

Theory of Condensed Matter and New Materials

Leaders: V.A. Osipov and J. Brankov

Projects:

Physical properties of complex materials
and nanostructures

Spokespersons: *N.M. Plakida, V.A. Osipov,
G. Roepke*

Mathematical Problems of Many-Particle
Systems

Spokesperson: *V.B. Priezzhev, V.I. Yukalov*

Main topics

- **Strongly correlated systems** (high- T_c superconductors, complex magnetic systems)
- **Physics of Nanostructures** (carbon nanosystems, layered structures, BEC in traps, fractal systems)
- **Modern problems of statistical mechanics** (sandpile model, random walk models, etc)

Топология и геометрия в современной теории конденсированных сред на примере графена и тд

- Условная классификация:
- Топологические кристаллы
- Топологические дефекты
- Топологические возбуждения

Топологические кристаллы

Topology in Condensed Matter Physics

seminar: May 13 - July 31, 2002

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Картинки

Topological Defects in Carbon Nanocrystals

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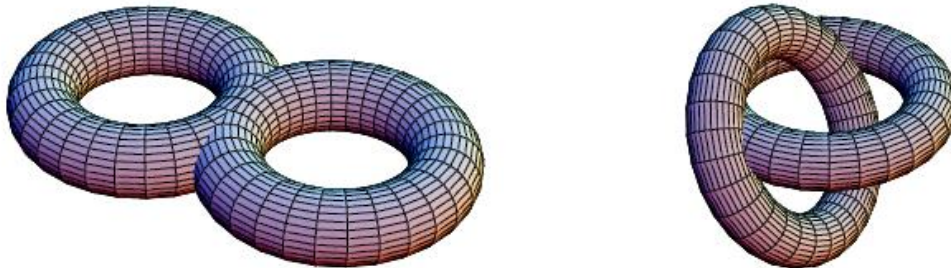


Fig. 5. Exotic configurations

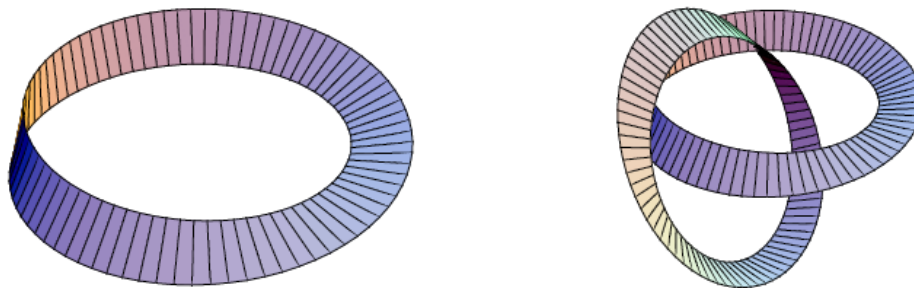
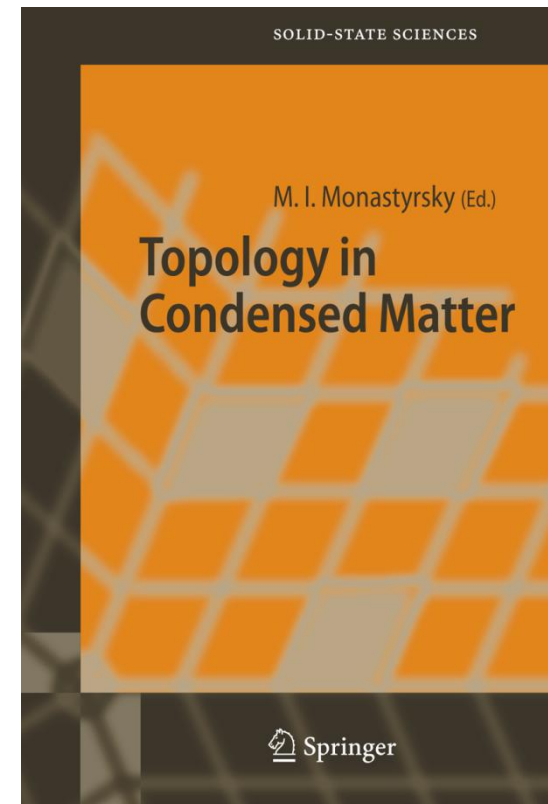


Fig. 6. Möbius stripe (left) and a more exotic configuration



Эксперимент

International weekly journal of science
nature

A Möbius strip of single crystals

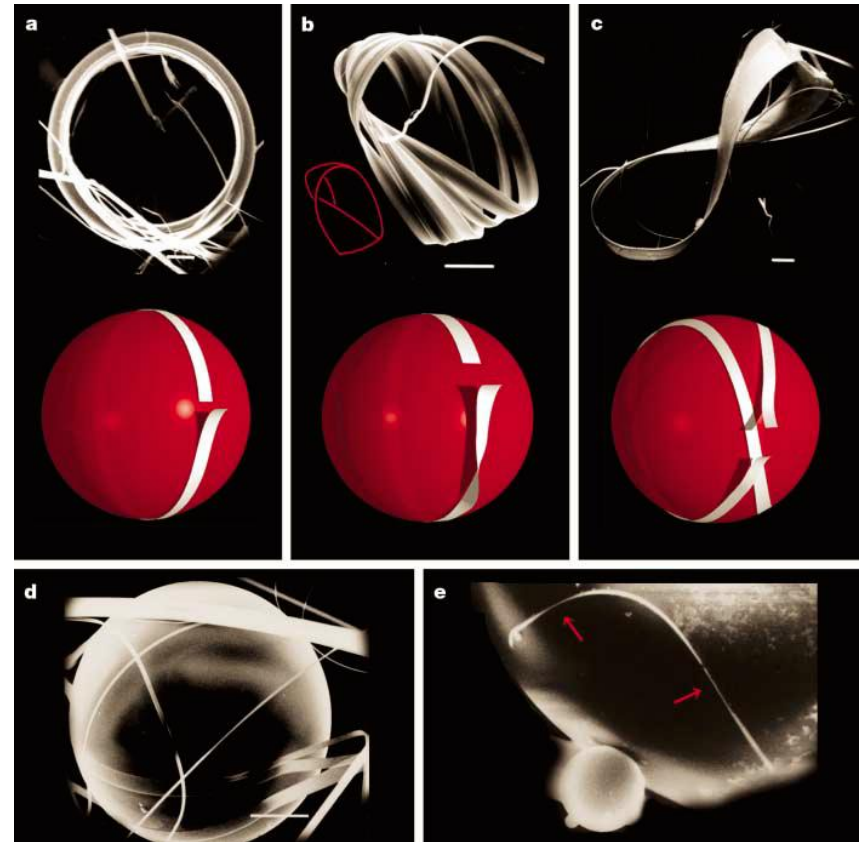
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Эксперимент



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Topologically linked crystals

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Abstract

We discovered a new class of topological crystals, namely linked rings of crystals. Two rings of tantalum triselenide (TaSe_3) single crystals were linked to each other while crystal growing. The topology of the crystal form is called a “Hopf link”, which is the simplest link involving just two component unknots linked together exactly once. The feature of the crystals is not covered by the conventional crystallography.

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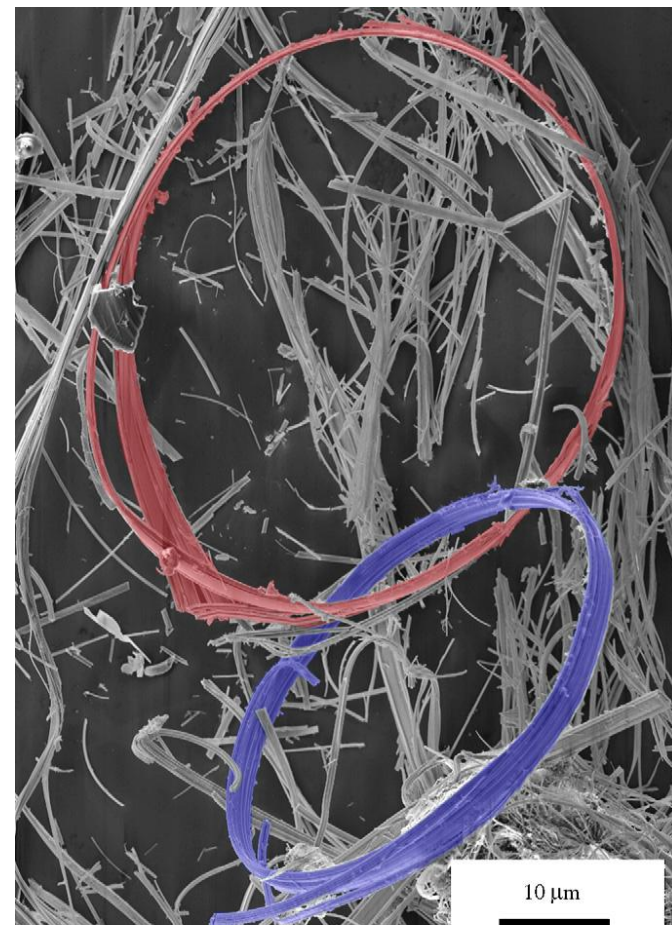
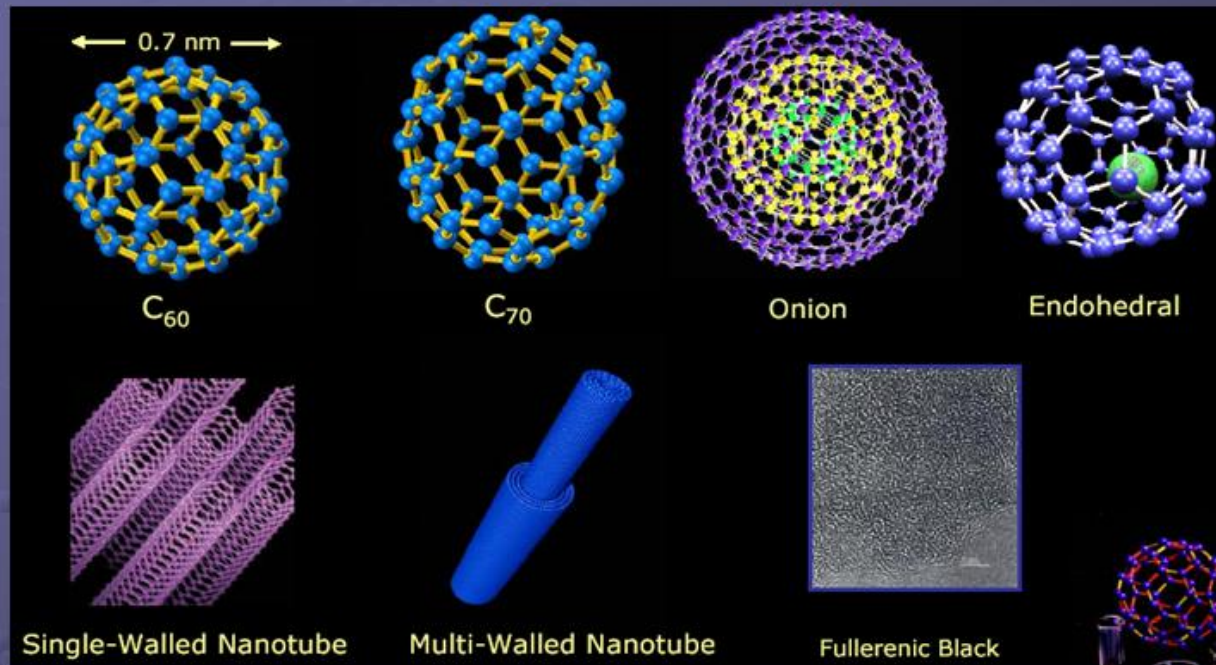


Fig. 1. Scanning electron microscope (SEM) image of linked rings of crystal formed of a compound of tantalum and selenium (TaSe_3). The blue and red rings have respective diameters of 46 and 54 μm . The two rings are linked with each other exactly once.

