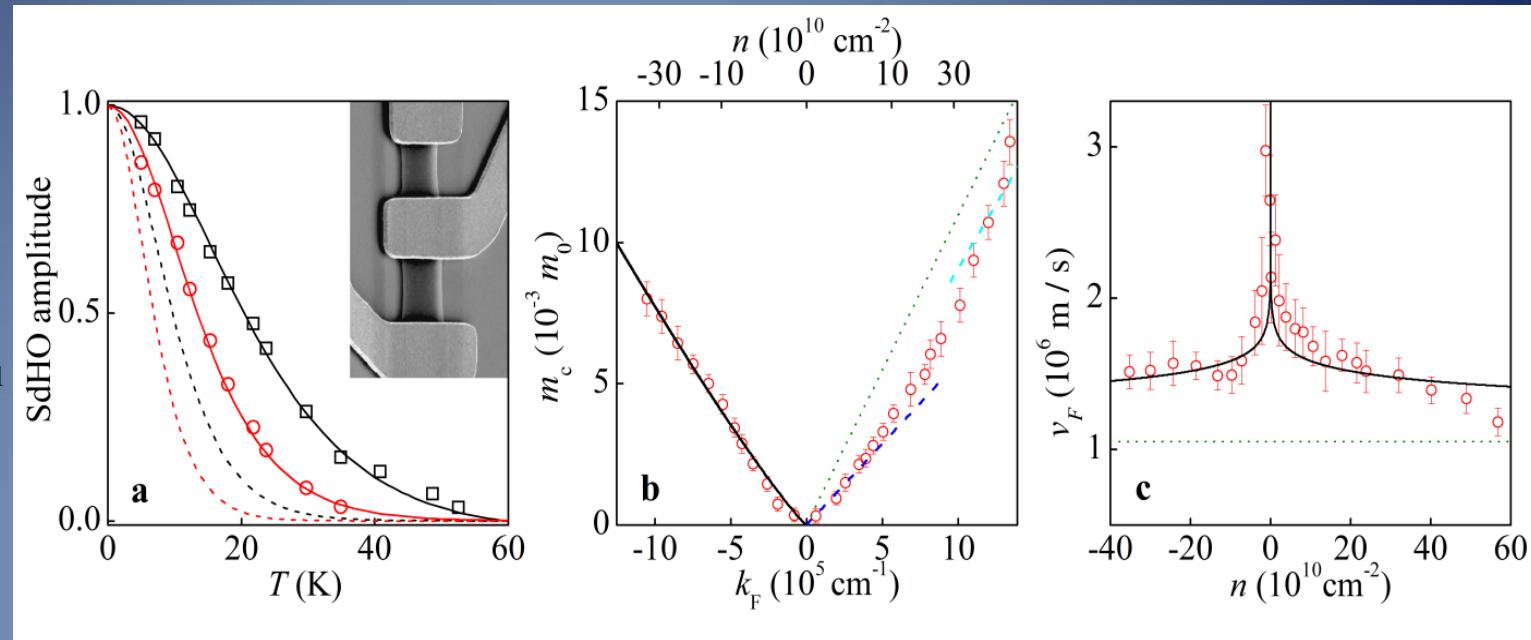
Measurements of the effective mass

Suspended samples.
Very high mobility

$$\mu \approx 10^6 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$$

$$n = 1.4 \times 10^{10} \text{ cm}^{-2}$$

$$n = -7 \times 10^{10} \text{ cm}^{-2}$$

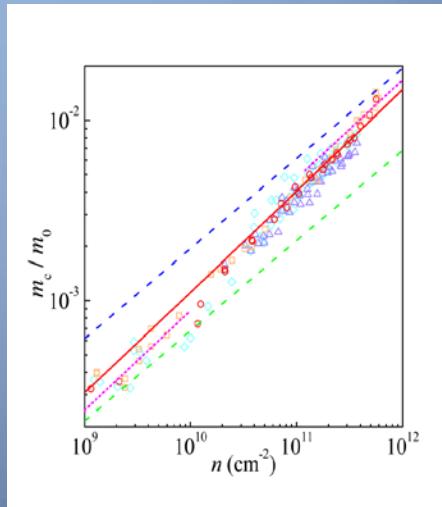


nature
physics

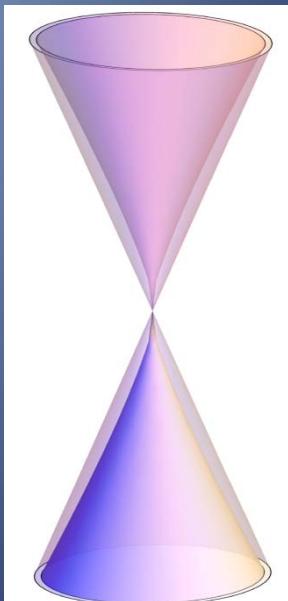
LETTERS
PUBLISHED ONLINE: 24 JULY 2011 | DOI: 10.1038/NPHYS2049

Dirac cones reshaped by interaction effects in suspended graphene

D. C. Elias¹, R. V. Gorbachev¹, A. S. Mayorov¹, S. V. Morozov², A. A. Zhukov³, P. Blake³, L. A. Ponomarenko¹, I. V. Grigorieva¹, K. S. Novoselov¹, F. Guinea^{4*} and A. K. Geim^{1,3}



Fits to Renormalization Group calculations



GRAPHENE'S SUPERLATIVES

- Thinnest imaginable material
- largest surface area ($\sim 2,700 \text{ m}^2$ 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 (106 times of copper)
- completely impermeable (even He atoms cannot squeeze through)
- 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)

Early experiments

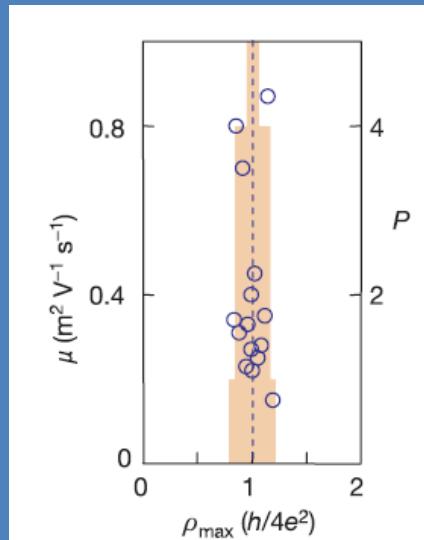
Vol 438 | 10 November 2005 doi:10.1038/nature04233

nature

LETTERS

Two-dimensional gas of massless Dirac fermions in graphene

K. S. Novoselov¹, A. K. Geim¹, S. V. Morozov², D. Jiang¹, M. I. Katsnelson³, I. V. Grigorieva¹, S. V. Dubonos² & A. A. Firsov²



Nature Materials 6, 183 (2007)

PROGRESS ARTICLE

The rise of graphene

A. K. GEIM AND K. S. NOVOSELOV

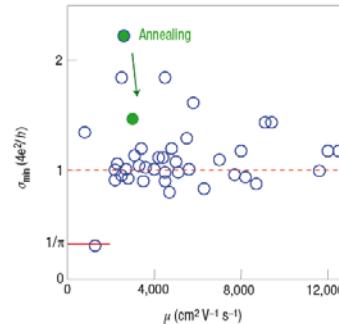


Figure 5 Minimum conductivity of graphene. Independent of their carrier mobility μ , different graphene devices exhibit approximately the same conductivity at the neutrality point (open circles) with most data clustering around $\approx 4e^2/h$ indicated for clarity by the dashed line (A.K.G. and K.S.N., unpublished work; includes the published data from ref. 9). The high-conductivity tail is attributed to macroscopic inhomogeneity. By improving the homogeneity of the samples, σ_{\min} generally decreases, moving closer to $\approx 4e^2/h$. The green arrow and symbols show one of the devices that initially exhibited an anomalously large value of σ_{\min} , but after thermal annealing at ≈ 400 K its σ_{\min} moved closer to the rest of the statistical ensemble. Most of the data are taken in the bend resistance geometry where the macroscopic inhomogeneity plays the least role.

$$\sigma \approx \frac{e^2}{\hbar} \mathcal{E}_F \tau$$

$$\tau^{-1} \propto N(\mathcal{E}_F) \approx \frac{\mathcal{E}_F}{V_F^2}$$

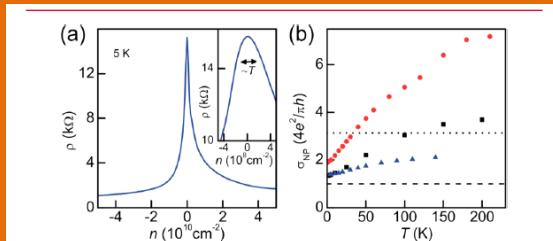
Recent experiments

NANO LETTERS

Letter
pubs.acs.org/NanoLett

How Close Can One Approach the Dirac Point in Graphene Experimentally?

