計算科学の戦略と次世代スーパーコンピュータ

つくば市（２００６年４月４日）

ナノ・バイオ分野 ディスカッション

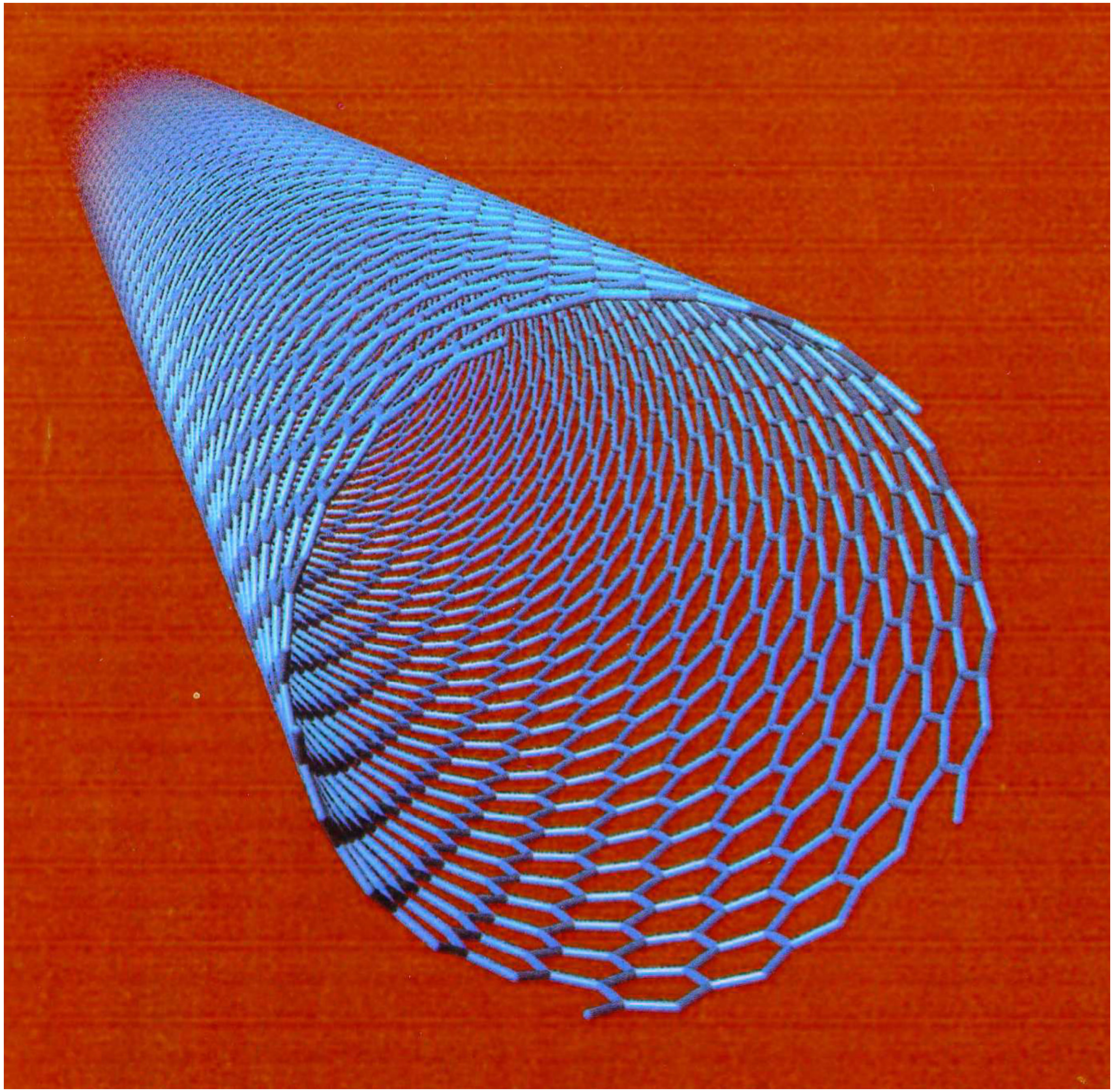
炭素ナノ科学と大規模計算

東京工業大学･物性物理学専攻
量子ナノ物理学研究センター

斎藤　晋

OUTLINE

- ◆ なぜ「炭素」か