Фуллерены, нанотрубки,
конуса, корзинки

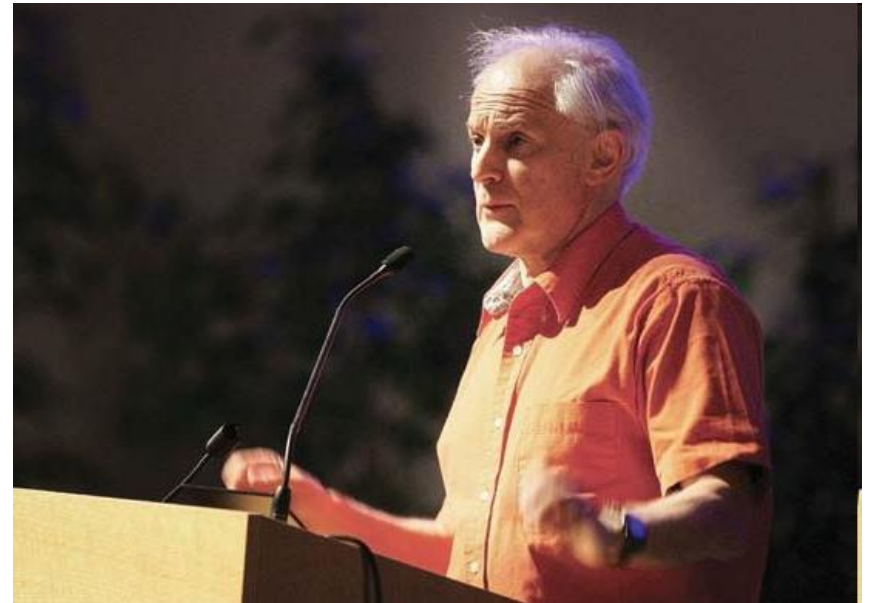
Carbon nanostructures

Several Nanocarbon Structures

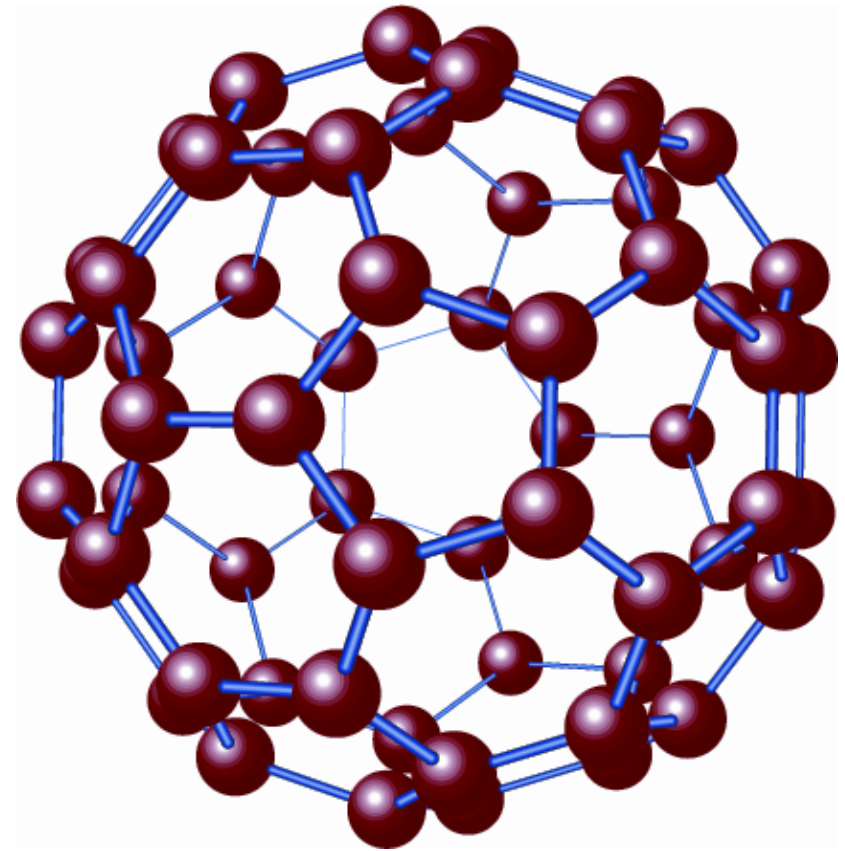


Нобелевская премия по химии (1996)

- English chemist Sir Harold Kroto was corecipient with Richard E. Smalley and Robert F. Curl, Jr., for their joint discovery of the carbon compounds called fullerenes.



Pentagons (why twelve?)



$$\Sigma(6-x)n_x=12(1-g)$$

Euler's theorem

Euler's theorem relates the number of vertices, edges and faces of an object

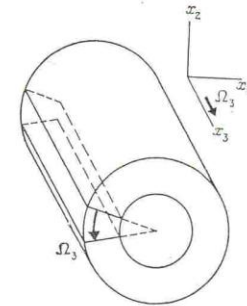
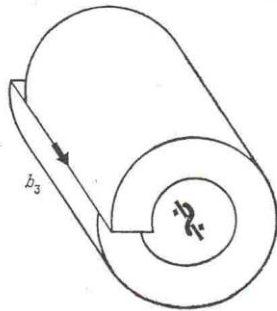
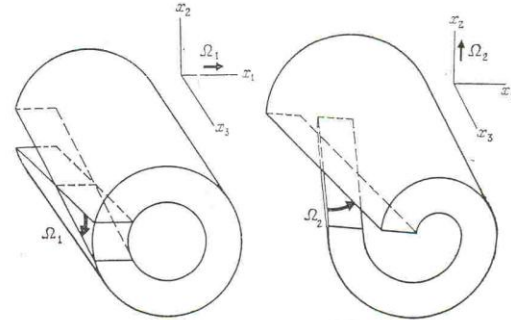
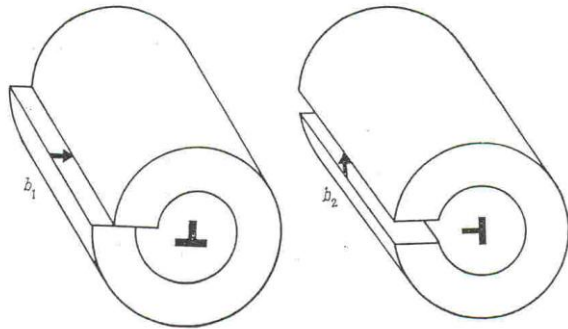
$$\dots 2n_4 + n_5 - n_7 - 2n_8 \dots = \sum (6-x)n_x = 12(1-g)$$

n_x is the number of polygons having x sides, g is the genus. For sphere $g=0$, $n_5=12$. Thus, these microcrystals can only be formed by having a total disclination of 4π . According to the geometry of the hexagonal network this means the presence of twelve pentagons (60° disclinations) on the closed hexatic surface.

Important: Disclinations are generic defects in closed carbon structures

Топологические дефекты

Дислокации и дисклинации



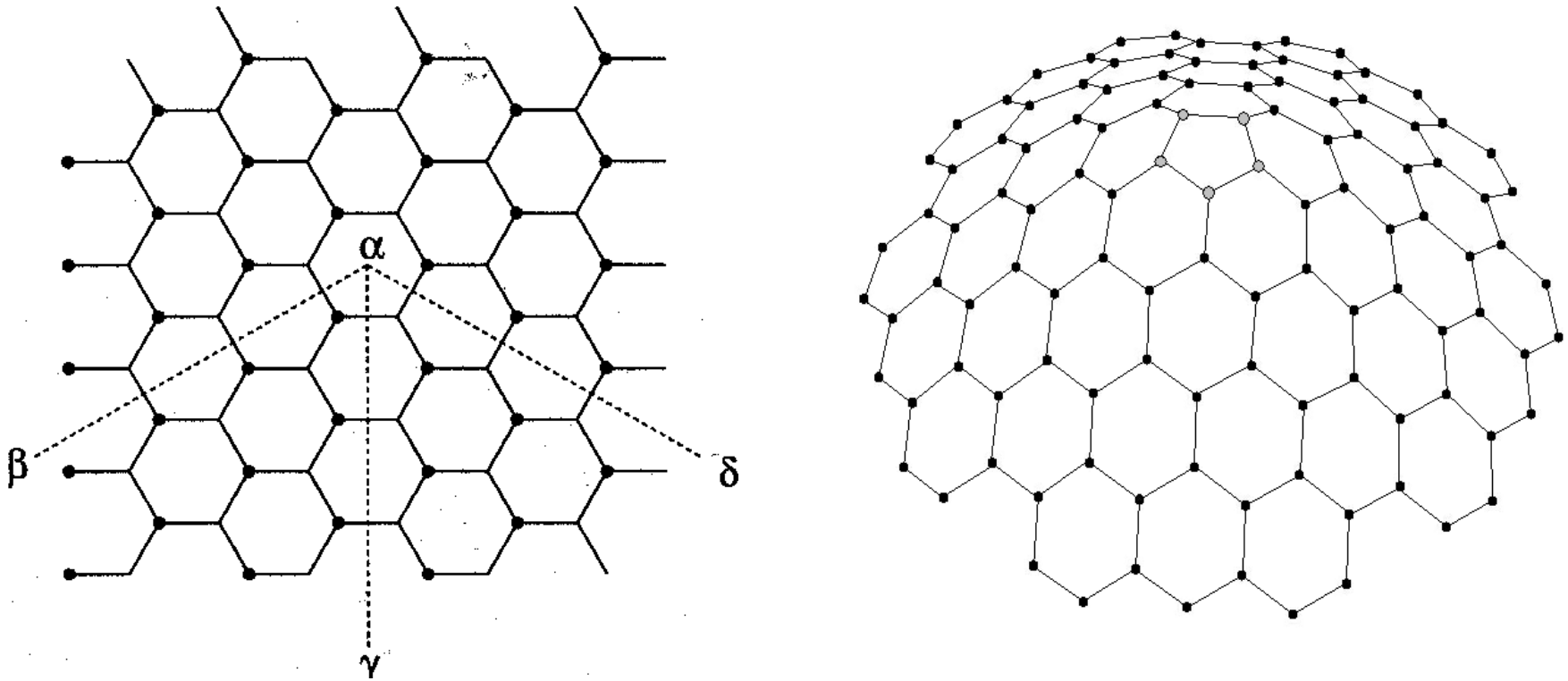
$$\oint_L du_i = \oint_L \frac{\partial u_i}{\partial x_k} dx_k = -b_i.$$

$$\oint_L d\omega_i = \oint_L \frac{\partial \omega_i}{\partial x_k} dx_k = -\Omega_i,$$

$$\vec{u}^P = \vec{u}^+ - \vec{u}^- = \vec{b} + [\vec{\Omega} \vec{R}],$$

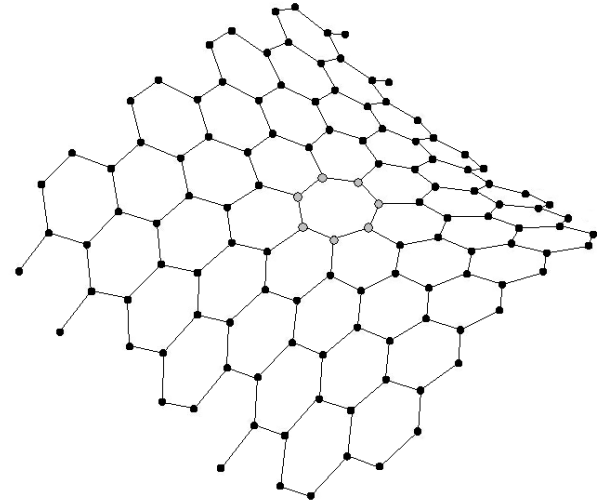
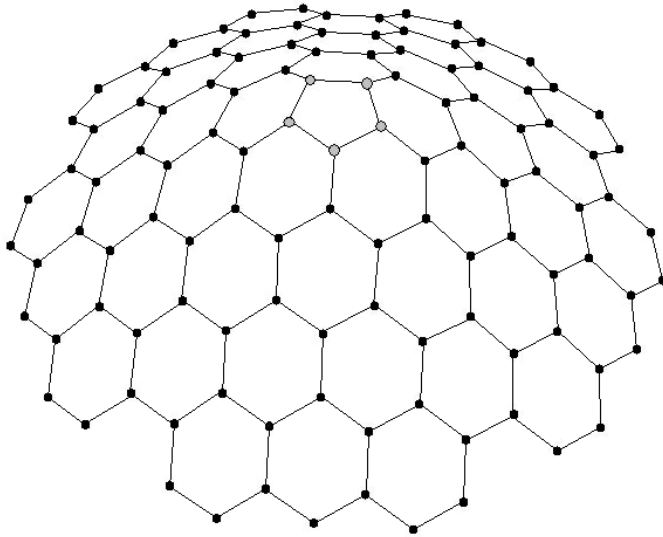
$$\vec{\omega} = (1/2) \text{rot} \vec{u}$$

Pentagons and disclination buckling transition



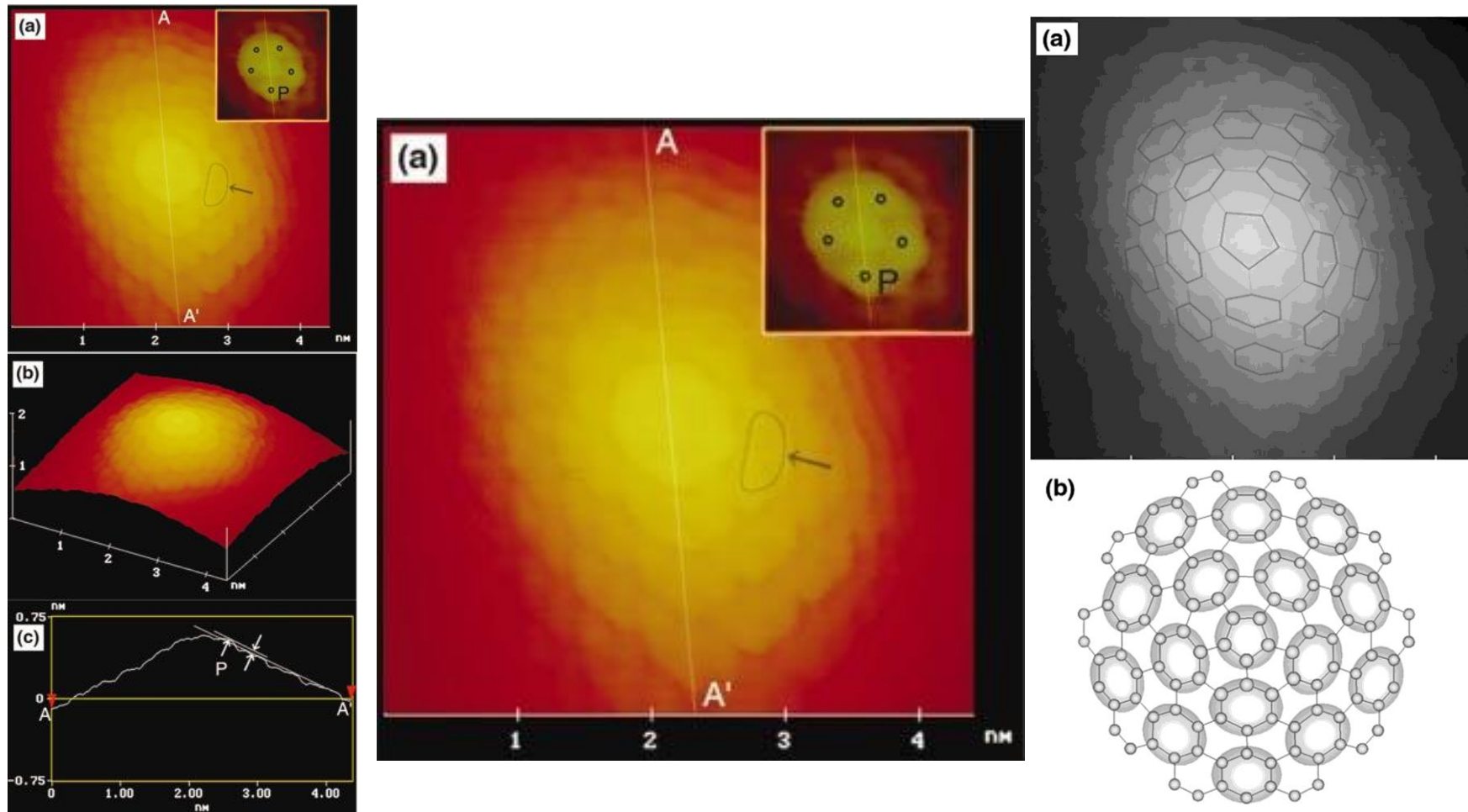
By its nature, the pentagon in a graphite sheet is a topological defect. Actually, fivefold coordinated particles (pentagons) are orientational disclination defects in the otherwise sixfold coordinated triangular lattice.