Alexander S. Mayorov,^{*†} Daniel C. Elias,[†] Ivan S. Mukhin,[‡] Sergey V. Morozov,[§]
Leonid A. Ponomarenko,[†] Kostya S. Novoselov,[†] A. K. Geim,^{†,§} and Roman V. Gorbachev^{†,§}



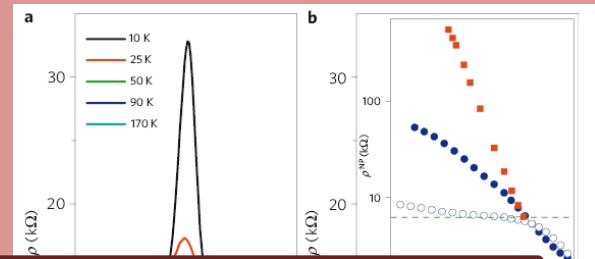
LETTERS

PUBLISHED ONLINE: 9 OCTOBER 2011 | DOI: 10.1038/NPHYS2114

nature physics

Tunable metal-insulator transition in double-layer graphene heterostructures

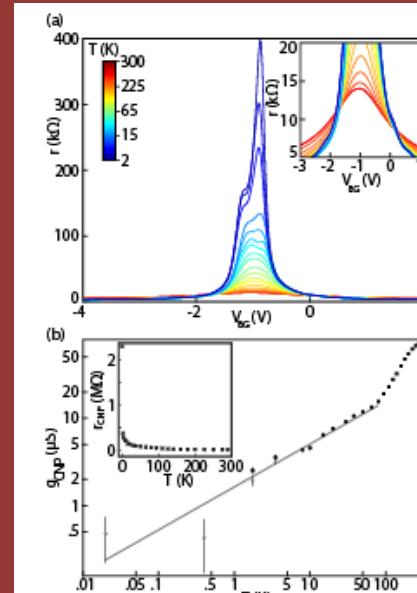
L. A. Ponomarenko¹, A. K. Geim^{1,2}, A. A. Zhukov², R. Jalil², S. V. Morozov^{1,3}, K. S. Novoselov¹, I. V. Grigorieva¹, E. H. Hill², V. V. Cheianov⁴, V. I. Fal'ko⁴, K. Watanabe⁵, T. Taniguchi⁵ and R. V. Gorbachev^{2*}



Insulating behavior at the neutrality point in single-layer graphene

F. Amet,¹ J. R. Williams,² K. Watanabe,³ T. Taniguchi,³ and D. Goldhaber-Gordon²

arXiv:1209.6364



Theory I

PHYSICAL REVIEW B **86**, 165413 (2012)

Conductivity of suspended graphene at the Dirac point

I. V. Gornyi,^{1,2} V. Yu. Kachorovskii,^{1,2,3} and A. D. Mirlin^{1,3,4}

$$\sigma_{\text{ee+ph}} = \frac{e^2}{\hbar} \frac{N \ln 2}{2\pi [C_2 Z^2 g^2 (T/\Delta_c)^\eta + C_3 g_e^2 N]}.$$

Flexural modes

$$g_e = \frac{g_e^0}{1 + (g_e^0/4) \ln(\Delta/T)}$$

Electron-electron interaction

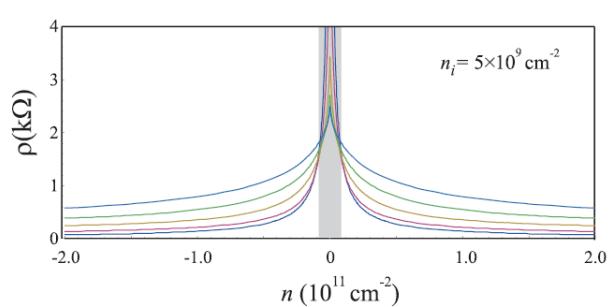


FIG. 8. (Color online) Resistivity as a function of electron concentration at $n_i = 5 \times 10^9 \text{ cm}^{-2}$ and different temperatures ($T/1\text{K} = 5, 40, 90, 150, 230$) increasing from the bottom to the top at large n . Within the grey area temperature dependence is “insulating,” while outside this region it is “metallic.”

At the neutrality point the conductivity increases as the temperature decreases

See also: L. Fritz, J. Schmalian, M. Müller, and S. Sachdev, Phys. Rev. B **78**, 085416 (2008).
V. Juricic, O. Vafek, and I. F. Herbut, Phys. Rev. B, **82**, 235402 (2010).

PHYSICAL REVIEW B **85**, 195451 (2012)



Disorder by order in graphene

S. Das Sarma, E. H. Hwang, and Qiuzi Li

Theory II

The pseudodiffusive regime

Eur. Phys. J. B 51, 157–160 (2006)
DOI: 10.1140/epjb/e2006-00203-1

THE EUROPEAN
PHYSICAL JOURNAL B

Zitterbewegung, chirality, and minimal conductivity in graphene

M.I. Katsnelson^a

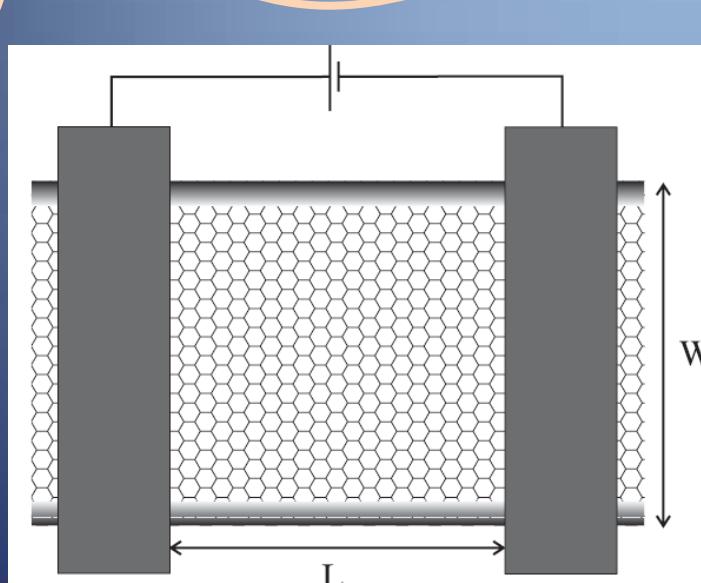
PRL 96, 246802 (2006)

PHYSICAL REVIEW LETTERS

week ending
23 JUNE 2006

Sub-Poissonian Shot Noise in Graphene

J. Tworzydlo,¹ B. Trauzettel,² M. Titov,³ A. Rycerz,^{2,4} and C. W. J. Beenakker²



$$T(k_y) \propto e^{-k_y L_x}$$
$$G = \sum_{k_y} T(k_y) \propto \frac{L_y}{L_x}$$