- ◆ 次世代スーパーコンピュータの必要性

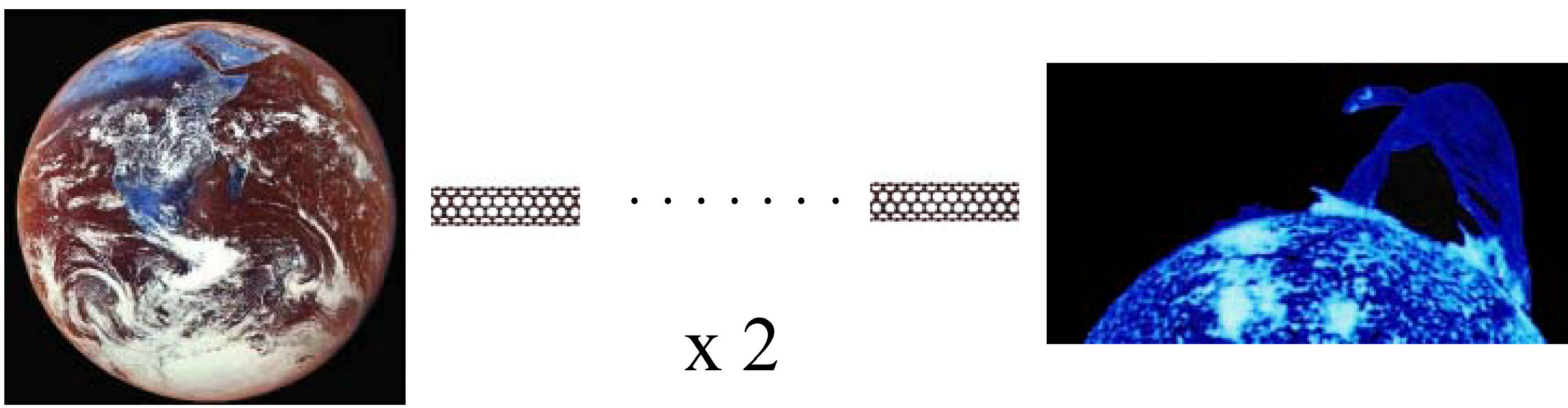


カーボンナノチューブ

カーボンナノチューブの「細さ」

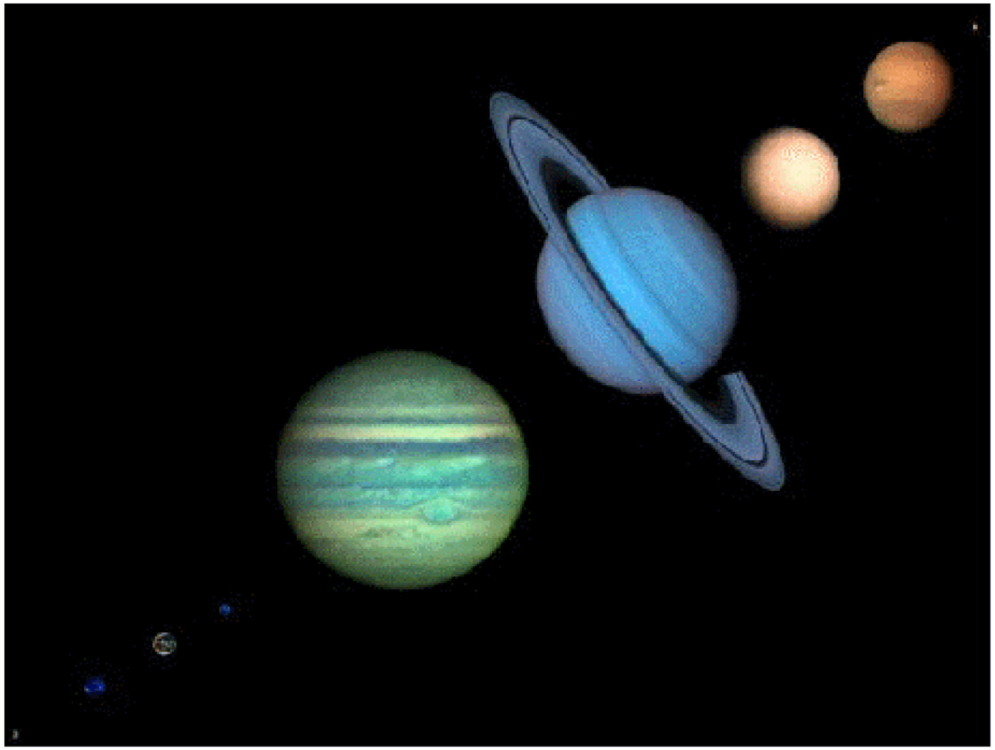
Q: １gのナノチューブの長さは？

Answer: Two astronomical units!!