Defects, Curvature



The pentagon (positive curvature) and the heptagon (negative curvature) in the hexagonal graphite lattice

Experimental observation of the pentagon by STM (scanning tunneling microscopy)



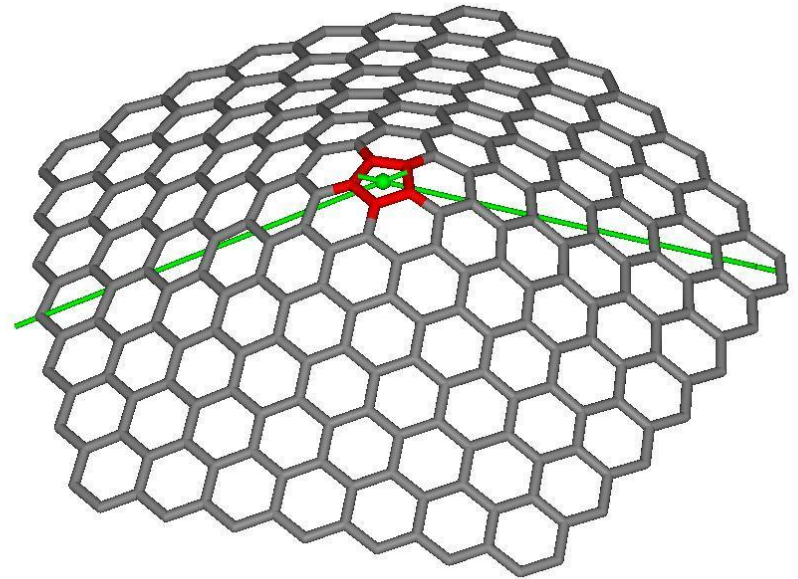
B.An et.al, Appl.Phys.Lett. 78, 3696 (2001): the enhanced charge density localized at each carbon atom in the pentagon was experimentally clarified. Typical images of the conical protuberance by STM: (a) Top view of the apex, (b) Bird's-eye view, (c) Cross section along line AA'. Five bright spots are clearly seen.

Cone geometry

Due to the symmetry of a graphite sheet only **five types of cones** can be created from a continuous sheet of graphite. The total disclinations of all these cones are multiples of 60° , corresponding to the presence of a given number (n) of pentagons at the apices.

Important: carbon nanocones with cone angles of 19° , 39° , 60° , 85° , and 113° have been observed in a carbon sample

A. Krishnan et al., *Nature* (London), **388**, 451 (1997).



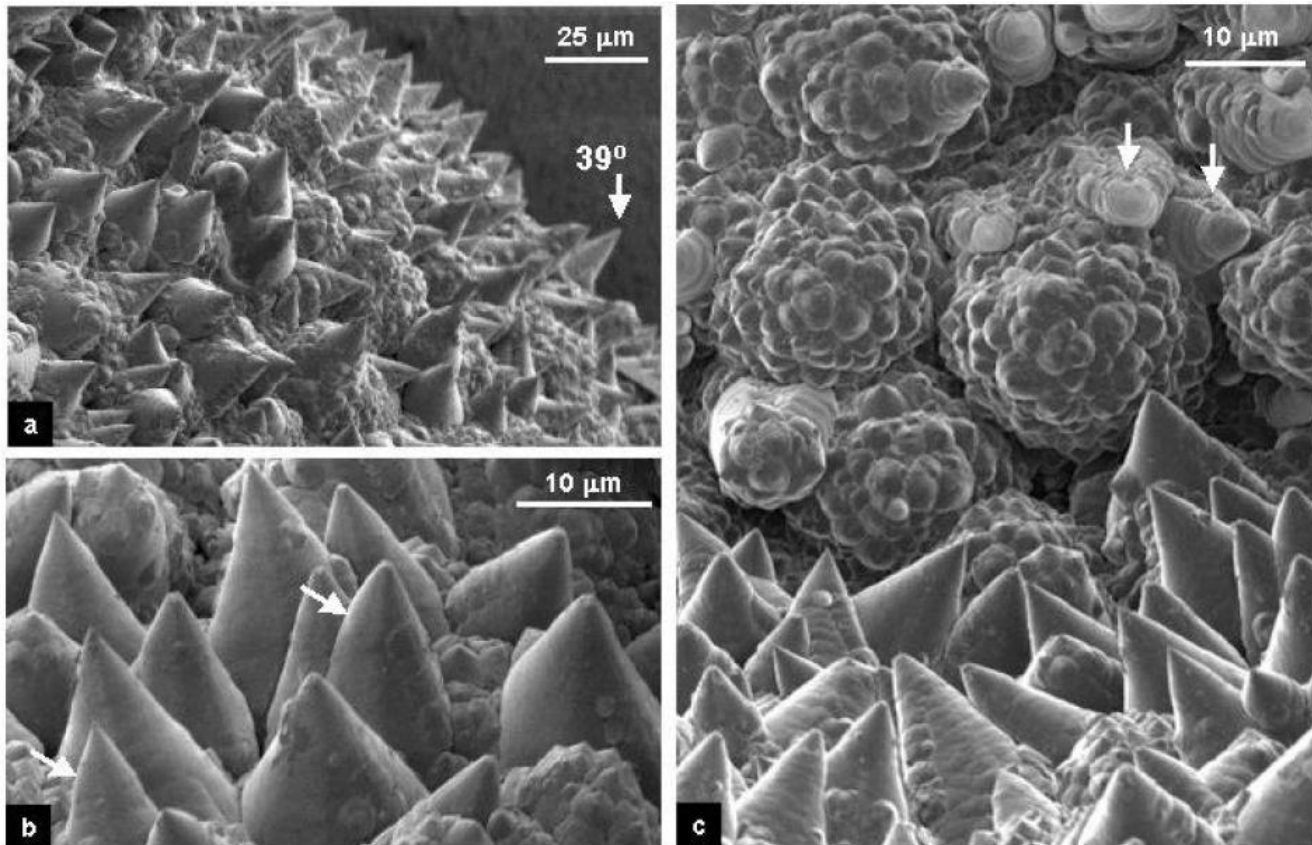


Fig. 2. FESEM images of a cone-covered graphite aggregate. (a) Low-magnification image showing complete coverage of the aggregate surface with conical structures. A $\sim 39^\circ$ cone is marked by an arrow. (b) Higher magnification image of the sample showing a variety of large cones with different apex angles and sharp and blunt tips. Arrows show changes in the apex angle. (c) Close up view of two surfaces which are almost perpendicular and show different cone morphologies – large cones on one surface and globular (artichoke-like) structures on the other. The latter ones are clusters of large-angle cones. Arrows show some of the cones that are ripped on the side

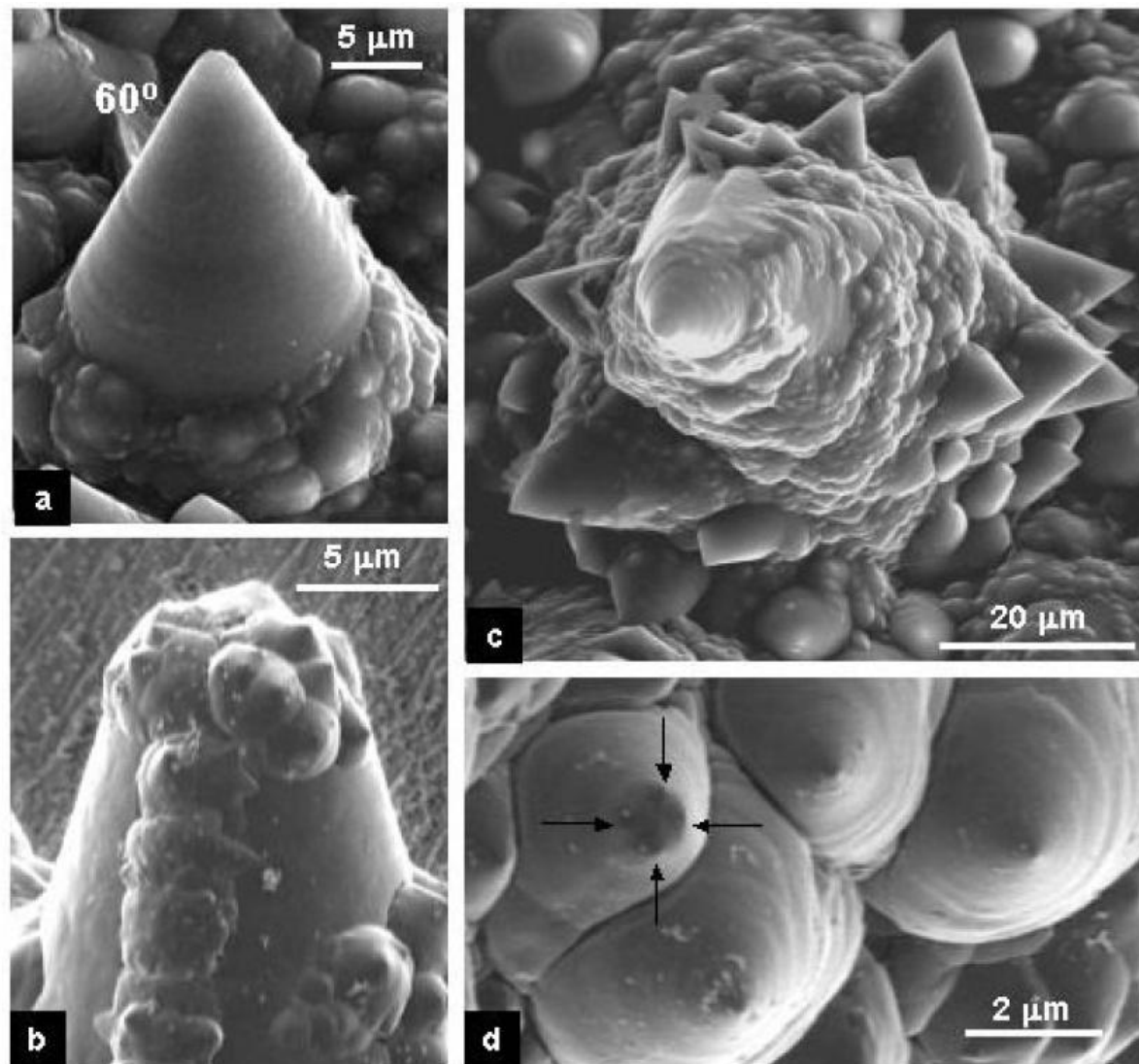
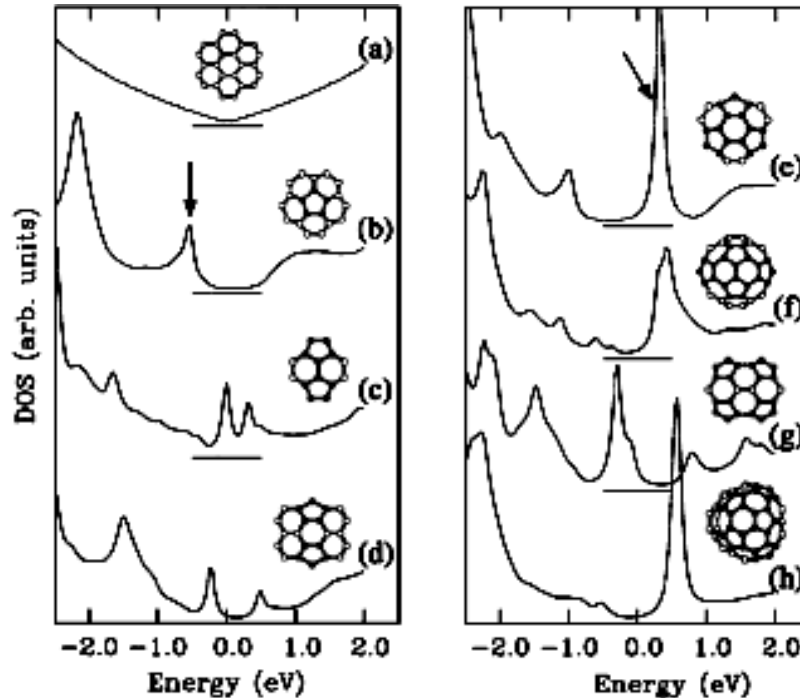


Fig. 3. Typical cone morphologies. (a) SEM image of a cone with a 60° apex angle, the most common apex angle. The slightly uneven surface of the cone suggests layer growth. (b) FESEM and (c) SEM images of large cones with numerous smaller cones growing on their surface. Smaller cones covering surfaces of large cones have a broad distribution of shapes, but large apex angles prevail (c). (d) FESEM image of four cones having sharp and broad tips (multiple tips are marked by arrows). The cones are oriented to reveal their circular cross sections around the tips and layered growth (ripples).