See also :

- **Pseudodiffusive transport in graphene**, E. Prada, P. San Jose, B. Wunsch, F. G., Phys. Rev. B 75, 113407 (2007).
- **Transport through evanescent waves in graphene quantum dots**, M. I. Katsnelson, F. G., Phys. Rev. B 79, 075417 (2008)

Tunneling and interactions

PHYSICAL REVIEW
LETTERS

VOLUME 46

26 JANUARY 1981

NUMBER 4

Influence of Dissipation on Quantum Tunneling in Macroscopic Systems

A. O. Caldeira and A. J. Leggett

School of Mathematical and Physical Sciences, University of Sussex, Brighton BN1 9QH, Sussex, United Kingdom



Annals of Physics

Volume 149, Issue 2, September 1983, Pages 374–456



Quantum tunnelling in a dissipative system

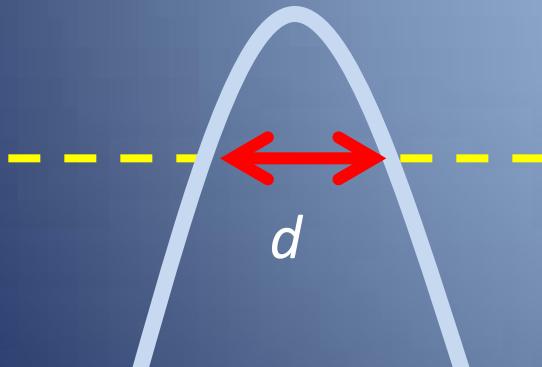
A.O. Caldeira

Instituto de Física "Gleb Wataghin" Universidade Estadual de Campinas, Cidade Universitária, Barão Geraldo, 13-100 Campinas, São Paulo, Brazil

A.J. Leggett*

School of Mathematical and Physical Sciences, University of Sussex, Falmer, Brighton BN1 9QH, England

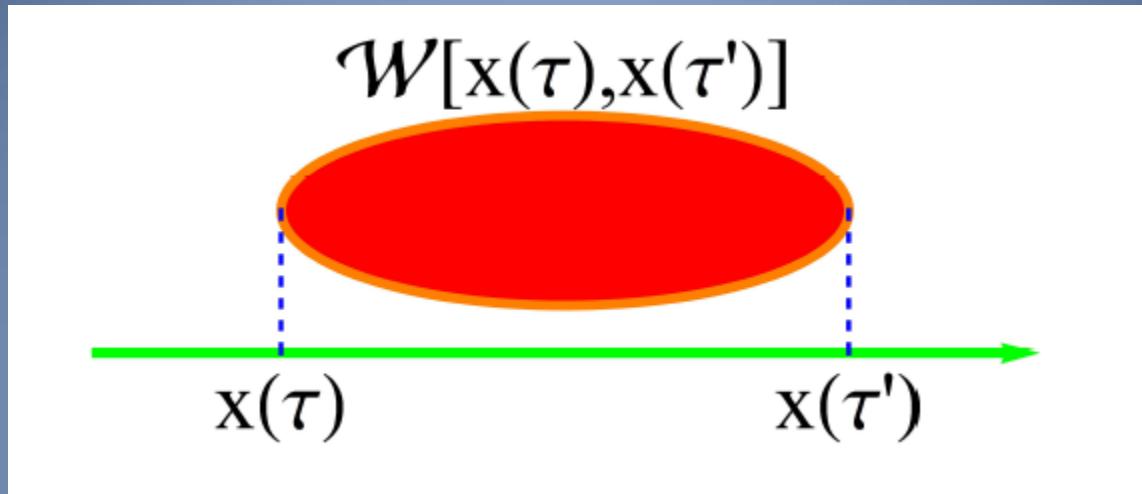
$$Mq'' + \eta q' = -dV/dq + F_{ext}(t)$$



$$T = T_0 e^{-c \frac{\eta d^2}{\hbar}}$$

- Semiclassical analysis
- The excitations of the environment are treated as a set of independent bosons

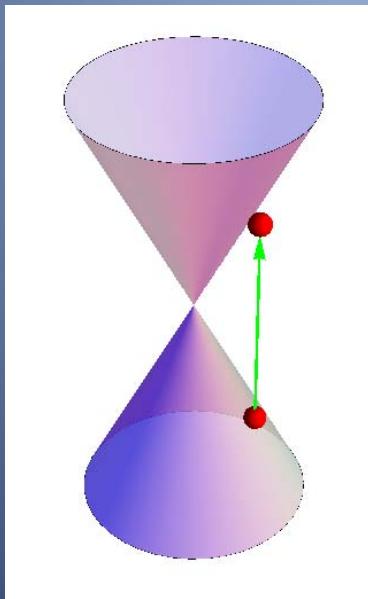
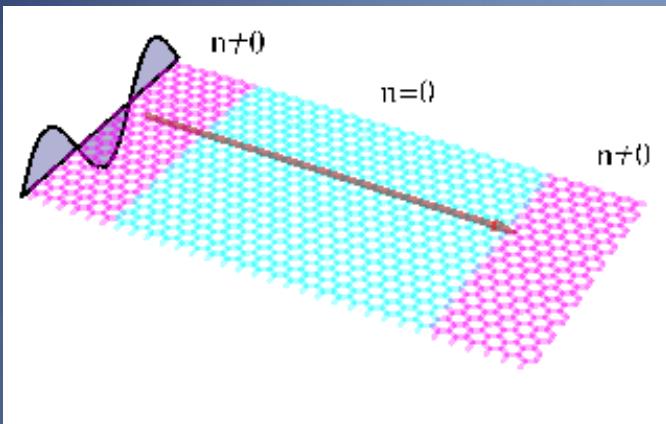
The Caldeira-Leggett model



$$\delta S = \int_{-\infty}^{+\infty} d\tau \int_0^{\beta} d\tau' \int_{-\infty}^{+\infty} \frac{dq}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{iq[x(\tau)-x(\tau')]} e^{-\omega|\tau-\tau'|} \text{Im}[W(q, \omega)]$$

$$W_{CL}[x(\tau) - x(\tau'), \tau - \tau'] = \frac{\eta}{2\pi} \frac{[x(\tau) - x(\tau')]^2}{[\tau - \tau']^2}$$

Graphene as a dissipative environment



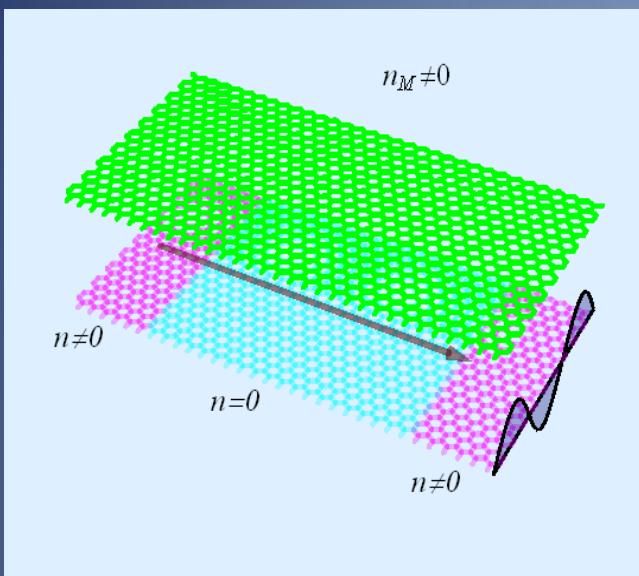
$$\text{Im}W(q, \omega) = \text{Im} \frac{v_q}{\epsilon(q, \omega)} = \text{Im} \frac{v_q}{1 + v_q \chi_{1D}(q, \omega)}$$

$$v_q \approx \begin{cases} -\frac{2e^2}{\epsilon_0} \text{Log}(qL_y) & qL_y \ll 1 \\ \frac{2\pi e^2}{\epsilon_0 q L_y} & qL_y \gg 1 \end{cases}$$

$$\chi_{1D}(q, \omega) \approx \begin{cases} \frac{L_y q^2}{4\sqrt{v_F^2 q^2 - \omega^2}} & \text{graphene} \\ \frac{\nu_{1D} D q^2}{i\omega + D q^2} & \text{diffusive metal, } q \leq \ell_{el}^{-1} \\ \frac{\nu_{1D} v_F q}{i\omega + v_F q} & \text{ballistic metal, } \ell_{el}^{-1} \leq q \leq k_F \end{cases}$$

$$q_c \approx \text{Max}\left(L_x^{-1}, \frac{v_F}{T}, \ell_B^{-1} \right)$$

Results



$$\delta S_G \approx \frac{L_x}{8\pi L_y} \frac{\alpha^2}{4\sqrt{2} + \alpha} \log\left(\frac{L_x}{a}\right)$$

$$\delta S_M \approx \frac{L_x^2}{4\pi g \ell L_y} + \frac{L_x}{8\pi L_y} \log(g)$$