for (10,10) CNT

カーボンナノチューブの「細さ」



Sun – Neptune:

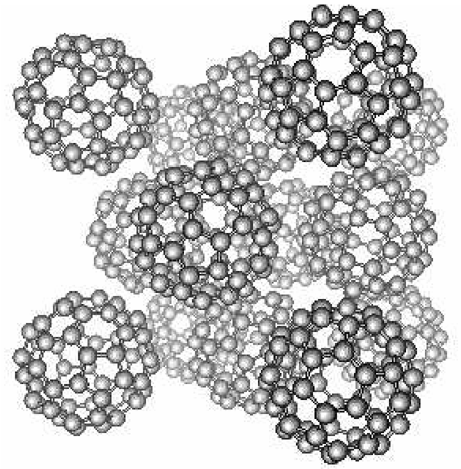
15g is enough!

カーボンナノチューブの「細さ」

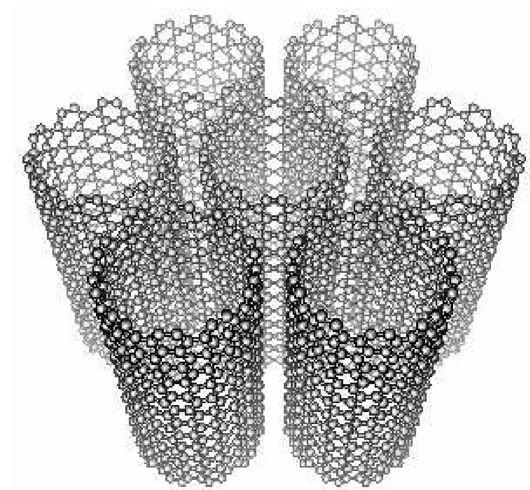
Diameter of galaxy
(100,000 light years):