A presence of sharp resonant states in the region close to the Fermi energy

J.-C. Charlier and G.-M. Rignanesse, Phys. Rev.Lett. 86, 5970 (2001)

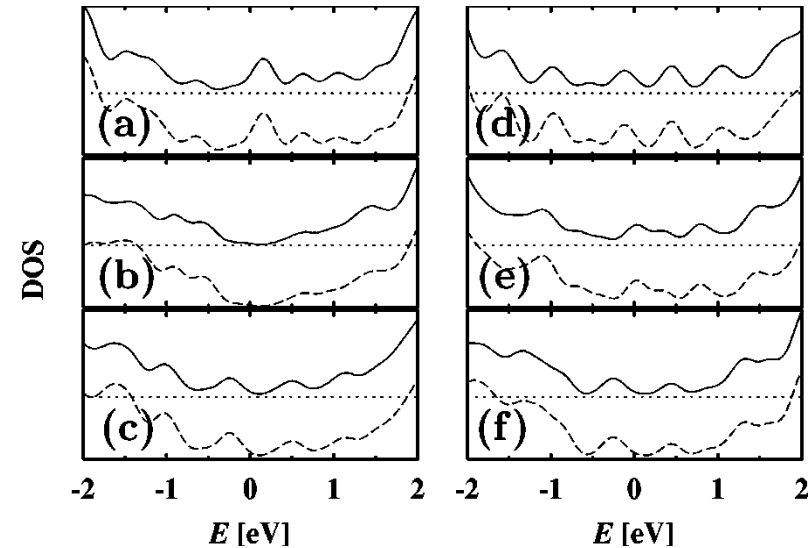
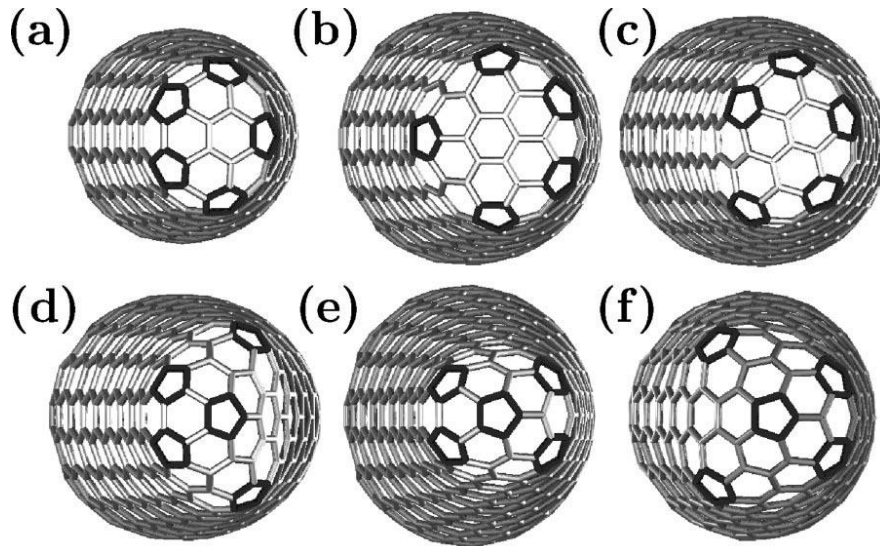


Computed tight-binding LDOS for a single graphene layer (a), and nanocones with one (b), two (c) and (d), three (e), four (f) and (g), and five (h) pentagons, respectively. The Fermi level is at zero energy.

The strength and the position of these states with respect to the Fermi level was found to depend sensitively on the number and the relative positions of the pentagons constituting the conical tip. In particular, a prominent peak which appears just above the Fermi level was found for the nanocone with three symmetrical pentagons (which corresponds to a 60° opening angle or, equivalently, to 180° disclination).

Nanohorns

Source: S. Berber et al., Phys.Rev.B 62, R2291 (2000)

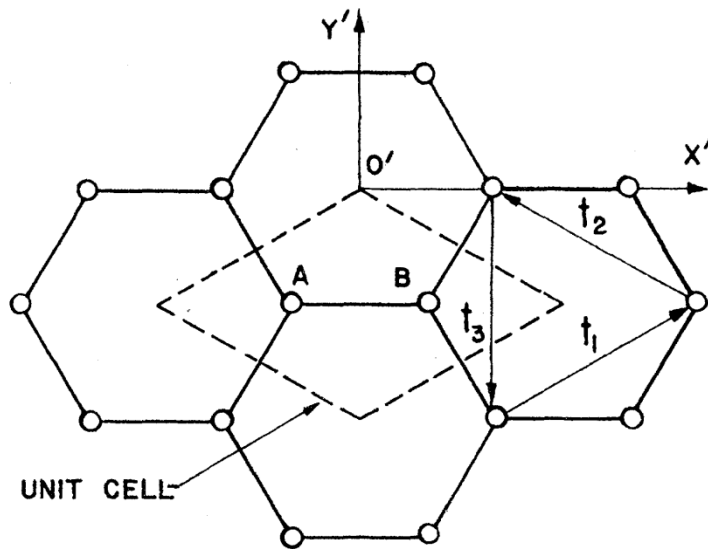


Carbon nanohorn structures with a total disclination angle of $5(\pi/3)$, containing five isolated pentagons at the terminating cap. Structures (a)–(c) contain all pentagons at the conical “shoulder,” whereas structures (d)–(f) contain a pentagon at the apex.

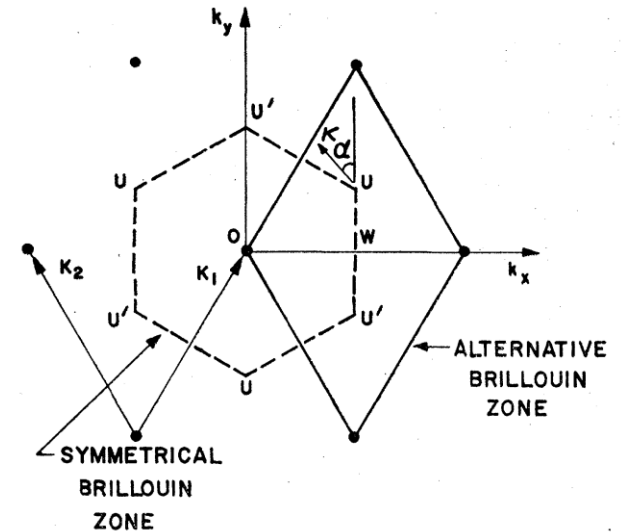
Graphite plane

J.C. Slonczewski and P.R. Weiss, Phys.Rev. 109, 272 (1958)

Real space



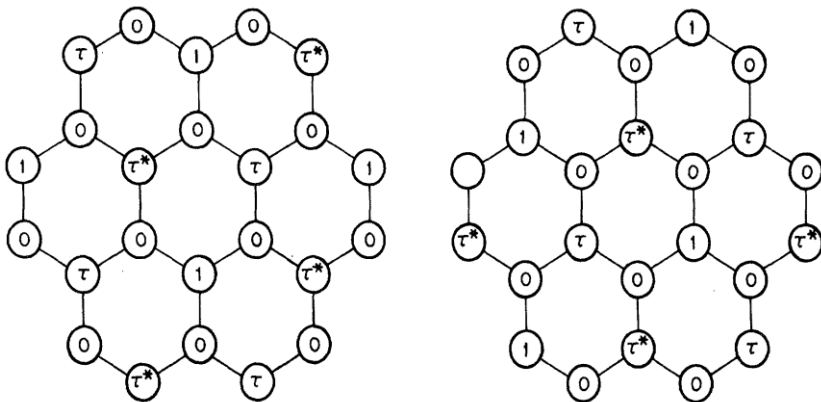
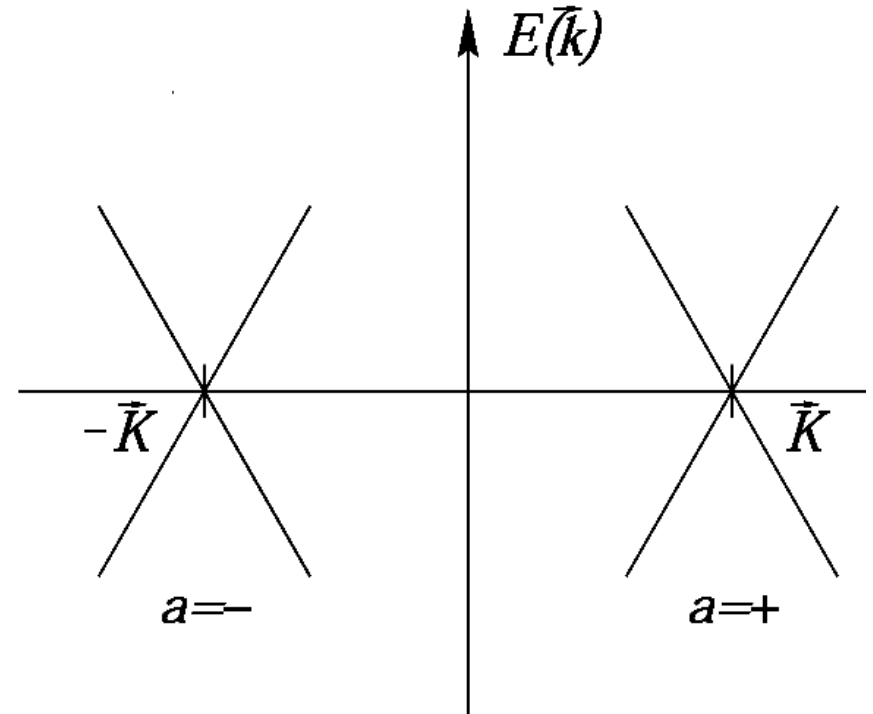
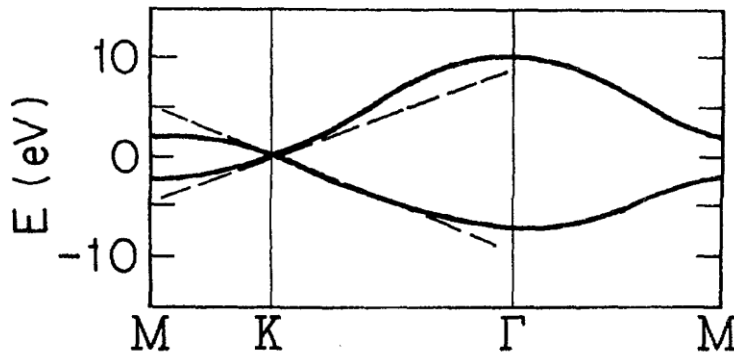
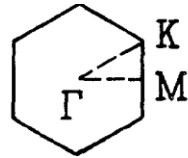
Reciprocal space



Important:

- there are two atoms per unit cell;
- there are to generate Bloch eigenstates at the Fermi point.

Lattice, spectrum



$$\tau = e^{i\frac{2\pi}{3}}$$

Energy-band structure of the bands of a two-dimensional graphite layer.

Two degenerate eigenstates which provide the basis set for the $\mathbf{k}p$ trial wave function.

Dirac equation

Step1: the effective-mass approximation, which is equivalent to the kp expansion about the K point in the Brillouin zone

$$\Psi(\mathbf{k}, \mathbf{r}) = f_1(\mathbf{k}') e^{i\mathbf{k}' \cdot \mathbf{r}} \Psi_1^S(\mathbf{K}, \mathbf{r}) + f_2(\mathbf{k}') e^{i\mathbf{k}' \cdot \mathbf{r}} \Psi_2^S(\mathbf{K}, \mathbf{r})$$

Step2: put it in the Schroedinger equation and diagonalize the secular equation for functions f_i . As a result,

$$-i\sigma^\mu \partial_\mu \psi(\mathbf{r}) = E\psi(\mathbf{r})$$

$$\psi = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$$

The most important fact is that the electronic spectrum of a single graphite plane linearized around the corners of the hexagonal Brillouin zone coincides with that of the Dirac equation in (2+1) dimensions

DOS in 2D

$$D_{oS}(E) = \frac{gV}{4\pi^2} \oint_{\epsilon=E} \frac{dS}{|\text{grad}_k \epsilon(\vec{k})|}. \quad g = 4 \text{ --degeneracy of electronic states}$$

For linear (Dirac-type) spectrum

$$D_{oS}(E) = \frac{gV|E|}{2\pi}, \quad \text{Linear in energy } E$$

Local DOS for arbitrary surface

$$LD_{oS}(E, x) = \sum_k |\psi_k(x)|^2 \delta(\epsilon(k) - E)$$

Педагогический пример

Defects in flexible membranes with crystalline order

H. S. Seung and David R. Nelson

Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138

(Received 3 March 1988)

We study isolated dislocations and disclinations in flexible membranes with internal crystalline order, using continuum elasticity theory and zero-temperature numerical simulation. These defects are relevant, for instance, to lipid bilayers in vesicles or in the L_β phase of lyotropic smectic liquid crystals. We first simulate defects in flat membranes, obtaining numerical results in good agreement with plane elasticity theory. Disclinations and dislocations eventually exhibit a buckling transition with increasing membrane radius. We generalize the continuum theory to include such buckled defects, and solve the disclination equations in the inextensional limit. The critical radius at which buckling starts to screen out internal elastic stresses is determined numerically. Computer simulation of buckled defects confirms predictions of the disclination energies and gives evidence for a finite dislocation energy.