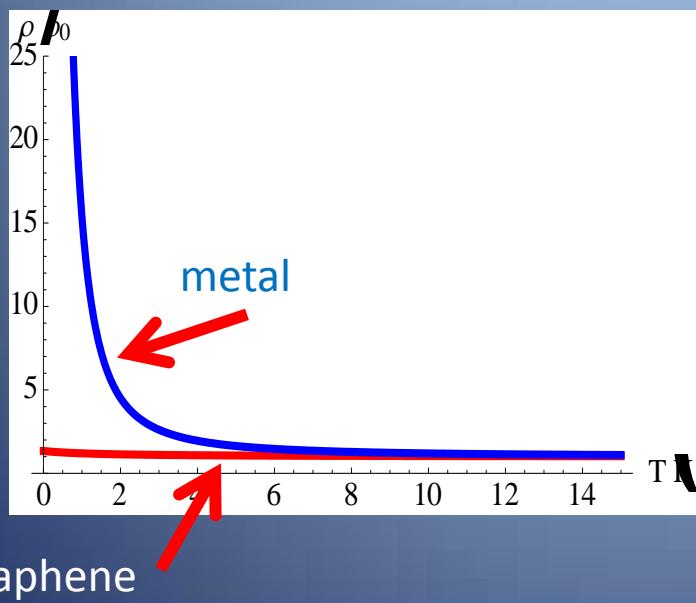
T=B=0

diffusive contribution,

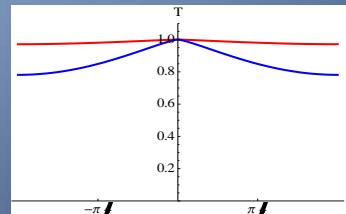
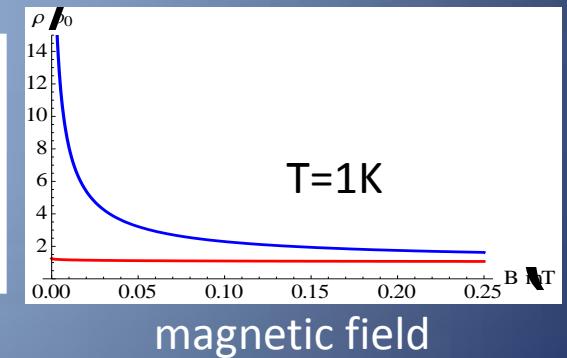
$$L_x^{-1} \leq q \leq \ell^{-1}$$

ballistic contribution,

$$\ell^{-1} \leq q \leq k_F$$



$L_x = 4\mu\text{m}$
 $L_y = 1\mu\text{m}$
 $n_M = 10^{11} \text{ cm}^{-2}$
 $l = 60\text{nm}$



p-n junction

GRAPHENE'S SUPERLATIVES

- Thinnest imaginable material
- largest surface area ($\sim 2,700 \text{ m}^2$ per gram)
- **strongest material 'ever measured'** (theoretical limit)
- stiffest known material (stiffer than diamond)
- most stretchable crystal (up to 20% elastically)
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- 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)

Why are there two dimensional crystals?

STATISTICAL PHYSICS

by

L. D. LANDAU AND E. M. LIFSHITZ

INSTITUTE OF PHYSICAL PROBLEMS,
U.S.S.R. ACADEMY OF SCIENCES

Volume 5 of *Course of Theoretical Physics*

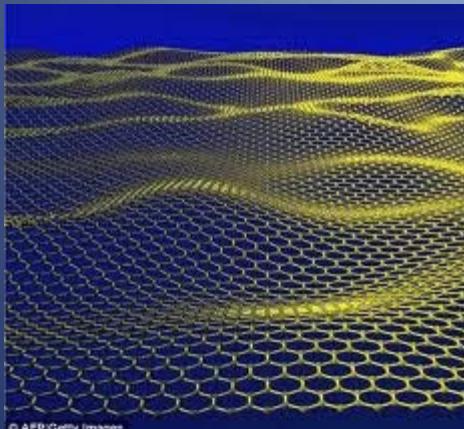
PART 1

THIRD EDITION, REVISED AND ENLARGED
by E. M. LIFSHITZ and L. P. PITAEVSKII

ered). It is easy to see, however, that the thermal fluctuations “smooth out” such a crystal, so that $\varrho = \text{constant}$ is the only possibility: the mean

Thermal fluctuations:

$$\langle \vec{u}(L)\vec{u}(0) \rangle \approx \frac{k_B T}{B} \log\left(\frac{L}{d}\right)$$



© AFP/Getty Images

$$B_{\text{graphene}} = 22 \text{ eV } \text{\AA}^{-2} = 352 \text{ N/m}$$
$$B_{\text{diamond}} \times d = 52.4 \text{ N/m}$$

$$T = 300 \text{ K}$$

$$L = 1 \text{ Km}$$

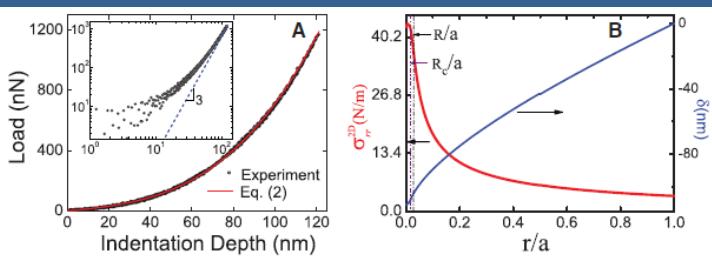
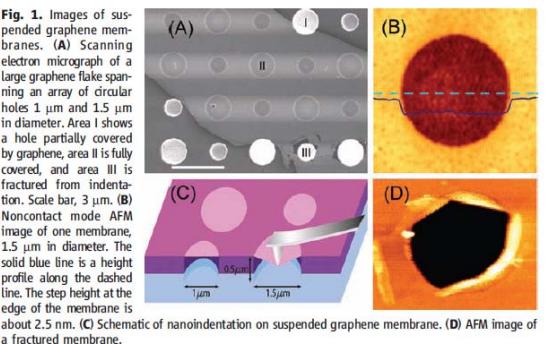
$$\langle \vec{u}(L)\vec{u}(0) \rangle \approx 0.03 \text{\AA}^2$$

Elastic properties of graphene

Measurement of the Elastic Properties and Intrinsic Strength of Monolayer Graphene

Changgu Lee,^{1,2} Xiaodong Wei,¹ Jeffrey W. Kysar,^{1,3} James Hone^{1,2,4*}

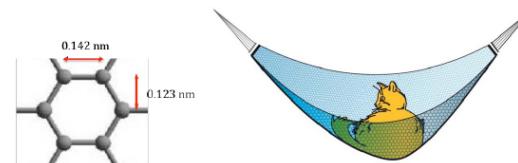
We measured the elastic properties and intrinsic breaking strength of free-standing monolayer graphene membranes by nanoindentation in an atomic force microscope. The force-displacement behavior is interpreted within a framework of nonlinear elastic stress-strain response, and yields second- and third-order elastic stiffnesses of 340 newtons per meter ($N\ m^{-1}$) and $\sim 690 N\ m^{-1}$, respectively. The breaking strength is $42 N\ m^{-1}$ and represents the intrinsic strength of a defect-free sheet. These quantities correspond to a Young's modulus of $E = 1.0$ terapascals, third-order elastic stiffness of $D = -2.0$ terapascals, and intrinsic strength of $\sigma_{in} = 130$ gigapascals for bulk graphite. These experiments establish graphene as the strongest material ever measured, and show that atomically perfect nanoscale materials can be mechanically tested to deformations well beyond the linear regime.