30,000 kg

Various Nanostructured Carbon Materials



Solid C_{60}

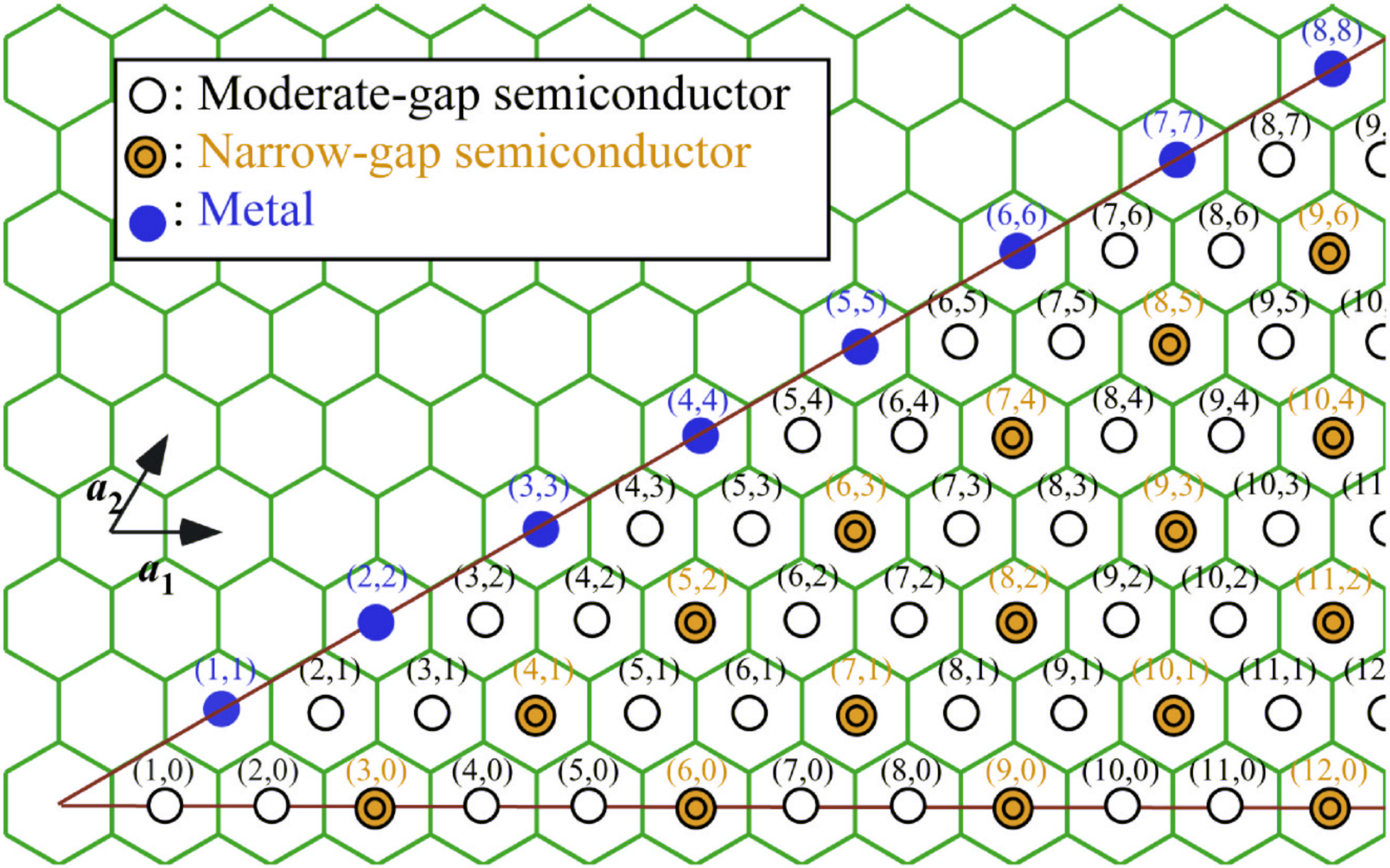


Crystalline CNT

C_{60}@(10,10) ("Peapod")

構造と物性に無限のバリエーション！

カーボンナノチューブの構造と物性

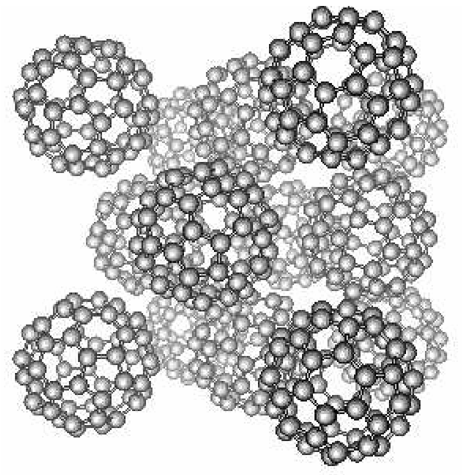


カーボンナノチューブの構造と物性

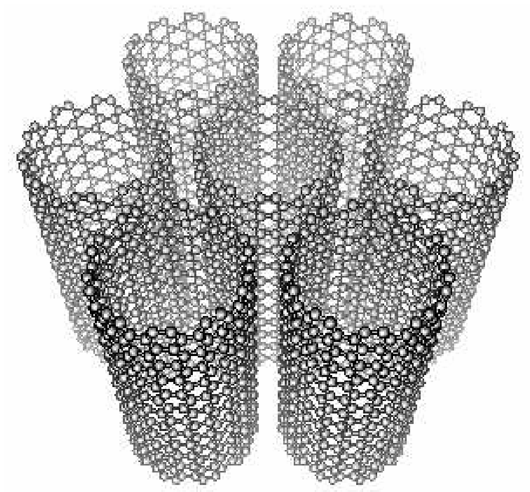
- 結合長:　１．４２（Å）？　１．４１？？　１．４３　？？？
- 結合角:　１２０°　？　１１８°　？？　１２２°　？？？
- エネルギーギャップ:　0.5 eV ?　1.0 eV ??　1.5 eV ???

第一原理電子構造計算による予言研究の重要性

Various Nanostructured Carbon Materials



Solid C_{60}



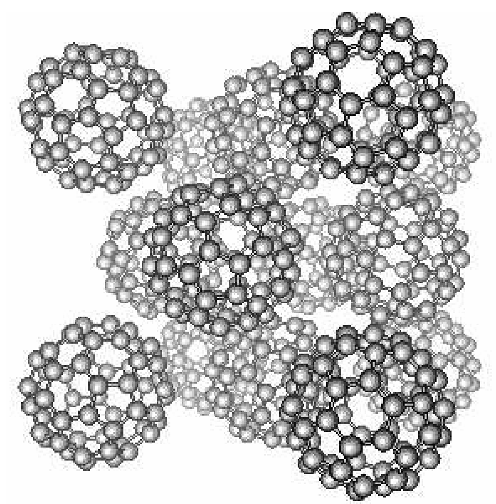
Crystalline CNT

C_{60}@(10,10) ("Peapod")