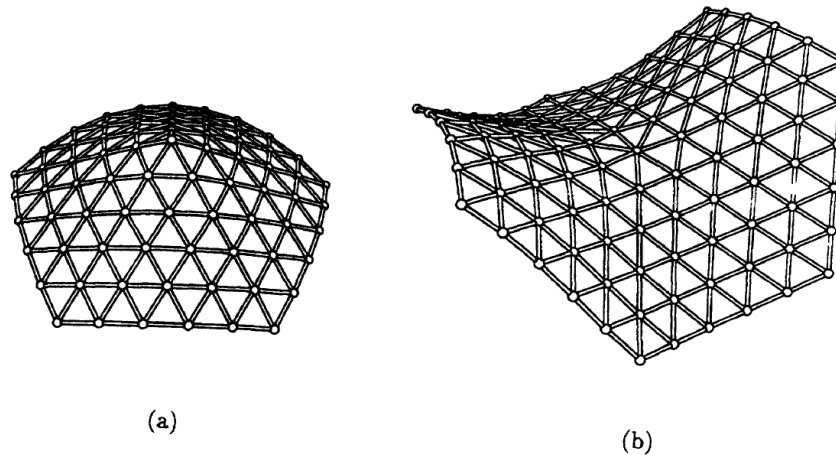


FIG. 5. (a) Buckled positive disclination ($K_0/\bar{\kappa}=2000$). (b) Buckled negative disclination ($K_0/\bar{\kappa}=2000$).

$$\kappa \nabla^4 f = \frac{\partial^2 \chi}{\partial y^2} \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 \chi}{\partial x^2} \frac{\partial^2 f}{\partial y^2} - 2 \frac{\partial^2 \chi}{\partial x \partial y} \frac{\partial^2 f}{\partial x \partial y}, \quad (4.10a)$$

$$\begin{aligned} \frac{1}{K_0} \nabla^4 \chi + \frac{\partial^2 f}{\partial x^2} \frac{\partial^2 f}{\partial y^2} - \left[\frac{\partial^2 f}{\partial x \partial y} \right]^2 \\ = \sum_{\alpha} s_{\alpha} \delta(\mathbf{r} - \mathbf{r}_{\alpha}) + \sum_{\beta} b_i^{\beta} \epsilon_{ik} \partial_k \delta(\mathbf{r} - \mathbf{r}_{\beta}). \end{aligned} \quad (4.10b)$$

For a defect-free membrane, the δ -function terms vanish, and we are left with the von Kármán equations for large deflections of thin plates.¹⁹ These coupled nonlinear partial differential equations are “very complicated, and cannot be solved exactly, even in very simple cases.”⁷

For an isolated positive disclination at the origin, we assume rotational symmetry and write Eqs. (4.10) away from the disclination core as

$$\kappa \nabla^4 f = \frac{1}{r} \frac{d}{dr} \left[\frac{d\chi}{dr} \frac{df}{dr} \right], \quad (4.11a)$$

$$\frac{1}{K_0} \nabla^4 \chi + \frac{1}{2r} \frac{d}{dr} \left[\frac{df}{dr} \right]^2 = 0, \quad (4.11b)$$

where

$$\nabla^2 = \frac{1}{r} \frac{d}{dr} r \frac{d}{dr}.$$

It is not difficult to guess a trial solution of these equations,

$$\chi = -\kappa \ln \left[\frac{r}{a} \right], \quad (4.12a)$$

$$f = \pm \left[\frac{s}{\pi} \right]^{1/2} r. \quad (4.12b)$$

Although it would appear that we have found an exact solution, comparison with the original form of the von Kármán equations (4.8) reveals that (4.12) is not a true solution because the left-hand side of Eq. (4.8b) is proportional to $\nabla^2\delta(\mathbf{r})$, while the right-hand side vanishes. If we attempt to bypass this issue by deleting a small disk of material around the origin, we create an inner boundary on which σ_{rr} and $\sigma_{r\phi}$ must vanish. One can easily calculate from the expression (4.12a) for χ that σ_{rr} behaves like $1/r^2$, so the inner boundary condition is badly violated if we excise a small disk.

Electronic properties of disclinated flexible membrane beyond the inextensional limit: application to graphene

E A Kochetov¹, V A Osipov¹ and R Pincak^{1,2}

Actually, a general solution must include a **homogeneous** term

$$\chi_0 = -\log \frac{r}{r_0} + q \frac{r}{r_0}$$

The stress tensor takes the form

$$\sigma_{rr} = -\frac{1}{r^2} + \frac{q}{rr_0}$$

$$\sigma_{rr}(r = r_0) = \sigma_0 \quad \text{yields} \quad q = 1 + \sigma_0 r_0^2$$

The stretching energy of
the membrane

$$E_s \propto \frac{\kappa^2 q^2}{K_0 r_0^2} \log \frac{R}{r_0}$$

Генерация метрики калибровочным полем

1. Поверхность вкладываем в \mathbb{R}^3

$$R_{(0)}^i(x^1, x^2)$$

2. Метрика

$$g_{ab}^{(0)} \equiv (g_{\Sigma_0})_{ab} = \partial_a \vec{R}_{(0)} \cdot \partial_b \vec{R}_{(0)}$$

инвариантна относительно вращений вектора R (группы $SO(3)$)

3. Требуем инвариантность относительно локальных вращений – генерируется новая метрика

$$g_{ab} = g_{ab}^{(0)}(\vec{W}^{(0)}) = \nabla_a \vec{R}_{(0)} \cdot \nabla_b \vec{R}_{(0)} = \partial_a \vec{R}_{(0)} \cdot \partial_b \vec{R}_{(0)} + \partial_a \vec{R}_{(0)} [\vec{W}_b^{(0)}, \vec{R}_{(0)}] + \partial_b \vec{R}_{(0)} [\vec{W}_a^{(0)}, \vec{R}_{(0)}] + (\vec{W}_a^{(0)} \vec{W}_b^{(0)}) \vec{R}_{(0)}^2 - (\vec{W}_a^{(0)} \vec{R}_{(0)}) (\vec{W}_b^{(0)} \vec{R}_{(0)}).$$

Пример

$$W_{\mu}^{(0)i=1,2} = 0 \text{ and } W_{\mu}^{(0)i=3} = W_{\mu}^{(0)}$$

$$W_x^{(0)} = \nu y / r^2, \quad W_y^{(0)} = -\nu x / r^2, \quad r = \sqrt{x^2 + y^2} \neq 0$$

$$\oint_C W_a^{(0)} dx^a = -2\pi\nu \neq 0$$

Плоскость

$$(r, \varphi) \rightarrow (r \cos \varphi, r \sin \varphi, 0), \quad 0 < r < \infty, \quad 0 \leq \varphi < 2\pi.$$

ПЛЮС

$$W_r^{(0)} = 0, \quad W_{\varphi}^{(0)} = -\nu \quad \text{дает метрику конуса}$$

$$g_{rr} = 1, \quad g_{\varphi\varphi} = \alpha^2 r^2, \quad g_{r\varphi} = g_{\varphi r} = 0.$$

Back to the Dirac equation

The Dirac equation on an arbitrary surface in the presence of the gauge field a_b and the external magnetic field with the vector potential A_b is written as

$$i\gamma^\alpha e_\alpha^b [\nabla_b - ia_b - iA_b]\psi = E\psi$$

with $\nabla_b = \partial_b + \Omega_b$

Geometrical characteristics

Covariant derivative

$$\nabla_{\mu} = \partial_{\mu} + \Omega_{\mu}$$

Spin connection term

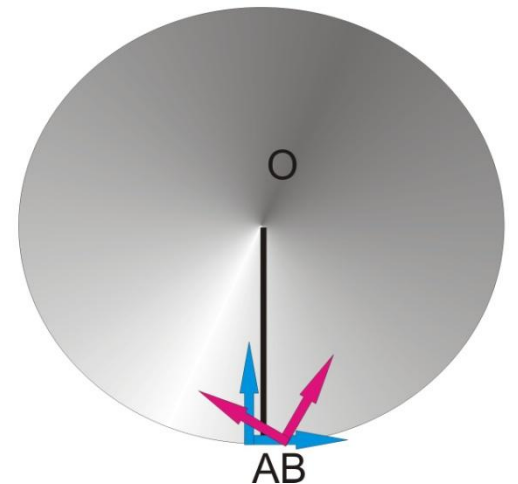
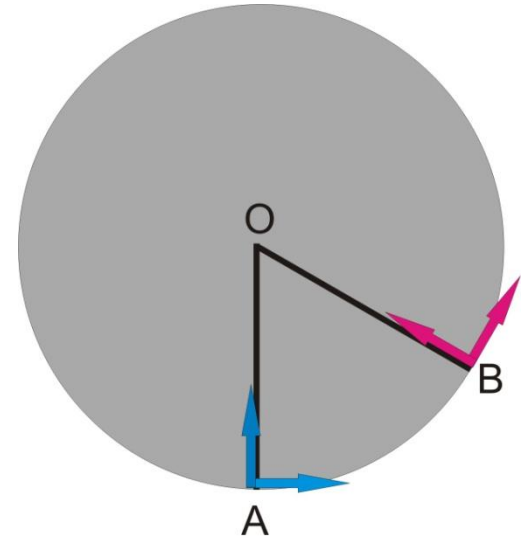
$$\Omega_{\mu} = (1/8)\omega_{\mu}^{\alpha\beta}[\sigma_{\alpha}, \sigma_{\beta}]$$

Spin connection coefficients:

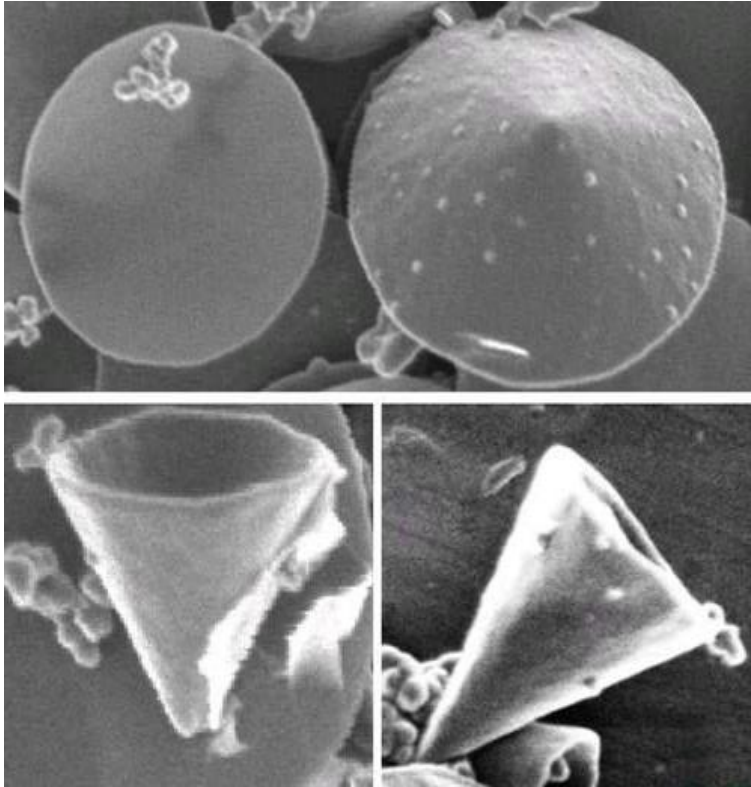
$$(\omega_{\mu})^{ab} = e_{\nu}^a(\partial_{\mu}e^{\nu b} - \Gamma_{\mu\chi}^{\nu}e^{\chi b}) = -(\omega_{\mu})^{ba}$$

Metric connection coefficients

$$\Gamma_{\mu\lambda}^{\nu} = \frac{g^{\nu\chi}}{2}(\partial_{\mu}g_{\chi\lambda} + \partial_{\lambda}g_{\chi\mu} - \partial_{\chi}g_{\mu\lambda})$$



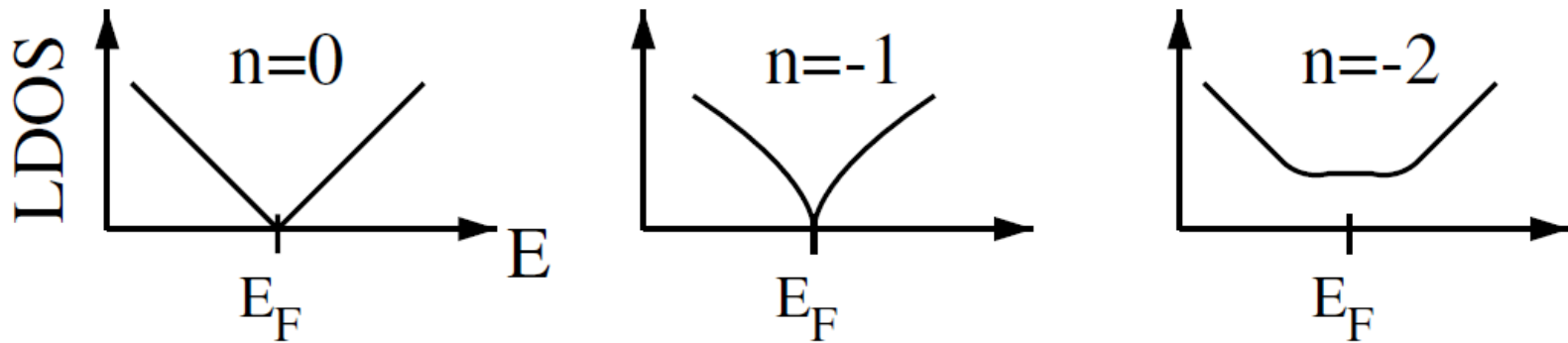
Elastic membrane



- The principally new model was formulated and applied to study the structure of the low energy electronic states of flexible graphene membrane with a topological defect.
- E.A. Kochetov, V.A. Osipov, and R. Pincak, *J. Phys.: Condens. Matter* **22** (2010)