KUNGL.
VETENSKAPS-
AKADEMIEN
THE ROYAL SWEDISH ACADEMY OF SCIENCES

OCTOBER 5, 2010

Appendix, some properties of graphene



CLAIM #1: GRAPHENE CAN HOLD AN ELEPHANT

“...graphene as the strongest material ever measured, some 200 times stronger than structural steel. ... If a sheet of cling film (which typically has a thickness of around $100\ \mu\text{m}$) were to have the same strength as pristine graphene, it would require a force of over $20,000\ N$ to puncture it with a pencil.”

Jim Hone, Columbia U

physicsworld.com

Graphic: Sci. Am., 11/2011



courtesy of M. M. Fogler

Self-Consistent Theory of Polymerized Membranes

Pierre Le Doussal^(a)

Institute for Advanced Study, Princeton, New Jersey 08540

Leo Radzhovsky

Lyman Laboratory, Harvard University, Cambridge, Massachusetts 02138

(Received 18 May 1992)

y a nontrivial fixed point, but with *anomalous* constants $\lambda(q) \sim \mu(q) \sim q^{\eta_u}$, $\eta_u > 0$, with η_u

Graphene

Carbon in Two Dimensions

Mikhail I. Katsnelson

of the order of a^{-1} to make A dimensionless. One can assume also a renormalization of effective Lamé constants:

$$\lambda_R(q), \mu_R(q) \sim q^{\eta_u}, \quad (9.103)$$

Experiments

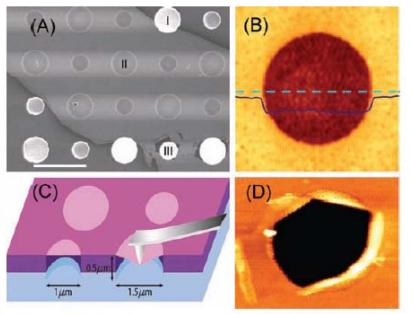
C. Gomez-Navarro, J. Gomez, G. Lopez-Polin, F. Perez-Murano

Measurement of the Elastic Properties and Intrinsic Strength of Monolayer Graphene

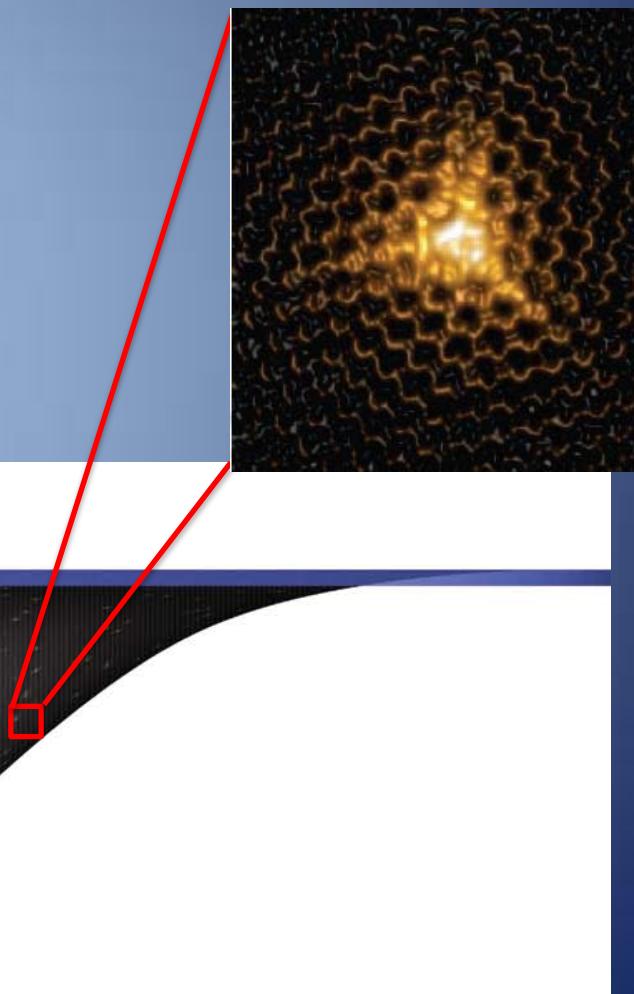
Changgu Lee,^{1,2} Xiaoding Wei,¹ Jeffrey W. Kysar,^{1,3} James Hone^{1,2,4*}

We measured the elastic properties and intrinsic breaking strength of free-standing monolayer graphene membranes by nanoindentation in an atomic force microscope. The force-displacement behavior is interpreted within a framework of nonlinear elastic stress-strain response, and yields second- and third-order elastic constants for bulk graphite. These experiments show that atomically perfect graphene is well beyond the linear regime respectively. The breaking stress of a defect-free sheet. These quantified third-order elastic stiffness of G for bulk graphite. These experiments show that atomically perfect graphene is well beyond the linear regime