Precursors to even more interesting new phases via *P* & *T* treatments

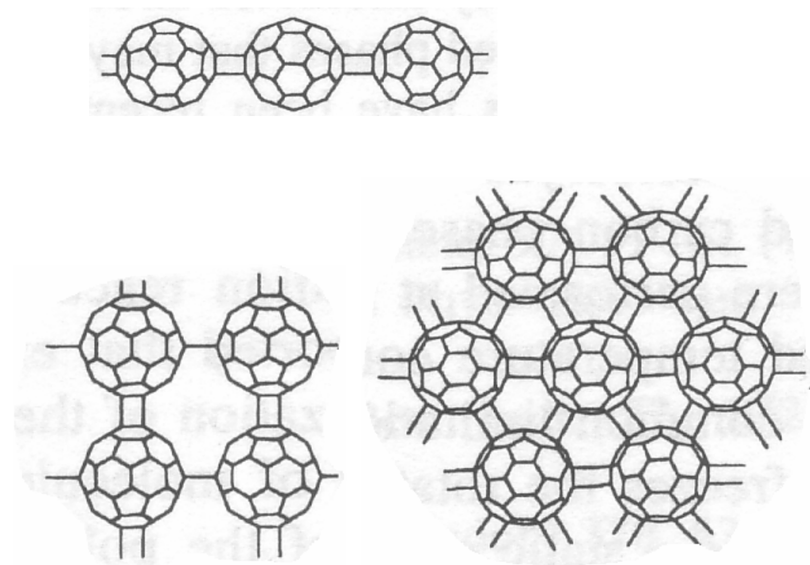
Polymerization of Fullerenes

[1] Y. Iwasa et al: Science **264**, 1570 (1994)
[2] M. Núñez-Regueiro et al: Phys. Rev. Lett. **74**, 278 (1995)



Solid C_{60}

P (and T) →



→ New dimensionality; *sp*^{2}-*sp*^{3} hybrid system

Constant-P Molecular Dynamics

M. Parrinello and A. Rahman: Phys. Rev. Lett. **45**, 1196 (1980)

Lagrangian

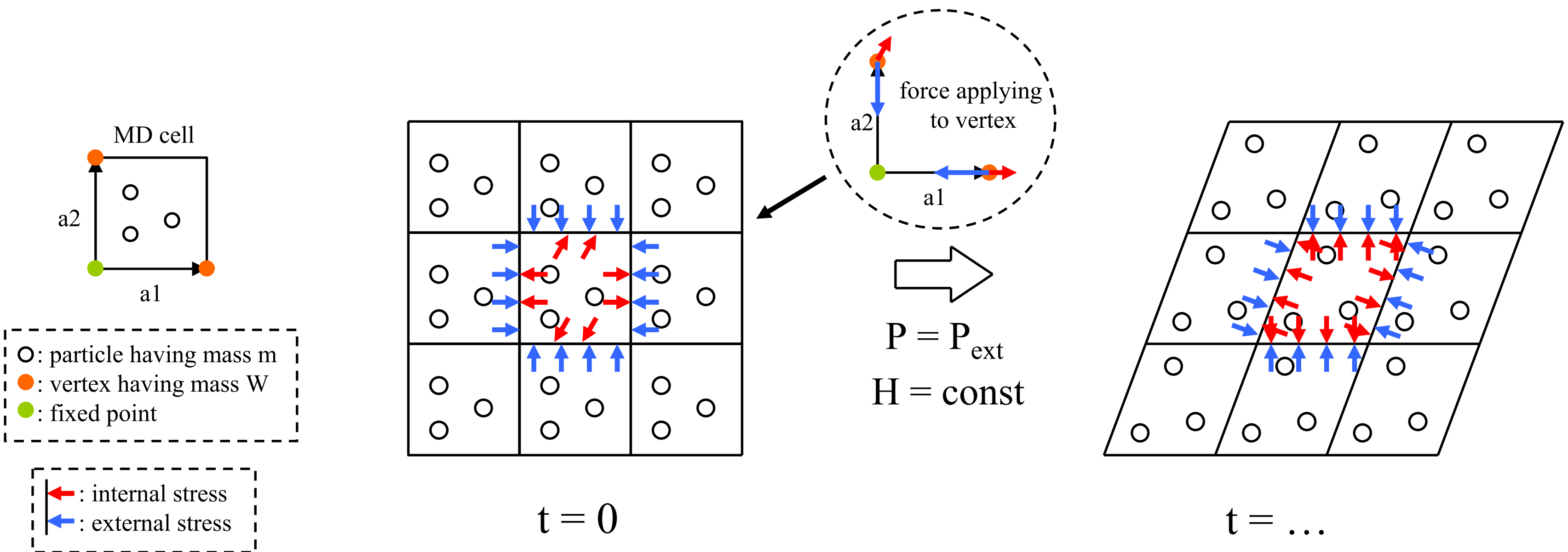
$$\mathcal{L} = \frac{1}{2}\sum_{i=1}^{N} m_i(\underline{\mathrm{h}}\dot{\boldsymbol{s}}_i)^{\mathrm{T}}(\underline{\mathrm{h}}\dot{\boldsymbol{s}}_i) - E(\{\boldsymbol{s}_i\},\underline{\mathrm{h}}) + \frac{W}{2}\,\mathrm{Tr}\,(\dot{\underline{\mathrm{h}}}^{\mathrm{T}}\dot{\underline{\mathrm{h}}}) - P_{\mathrm{ext}}V$$