SEM images of a carbon disk (top left image) and free-standing hollow carbon nanocones produced by pyrolysis of heavy oil

Schematic densities of states for a small patch near the apex of a cone at zero magnetic field and $K_0 \rightarrow \infty$

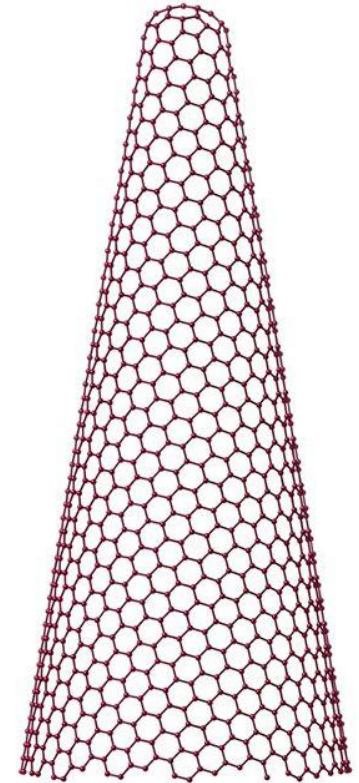
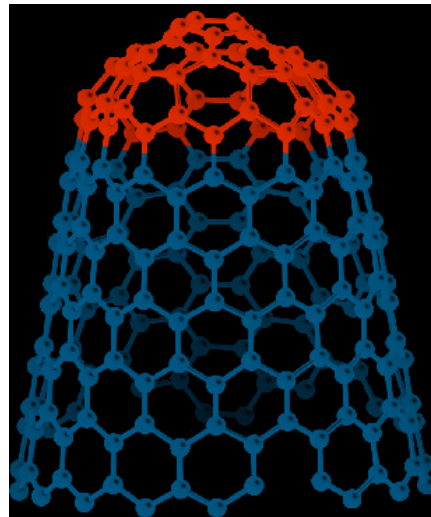
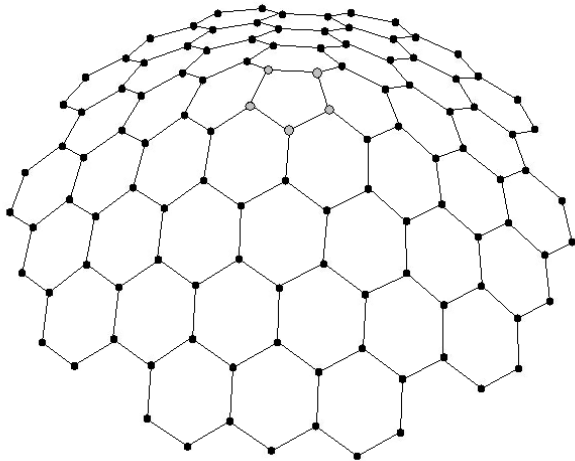


However, a cone with a point-like apex is a mathematical abstraction since in a real situation the media has a finite stiffness, which would inevitably result in a certain smearing of a conical singularity.

Nanocones: another geometry

Upper half of a two-sheet hyperboloid

$$(\chi, \varphi) \rightarrow (a \sinh \chi \cos \varphi, a \sinh \chi \sin \varphi, c \cosh \chi)$$



is suitable for the description of cone-like structures with pentagons situated at a smoothed apex. The most appropriate model for nanohorns with five pentagons at the tip.

However, one cannot incorporate finite elasticity into the theory by simply replacing a cone by a smooth surface that asymptotically approaches a cone far away from the origin. This would simply eliminate the defect. To illustrate this, consider an upper half of a hyperboloid as an embedding

$$(\xi, \varphi) \rightarrow (a \sinh \xi \cos \varphi, a \sinh \xi \sin \varphi, c \cosh \xi)$$
$$0 \leq \xi < \infty, \quad 0 \leq \varphi < 2\pi.$$

The components of the induced metric can be written as

$$g_{\xi\xi} = a^2 \cosh^2 \xi + c^2 \sinh^2 \xi, \quad g_{\varphi\varphi} = a^2 \sinh^2 \xi$$
$$g_{\varphi\xi} = g_{\xi\varphi} = 0,$$

which gives for the spin connection coefficients

$$\omega_{\xi}^{12} = \omega_{\xi}^{21} = 0,$$
$$\omega_{\varphi}^{12} = -\omega_{\varphi}^{21} = \left[1 - \frac{a \cosh \xi}{\sqrt{g_{\xi\xi}}} \right] =: \omega(\xi)$$

Since $\omega(\xi)$ goes to zero as $\xi \rightarrow 0$ a circulation of that field over a loop encircling the origin gives a flux which tends to zero as the counter shrinks to zero:

$$\lim_{\epsilon \rightarrow 0} \oint_{C_{\epsilon}} \omega_{\varphi}^{12} d\varphi = 0,$$

To incorporate flux we suggest the following metrics

$$g_{\xi\xi} = a^2 \cosh^2 \xi + c^2 \sinh^2 \xi,$$

$$g_{\varphi\varphi} = a^2 \alpha^2 \sinh^2 \xi, \quad g_{\varphi\xi} = g_{\xi\varphi} = 0,$$

with $\alpha = 1 - \nu$

This metric generates the spin connection term

$$\omega_{\varphi}^{12} = -\omega_{\varphi}^{21} = \left[1 - \frac{a\alpha \cosh \xi}{\sqrt{g_{\xi\xi}}} \right] = \omega_{\alpha}(\xi)$$

and now

$$\lim_{\epsilon \rightarrow 0} \oint_{C_{\epsilon}} \omega_{\varphi}^{12} d\varphi = 2\pi \nu.$$

$$\partial_\xi \tilde{u} - \frac{(j + 1/2 - a_\varphi + A_\varphi)}{\alpha} \sqrt{\coth^2 \xi + \eta \tilde{u}} = \tilde{E} \tilde{v},$$

$$-\partial_\xi \tilde{v} - \frac{(j + 1/2 - a_\varphi + A_\varphi)}{\alpha} \sqrt{\coth^2 \xi + \eta \tilde{v}} = \tilde{E} \tilde{u},$$

$$\eta \sim \sqrt{\nu \epsilon}.$$

$$\epsilon = \kappa / (K_0 r_0^2)$$

The zero-energy mode

$$\begin{aligned} \tilde{u}_0(\xi) = & C (\Delta + k \cosh \xi)^{k\tilde{j} + \frac{\eta\tilde{\Phi}}{2k}} \left(\frac{\Delta + \cosh \xi}{\sinh \xi} \right)^{-\tilde{j}} \\ & \times \exp\left(-\frac{\tilde{\Phi} \Delta \cosh \xi}{2}\right), \end{aligned}$$

$$\begin{aligned} \tilde{v}_0(\xi) = & C' (\Delta + k \cosh \xi)^{-k\tilde{j} - \frac{\eta\tilde{\Phi}}{2k}} \left(\frac{\Delta + \cosh \xi}{\sinh \xi} \right)^{\tilde{j}} \\ & \times \exp\left(\frac{\tilde{\Phi} \Delta \cosh \xi}{2}\right), \end{aligned}$$

where

$$k = \sqrt{1 + \eta}; \quad \Delta = \Delta(\xi) = \sqrt{1 + k^2 \sinh^2 \xi},$$

$$\tilde{j} = (j + 1/2 - a_\varphi)/\alpha, \quad \tilde{\Phi} = \Phi/\alpha,$$

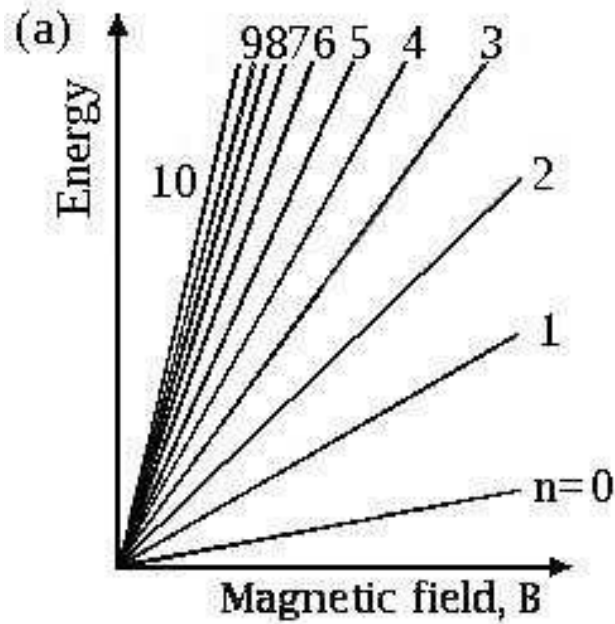
Landau states

$$E_n^0 = \pm\sqrt{2n}, \quad n = 0, 1, 2, \dots,$$

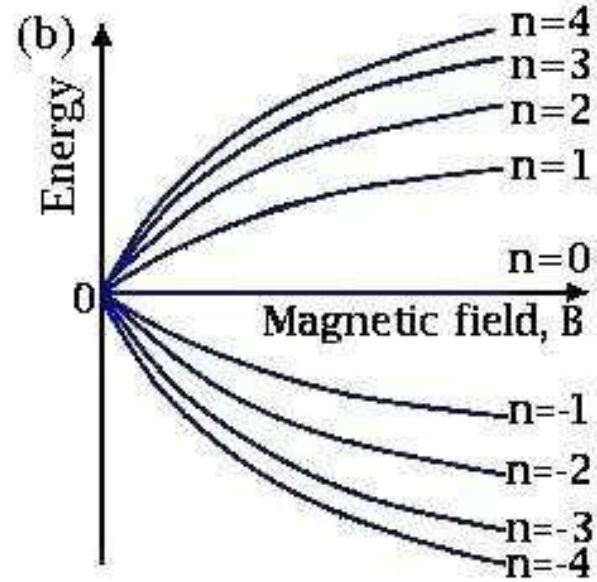
where the energy is measured in units of $\hbar v_F/l_B$ with the magnetic length $l_B = (\hbar c/eB)^{1/2}$.

$$E_{n=1}^\eta \simeq \pm\sqrt{2} \pm \eta \frac{\Gamma}{2\sqrt{2}} \simeq \pm\sqrt{2} \pm 0.3\eta,$$

Landau levels



(a) обычные

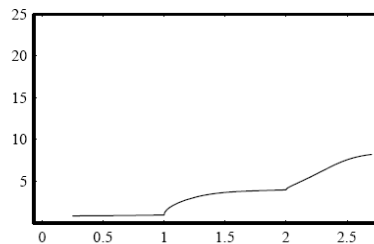
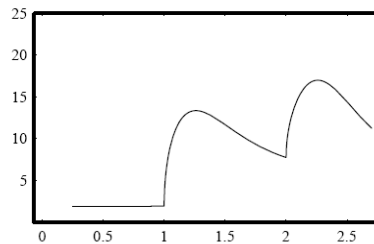
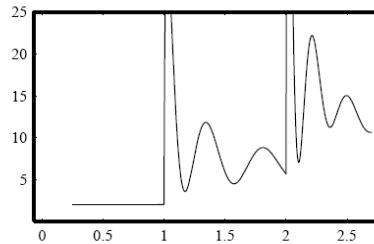


(b) в графене

Electronic structure

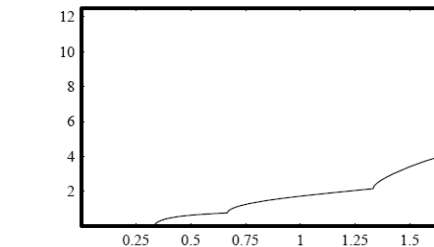
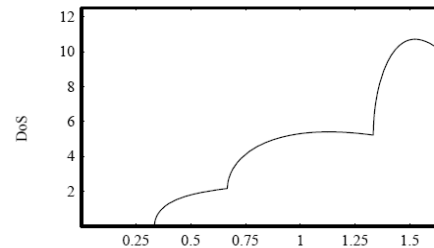
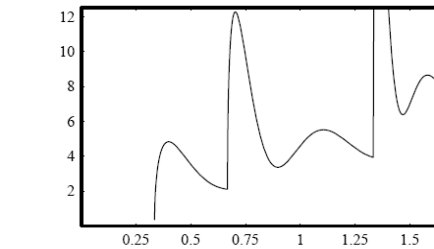
Carbon nanotubes (closed)

metallic



E

semiconducting



E



Far from the cap (top), near (middle), in the cap (bottom)

ФИЗИКА ЭЛЕМЕНТАРНЫХ ЧАСТИЦ И АТОМНОГО ЯДРА
2009. Т. 40. ВЫП. 4

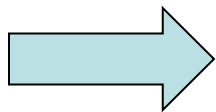
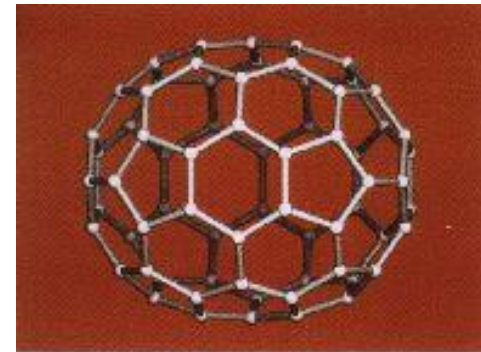
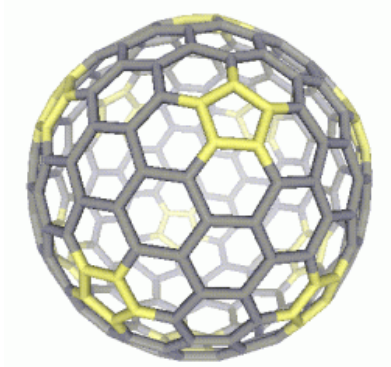
ТЕОРЕТИКО-ПОЛЕВОЙ ПОДХОД К ОПИСАНИЮ
ЭЛЕКТРОННЫХ СВОЙСТВ УГЛЕРОДНЫХ
НАНОСТРУКТУР