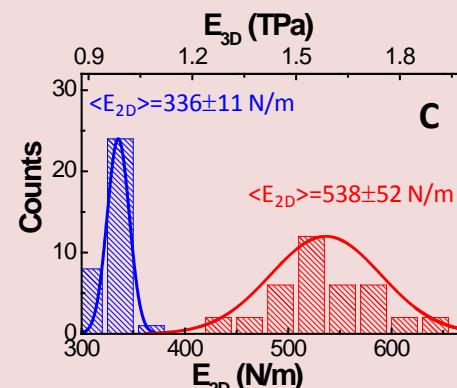
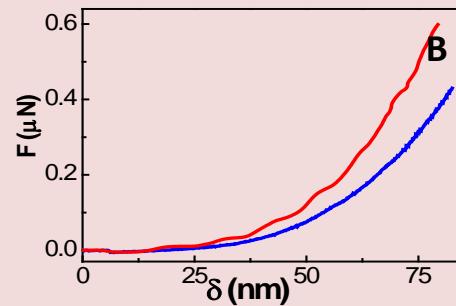
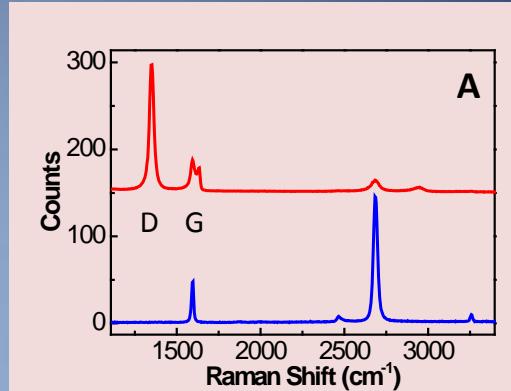
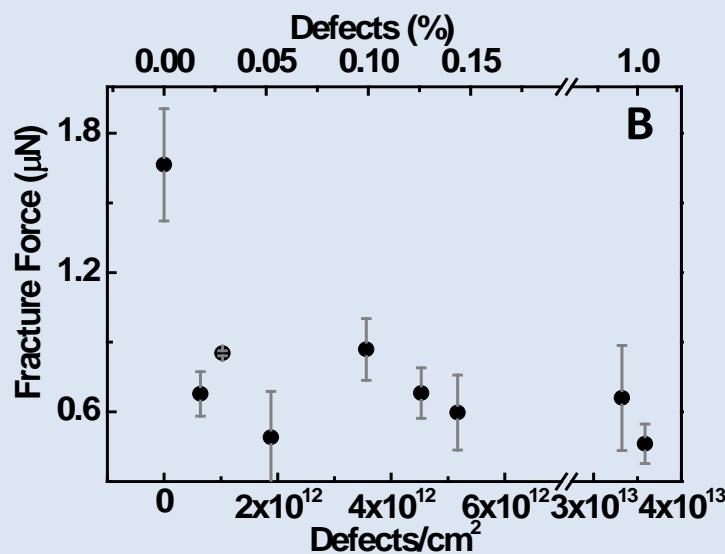
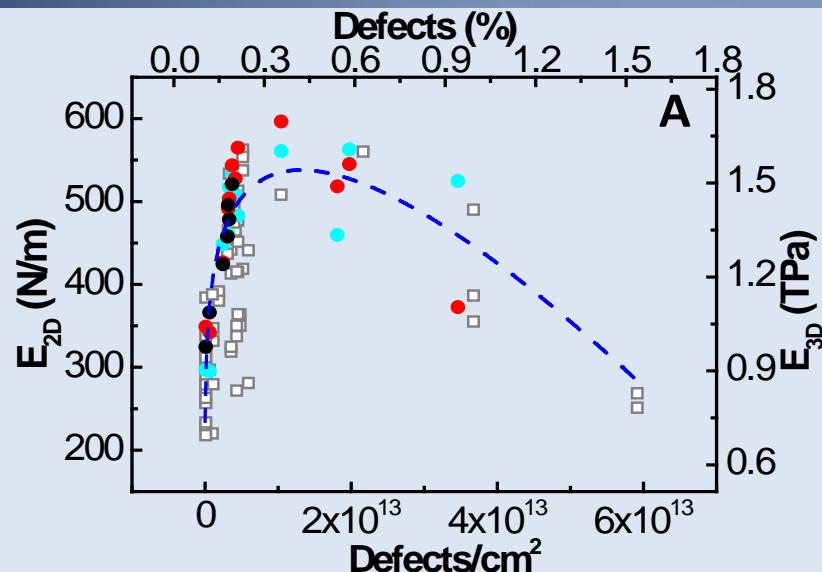
Fig. 1. Images of suspended graphene membranes. (A) Scanning electron micrograph of a large graphene flake spanning an array of circular holes 1 μm and 1.5 μm in diameter. Area I shows a hole partially covered by graphene, area II is fully covered, and area III is fractured from indentation. Scale bar, 3 μm . (B) Noncontact mode AFM image of one membrane, 1.5 μm in diameter. The solid blue line is a height profile along the dashed line. The step height at the edge of the membrane is about 2.5 nm. (C) Schematic of nanoindentation on suspended graphene membrane. (D) AFM image of a fractured membrane.



Load 2



Experiments

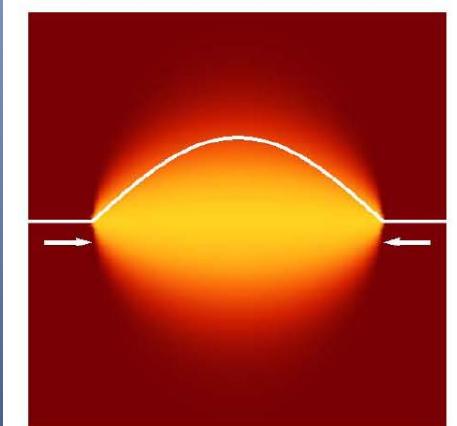
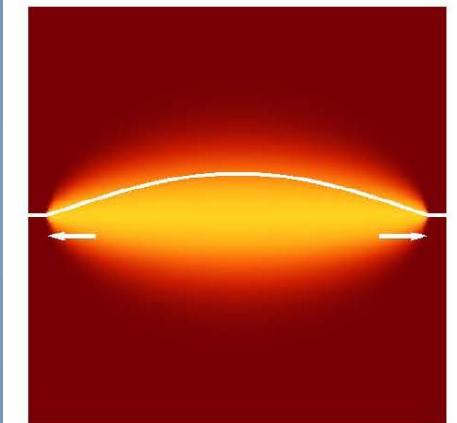
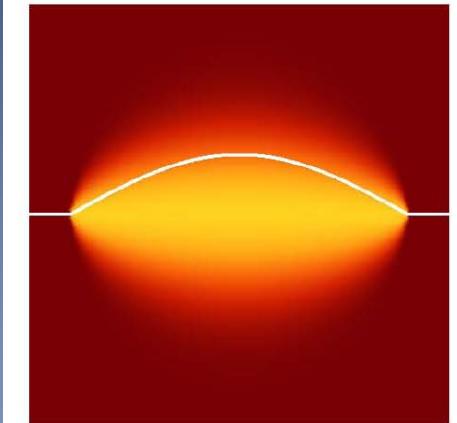


Out of plane fluctuations
renormalize the in plane
elastic constants

$$E \approx \left(c_1 Y \bar{u} + c_2 \frac{\kappa}{\ell^2} \right) h^2$$

$$F \approx T \log \left(\frac{T}{c_1 Y \bar{u} + c_2 \frac{\kappa}{\ell^2}} \right)$$

$$\delta Y = \frac{1}{\ell^2} \frac{\partial^2 F}{\partial \bar{u}^2} \propto -\frac{Y^2 T \ell^2}{\kappa^2}$$



Anharmonic effects: thermal expansion coefficient in graphene and graphite

PHYSICAL REVIEW B 86, 144103 (2012)

Bending modes, anharmonic effects, and thermal expansion coefficient in single-layer and multilayer graphene

P. L. de Andres,¹ F. Guinea,¹ and M. I. Katsnelson²

$$\alpha \approx -\frac{k_B}{8\pi\kappa} \log\left(\frac{\kappa^3\rho}{\hbar^2 Y^2}\right)$$