Variables

$$\underline{\mathrm{h}} \equiv \{\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3\}$$

$$\boldsymbol{r}_i = \underline{\mathrm{h}}\boldsymbol{s}_i$$

- Enthalpy *H*: Conserved
- MD cell can be deformed during the simulation.



§ Constant-*P* Molecular Dynamics Study of Nanostructured Carbon Solids:

- simple cubic C_{60}
- (10,10) CNT
- C_{60}@(10,10) peapod
- (5,5)@(10,10) double-walled CNT

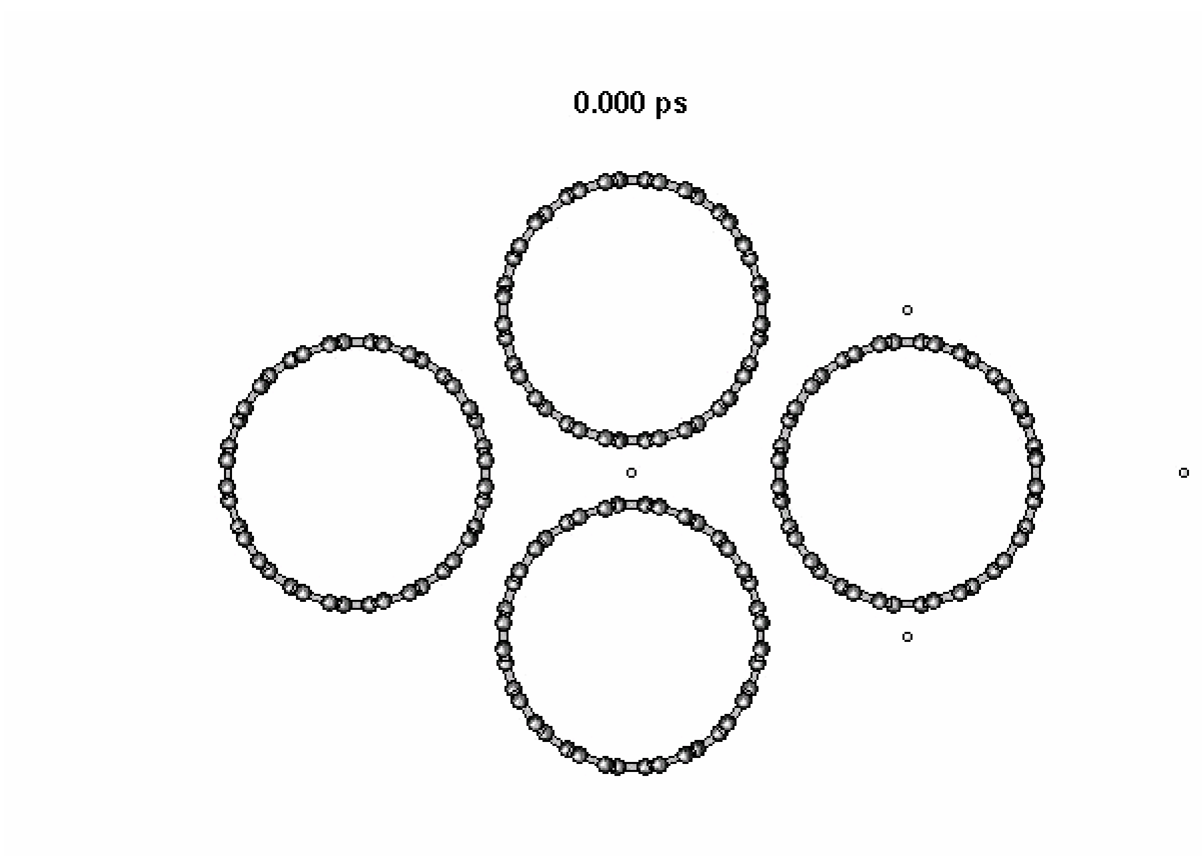
Constant-*P* Molecular Dynamics - Summary