Д. В. Колесников *, *В. А. Осипов* **

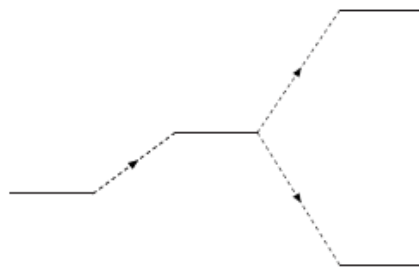
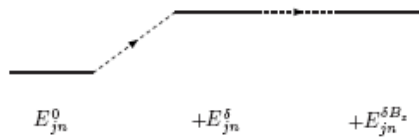
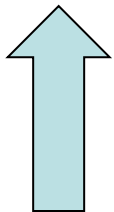
Объединенный институт ядерных исследований, Дубна

Electronic structure

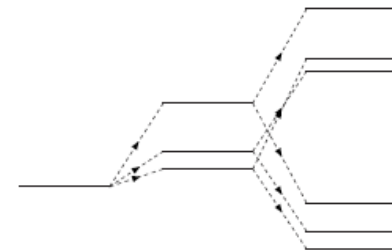
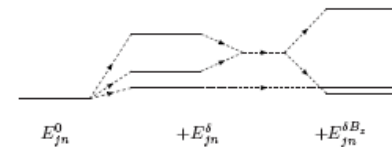
Spherical and spheroidal fullerenes



B



The first electronic level



The second electronic level

Zeeman splitting

Поликристаллический графен

Grains and grain boundaries in single-layer graphene atomic patchwork quilts

Pinshane Y. Huang^{1*}, Carlos S. Ruiz-Vargas^{1*}, Arend M. van der Zande^{2*}, William S. Whitney², Mark P. Levendorf³, Joshua W. Kevek⁴, Shivank Garg³, Jonathan S. Alden¹, Caleb J. Hustedt⁵, Ye Zhu¹, Jiwoong Park^{3,6}, Paul L. McEuen^{2,6} & David A. Muller^{1,6}

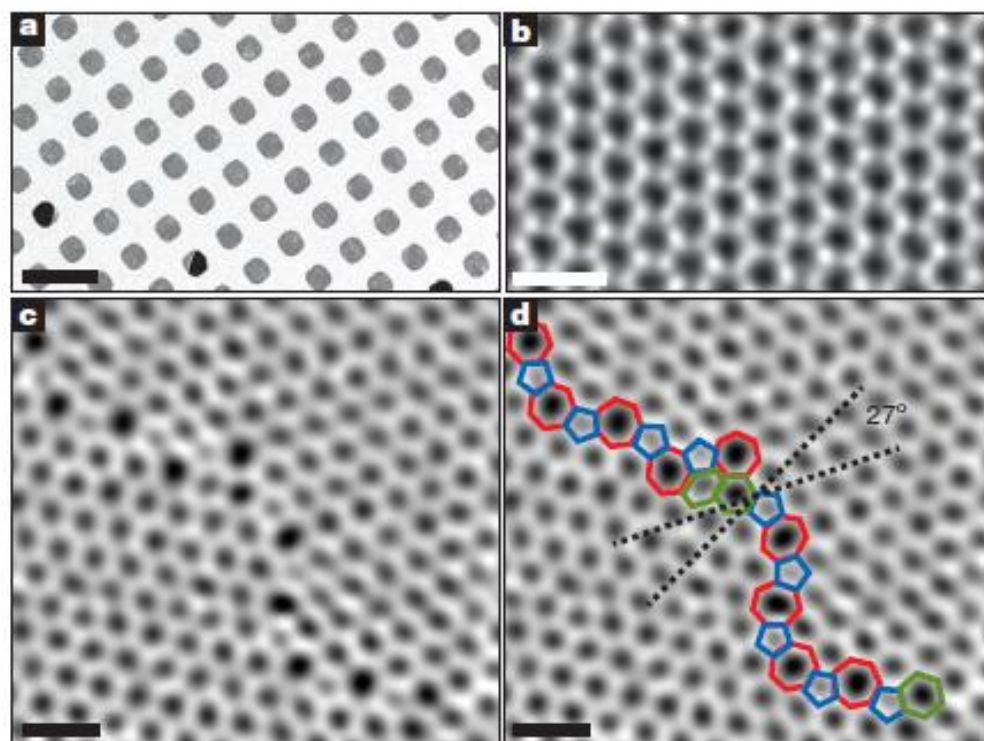
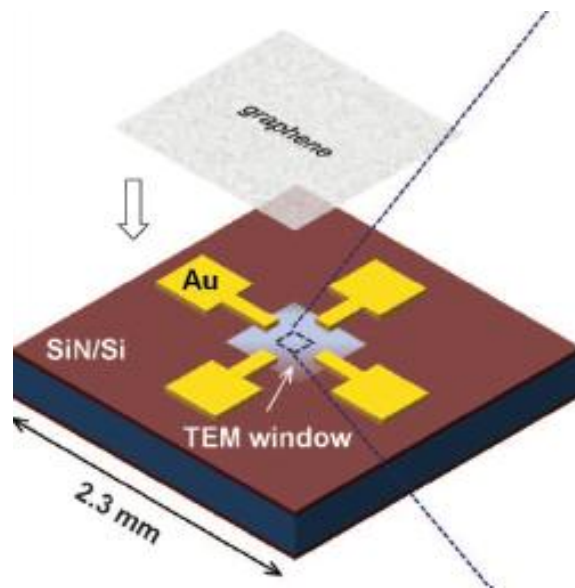


Figure 1 | Atomic-resolution ADF-STEM images of graphene crystals.

Tailoring Electrical Transport Across Grain Boundaries in Polycrystalline Graphene

Adam W. Tsen,¹ Lola Brown,² Mark P. Levendorf,² Fereshte Ghahari,³ Pinshane Y. Huang,¹ Robin W. Havener,¹ Carlos S. Ruiz-Vargas,¹ David A. Muller,^{1,4} Philip Kim,³ Jiwoong Park^{2,4*}



Low-temperature thermal conductivity in polycrystalline graphene

D. V. KOLESNIKOV and V. A. OSIPOV

*Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research
141980 Dubna, Moscow region, Russia*

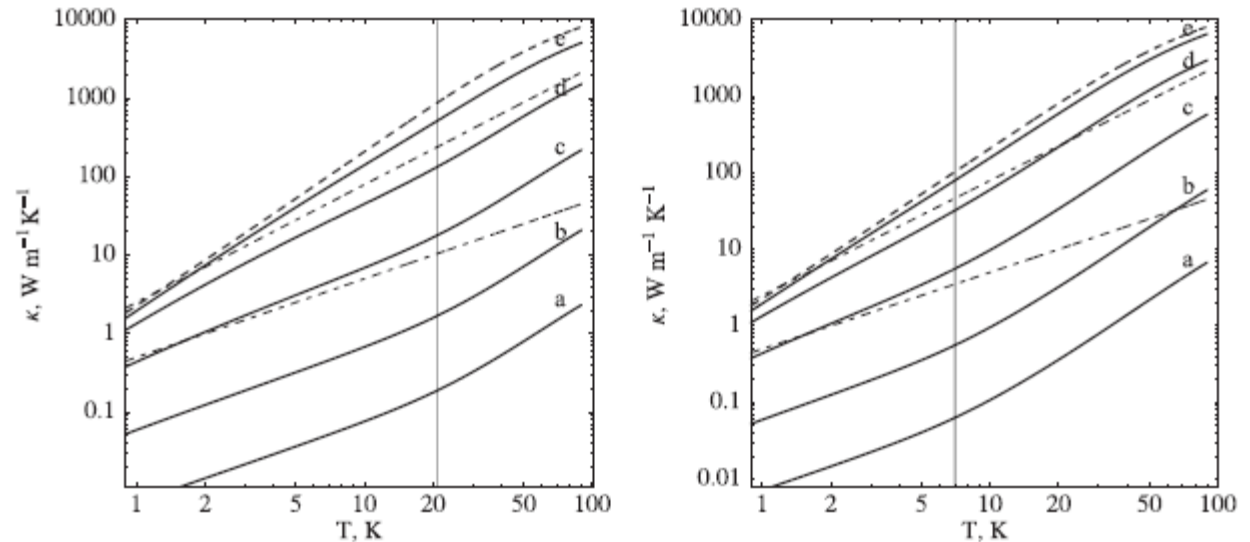
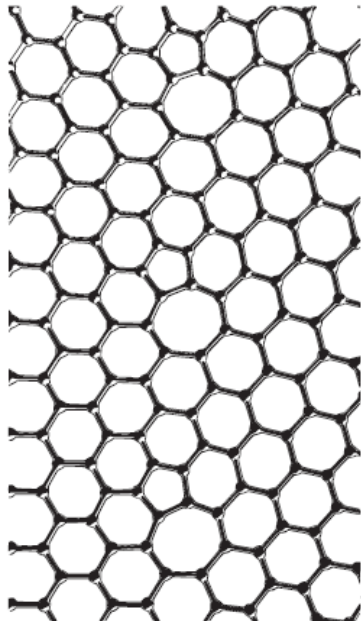


Fig. 2: The total thermal conductivity of polycrystalline graphene with high-angle grain boundaries for $L = 2.46$ nm (left) and $L = 7.38$ nm (right) at different packing coefficients: (a) $a/L = 0$, (b) $a/L = 2$, (c) $a/L = 9$, (d) $a/L = 30$, and (e) $a/L = 100$ (see table 2). The dashed curve corresponds to the case of the graphene single crystal. The dot-dashed straight lines show $T^{1.5}$ and T . The approximate crossover temperatures are indicated with vertical lines.

Field emission

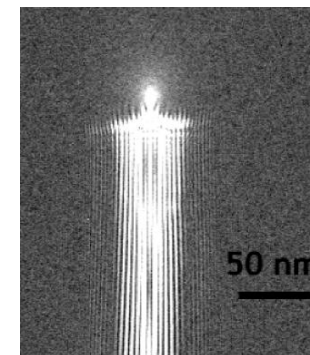
graphite

carbon nanotubes

few-layer graphene

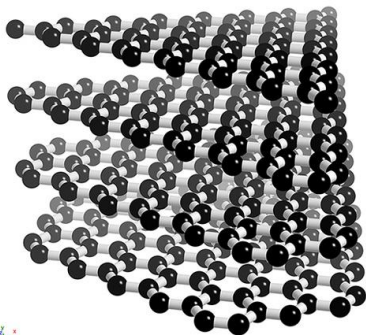
EFFECT OF BAND STRUCTURE ON FIELD EMISSION

Katkov V.L., Osipov V.A.: J. Phys.: Cond. Matt. 20 (2008) 035204

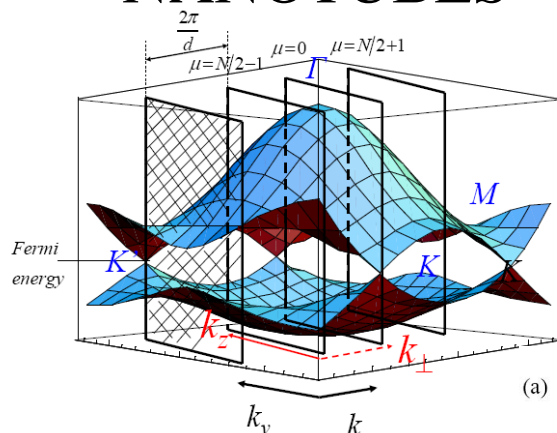
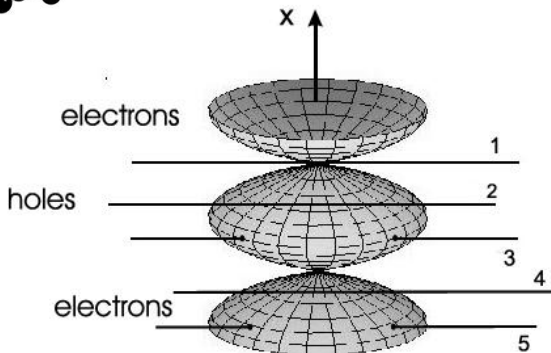


GRAPHITE

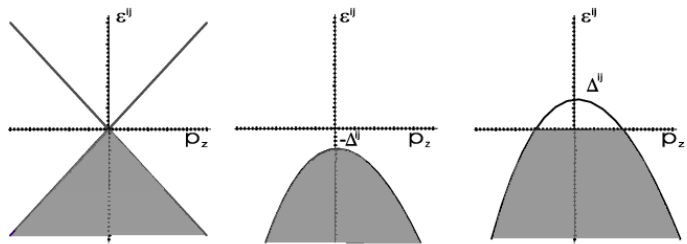
NANOTUBES



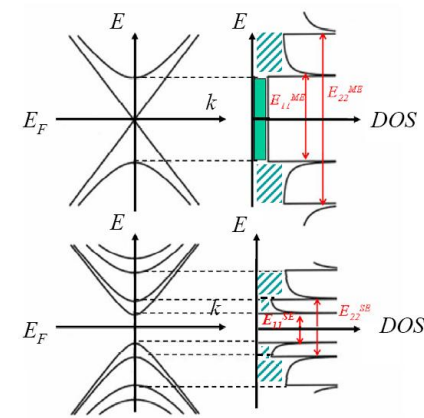
3D



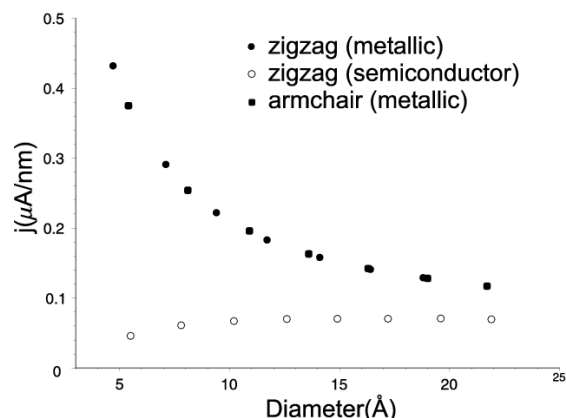
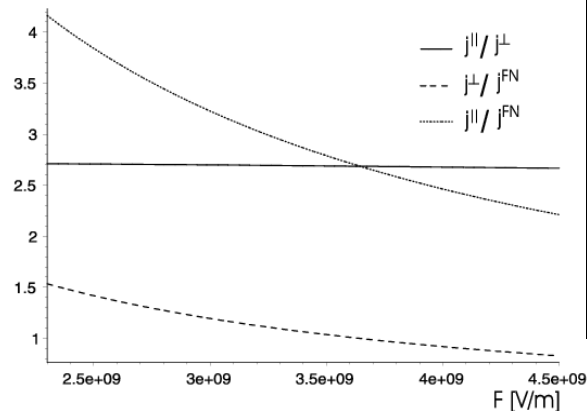
2D



Both cases were reduced to 1D problem.