graphite: crossover wavelength

$$q_c^* \approx \sqrt{\frac{g/d^2}{\lambda + 2\mu}}$$

$$g \approx 30 \text{ meV}/\text{\AA}^2$$

$$d \approx 3.3 \text{ \AA}$$

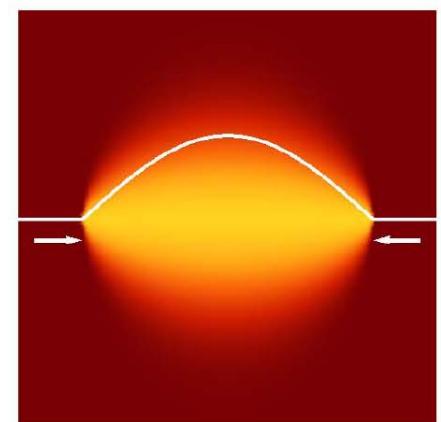
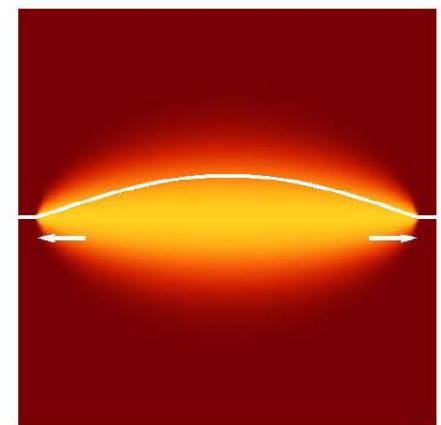
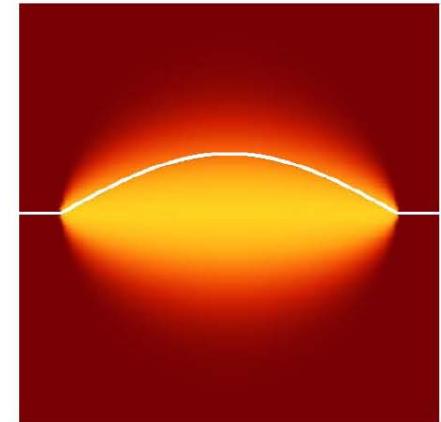
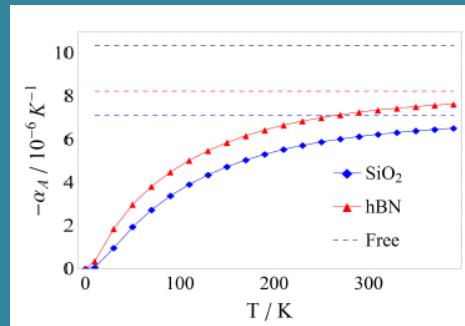
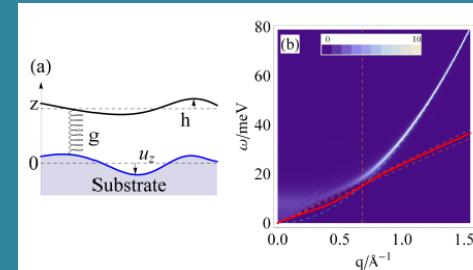
$$\lambda + 2\mu \approx 22 \text{ eV}/\text{\AA}^2$$

$$1/q_c^* \approx 5.5 \text{ \AA}^{-1}$$

The flexural modes of graphene on a substrate

Bruno Amorim¹ and Francisco Guinea¹

Arxiv:1304.6567



Vacancies and flexural modes

$$G(q, \omega) = \frac{1}{\rho\omega^2 - \kappa q^4 - \Sigma(q, \omega)}$$

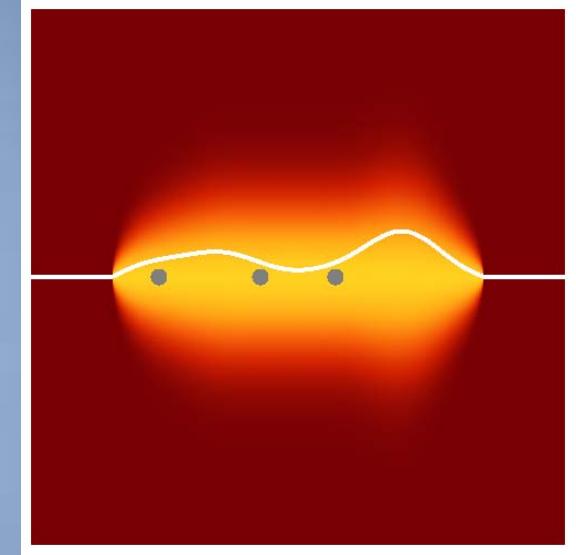
T-matrix approximation

$$\Sigma(\omega) \approx \begin{cases} n_v \sqrt{\kappa \rho \omega^2} & h^2 = 0 \\ n_v \frac{\sqrt{\kappa \rho \omega^2}}{\log\left(\frac{\kappa}{a^4 \rho \omega^2}\right)} & |\nabla h|^2 = 0 \end{cases}$$

infinite mass
vacancies

localization length

$$\frac{\kappa}{\ell^4} \approx \Sigma \left(\sqrt{\frac{\kappa}{\rho \ell^4}} \right)$$
$$\ell \approx n_v^{-1/2}$$



- Vacancies localize flexural modes
- Long wavelength flexural modes do not contribute to the screening of the elastic constants

geometric factor

percolation

$$Y \approx K \left(\frac{1}{R^2} + \frac{1}{\ell_0^2} + n_V \right)^{\frac{\eta_u}{2}} \left[1 - c \left(\frac{1}{\ell_0^2} + n_V \right) \right]$$

intrinsic localization length

PRL 105, 266601 (2010)

PHYSICAL REVIEW LETTERS

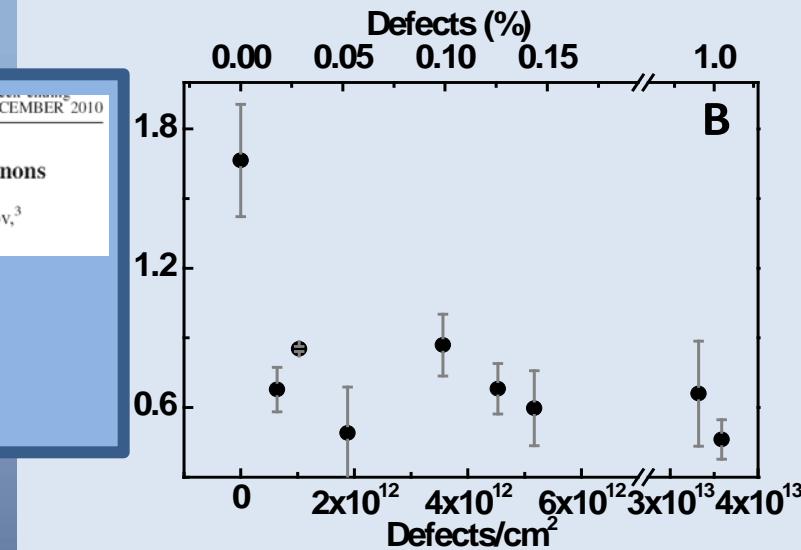
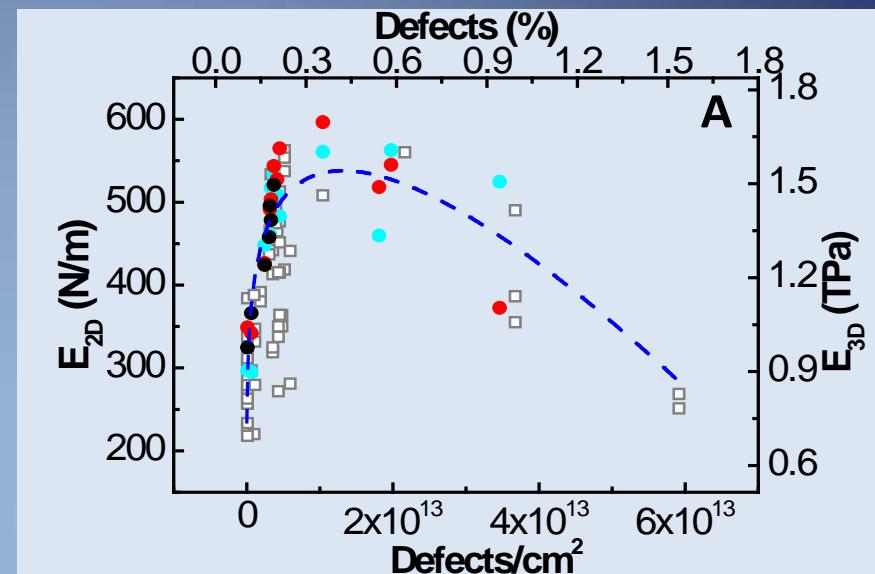
31 DECEMBER 2010

Limits on Charge Carrier Mobility in Suspended Graphene due to Flexural Phonons

Eduardo V. Castro,¹ H. Ochoa,¹ M. I. Katsnelson,² R. V. Gorbachev,³ D. C. Elias,³ K. S. Novoselov,³ A. K. Geim,³ and F. Guinea¹