	10 GPa	20 GPa	30 GPa
Solid C_{60}	new polymer phase		amorphous (*sp*^{3})
(10,10) CNT	graphite	new phase	amorphous (*sp*^{3})
C_{60}@(10,10)	(stable)	polymerize	amorphous (*sp*^{3})
(5,5)@(10,10)	(stable)	*sp*^{2}+*sp*^{3}	amorphous (*sp*^{3})*

*anisotropic

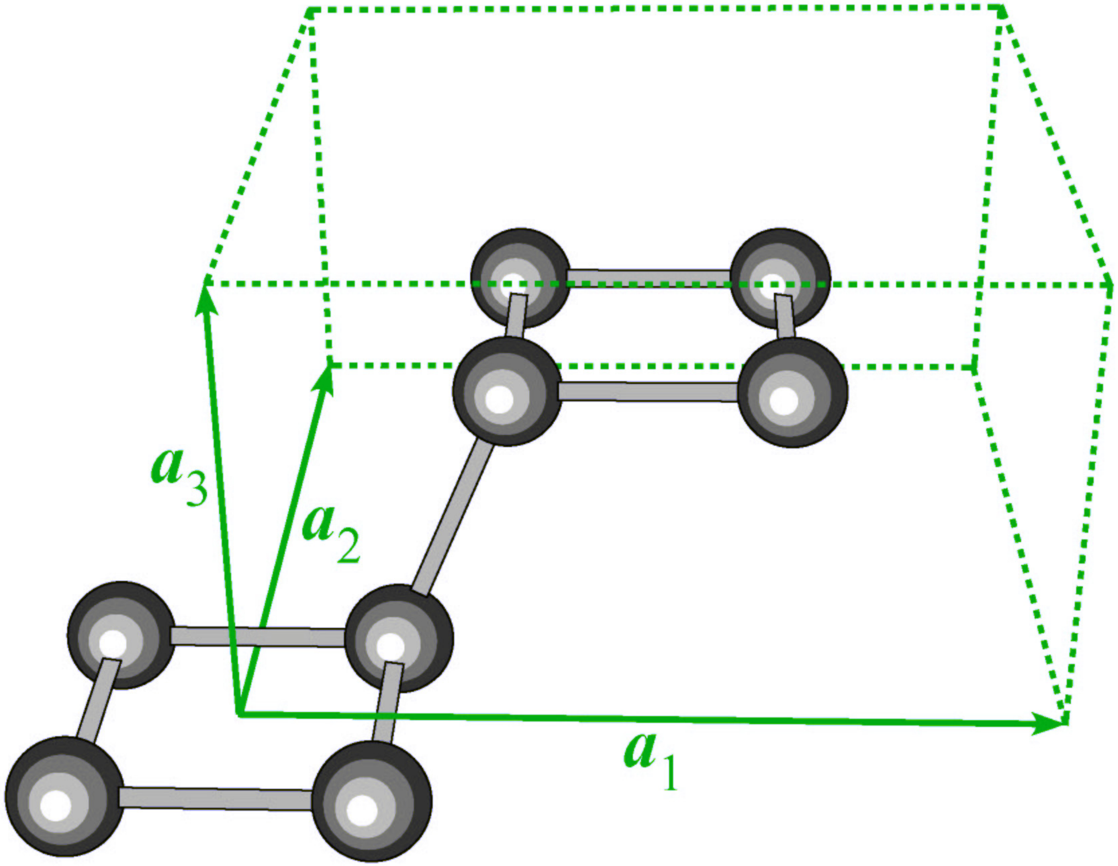
-- Y. Omata, Y. Yamagami, K. Tadano, T. Miyake, and S. Saito, Physica E **29**, 454 (2005)

(10,10) Solid under 20 GPa



New crystalline phase

New crystalline phase



Body-Centered Tetragonal Phase ("C_4")