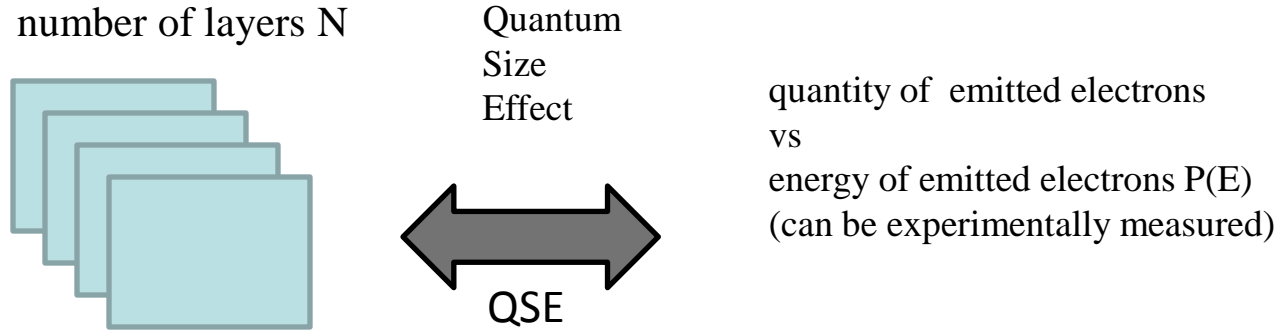


Field emission law for graphite in two orientations.

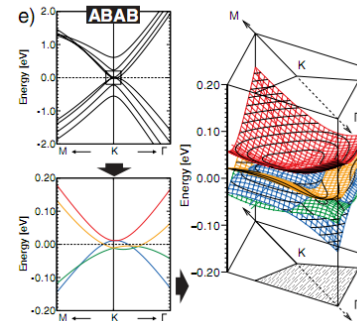
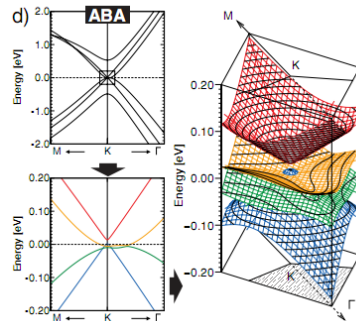
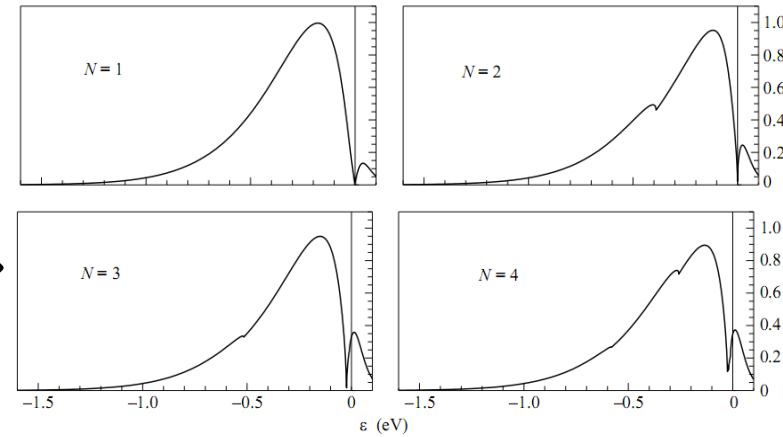
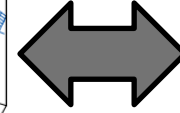
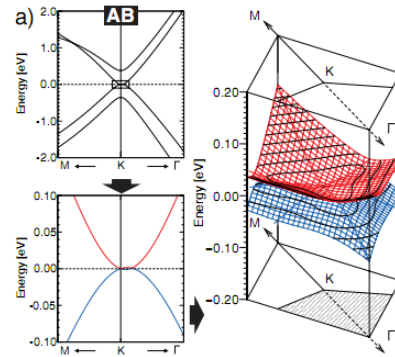
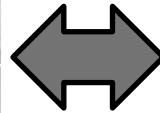
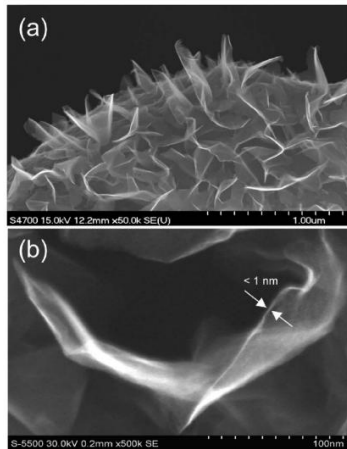


Analytical expressions explain numerical calculations.

Energy distribution of field emitted electrons from carbon nanosheets: manifestation of the quantum size effect



FLG



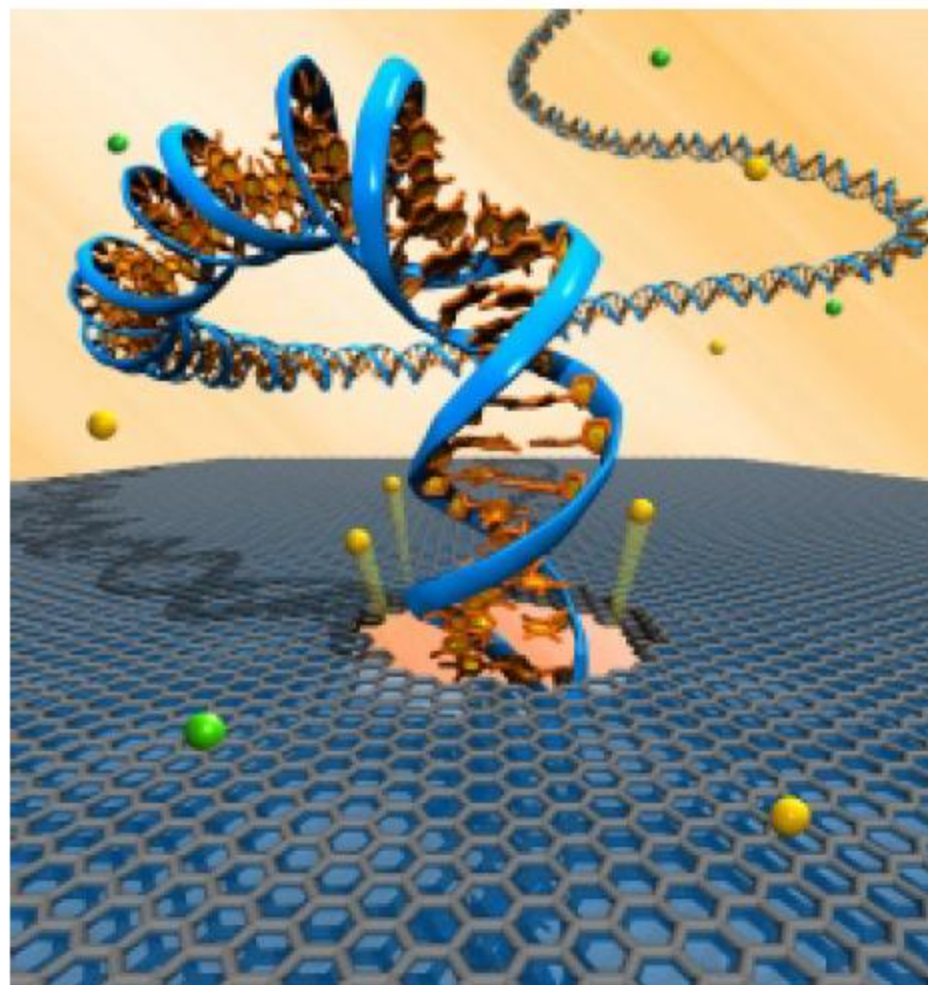
$$P(\epsilon) = \frac{2g}{v_F} f(\epsilon) D(\epsilon) \sum_{n=1}^{n=N} \theta(\epsilon_n) \sqrt{|\epsilon| \epsilon_n}$$

$$\epsilon_n = |\epsilon| + \gamma_1^n, \quad g = 4e / (h^2 N c)$$

Первый шаг к электронному анализу последовательности ДНК: перемещение через нанопоры в графене

(Июль 23, 2010)

(Pennsylvania University,
Philadelphia, USA)

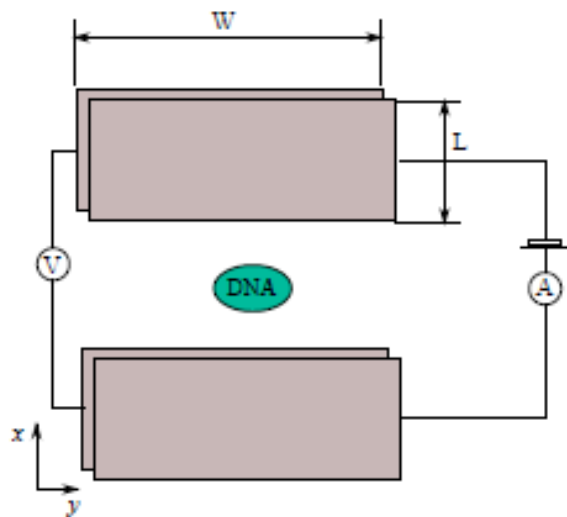


Resonant Tunneling In Graphene-DNA Base-Graphene Junctions

V.L. Katkov, O.G. Isaeva and V.A. Osipov

Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna,
Russia

Наши расчеты



Схематическое изображение устройства

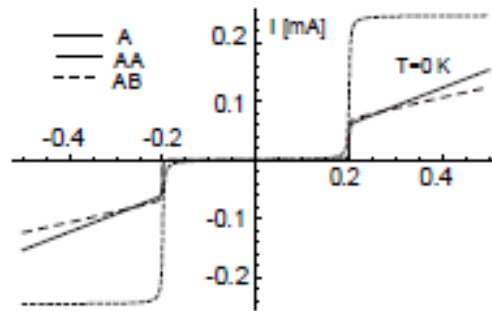


Рис. 2. $I - V$ характеристика туннельного контакта при нулевой температуре

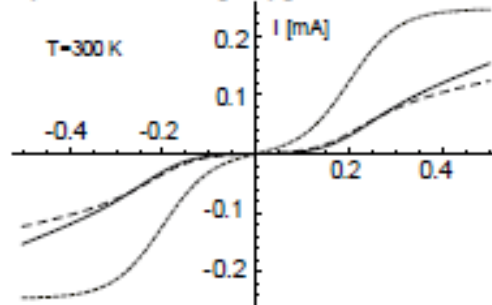


Рис. 4. $I - V$ характеристика туннельного контакта при комнатной температуре.

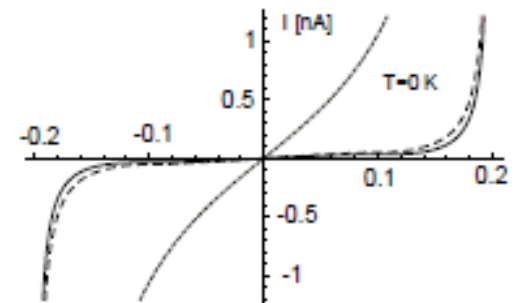


Рис. 3. Центральная часть вольт-амперной характеристики

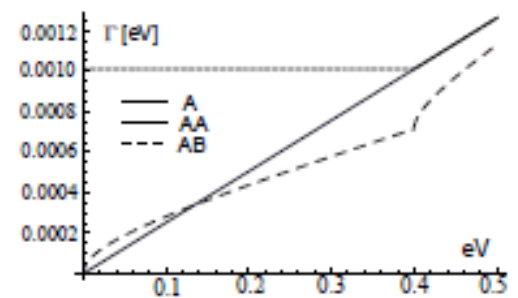


Рис. 5. Зависимость темпа тунnelирования от энергии, отсчитанной от уровня Ферми