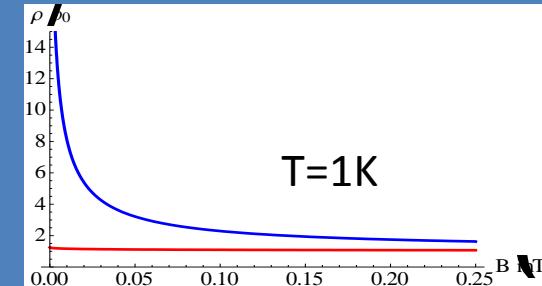
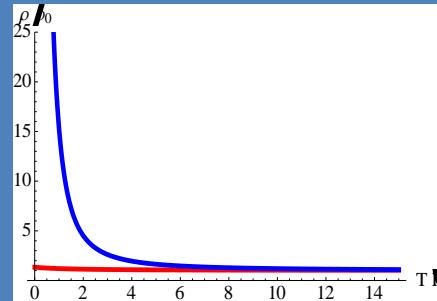
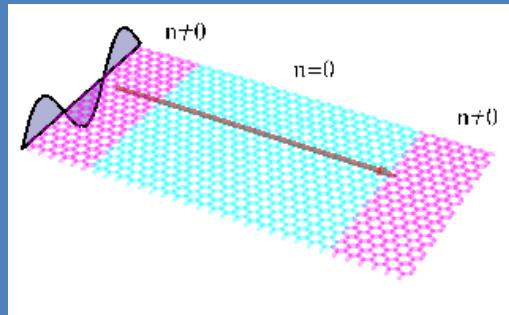
$$\ell_0 \approx 20 - 100 \text{ nm}$$

$$\ell_0 \geq k_F^{-1}$$



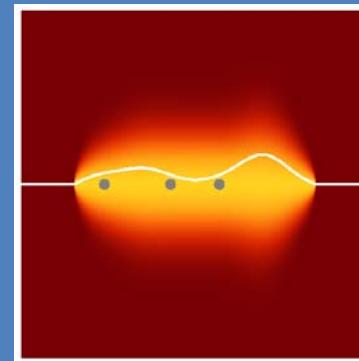
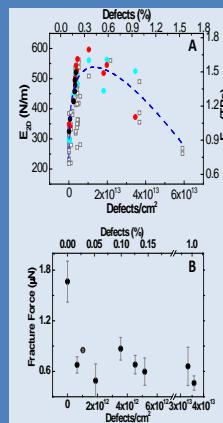
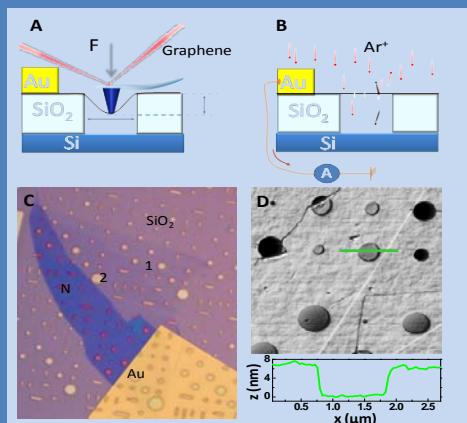
Minimal conductivity+interactions

F. G., M. I. Katsnelson, arXiv:1307.6221



The pseudodiffusive regime is highly sensitive to interactions

Elastic properties of graphene with defects



- Flexural phonons modify the elastic properties
- The value of the Young modulus depends on the experimental setup

First-principles determination of the structural, vibrational and thermodynamic properties of diamond, graphite, and derivatives

Nicolas Mounet* and Nicola Marzari†

FIRST-PRINCIPLES DETERMINATION OF THE...

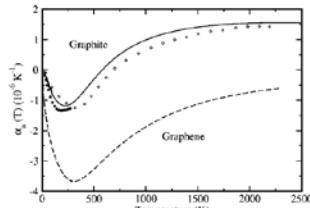


FIG. 15. In-plane coefficient of linear thermal expansion as a function of temperature for graphite (solid line) and graphene (dashed line) from our QHA-GGA *ab initio* study. The experimental results for graphite are from Ref. 14 (filled circles) and Ref. 7 (open diamonds).

Bending modes, anharmonic effects, and thermal expansion coefficient in single-layer and multilayer graphene

P. L. de Andres,¹ F. Guinea,¹ and M. I. Katsnelson²

$$\gamma_{\vec{q}} = -\frac{\mathcal{A}}{\omega_{\vec{q}}} \frac{\partial \omega_{\vec{q}}}{\partial \mathcal{A}} = -\left. \frac{1}{2\omega_{\vec{q}}} \frac{\partial \omega_{\vec{q}}}{\partial \bar{u}} \right|_{\bar{u}=0} = -\frac{\lambda + \mu}{2\kappa |\vec{q}|^2},$$

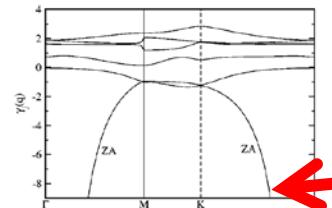
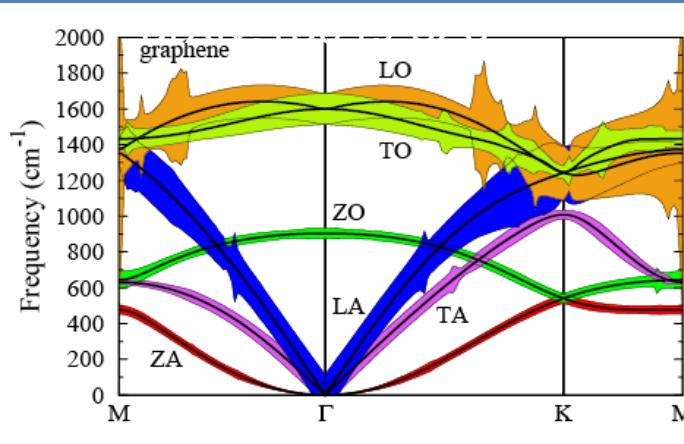


FIG. 17. *Ab initio* mode Gruneisen parameters for graphene.
= $-\left[a/2\omega_{\vec{q}}(\vec{q}) \right] [d\omega_{\vec{q}}(\vec{q})/da]$. While not visible in the figure, the Gruneisen parameters for the lowest acoustic branch of graphite become as low as -40, and as low as -80 in

Anharmonic properties from a generalized third order *ab initio* approach: theory and applications to graphite and graphene

Lorenzo Paulatto,* Francesco Mauri, and Michele Lazzeri



First-principles investigation of graphene fluoride and graphane

O. Leenaerts,^{1,*} H. Peelaers,^{1,†} A. D. Hernández-Nieves,^{1,2,‡} B. Partoens,^{1,§} and F. M. Peeters^{1,||}

TABLE III. Elastic constants of the different hydrogenated and fluorinated graphene derivatives. The 2D Young's modulus, E' , and Poisson's ratio, ν , are given along the cartesian axes. E' is expressed in N m⁻¹.

	Chair	Boat	Zigzag	Armchair
Graphane				
E'_x	243	230	117	247
E'_y	243	262	271	142
ν_x	0.07	-0.01	0.05	-0.05
ν_y	0.07	-0.01	0.11	-0.03
Fluorographene				
E'_x	226	238	240	215
E'_y	226	240	222	253
ν_x	0.10	0.00	0.09	0.02
ν_y	0.10	0.00	0.11	0.02

walls due to the charged F atoms. The values that are found for the chair configurations agree well with recent calculations (245 N m^{-1} and 228 N m^{-1} for graphane and fluorographene, respectively, in Ref. 20). Nair *et al.*¹¹ performed a nanoindentation experiment on fluorographene and measured a value of $100 \pm 30 \text{ N m}^{-1}$ for E'_{PG} . This value is approximately half the theoretical value. Because the theoretical values are trustworthy, i.e., they agree with earlier theoretical calculations, and this kind of calculations are believed to be accurate (as in the case of graphene), this suggests that the experimental samples contain an appreciable