次世代スーパーコンピュータとナノ炭素科学

◆ 謎につつまれた成長過程の解明

MDシミュレーション時間: ミクロ（μs）からマクロ（ms）へ

→ フラーレン・ナノチューブの選択的精製へ

◆ 多様な構造体の物性・伝導特性予言

「完全な第一原理計算」: 数百原子から数千・数万原子へ

→ナノエレクトロニクスにおけるデバイス機能予言・設計

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SCIENCE

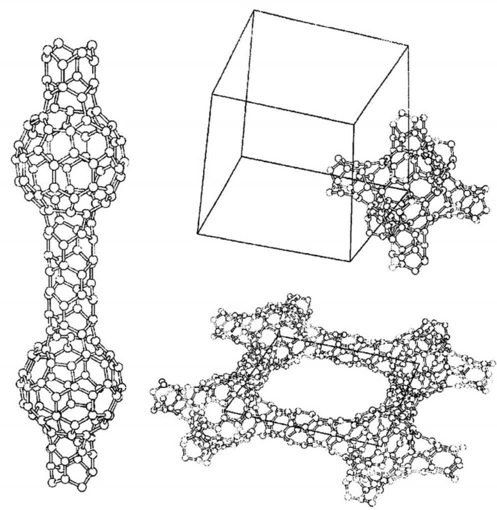
Carbon Nanotubes for Next-Generation Electronics Devices

Susumu Saito

Carbon Nanotubes for Next-Generation Electronics Devices

Susumu Saito

The age of semiconductor technology started in 1947, just a half century ago, when the first semiconductor device, a germanium-based transistor, was invented at Bell Telephone Laboratories. Since then, the miniaturization of devices has been continuous, and computers have become faster and smaller. Meanwhile, silicon has become the most popular device material, owing to its geological abundance and suitable physical properties. Nowadays, the size of the typical device is halved every 3 years. But how far can we go along this road? Although the present devices consist of tiny material domains and junctions between them, each domain is designed to behave in the same way as its macroscopic counterpart. Hence, the present path should end when we go from the present micrometer (~10 μm) world to the nanometer (~10 nm) world where materials are known to behave quite differently because of quantum effects.



Nanotubes and fullerenes may be useful as constituent units of carbon nanoelectronics device. [Adapted from Hamada (*5*)]

At the present pace of miniaturization, we will reach this end within a decade. In order to overcome this technological limit, several types of devices are being investigated that make use of quantum effects rather than trying to overcome them. For this reason, the nanometer-scale carbon materials, namely the fullerenes and nanotubes (see figure), have attracted great interest not only in the scientific fields but also in the field of semiconductor technology. Solid C_{60} is semiconducting (*1*), whereas nanotubes are predicted to be semiconducting or metallic, depending on their network topology (*2*), and several device structures have been theoretically proposed (*3*). On page 100 of this issue, Collins *et al.* report an experimentally functioning carbon nanodevice based on nanotubes (*4*).

In general, there are two kinds of elemental device structures: two-terminal and three-terminal devices. The transistor is a three-terminal device with a variety of structures, materials, and basic functional mechanisms. A typical two-terminal device is the diode, having also a variety of structures and applications, such as switching, rectification, and solar cells. The "nanotube nanodevice" reported by Collins *et al.* is a kind of nanodiode.

Collins *et al.* took a novel approach in using a scanning tunneling microscope (STM) as nanotube manipulator. The tip is first used to pick up and retract the nanotube rope, and then it is used as a sliding local probe to measure the electrical conductivity between the tip and substrate, connected by means of retracted tubes. They found an abrupt change in the current flow from that in a graphite wire to that in a device upon sliding the tip in one direction. Beyond certain well-localized positions, the current can flow only in one direction, which is called rectification, the fundamental function of the two-terminal diode device.

In semiconducting materials, a small amount of impurity added as a dopant can make electron-excess *n*-type or electron-deficient *p*-type semiconductors. A junction between *p*- and *n*-type semiconductors works as a diode. A rectifying junction can also be formed between a semiconductor and a metal. In the case of carbon nanotubes, they can be either metallic or semiconducting, depending on the topology. Hence, experimentally observed diode properties can be explained by the presence of the junction between two topologically or electronically different nanotubes.

Such junctions can be designed by introducing pentagon-heptagon pair defects into otherwise hexagonal nanotube networks (*3*). Fullerenes are also known to work as junction units for nanotubes (*5*). Therefore, the next milestone toward fullerene-nanotube electronics would be the construction of topologically designed two- and three-terminal nanostructures.

Carbon is also one of the geologically most abundant elements. Moreover, it can take a variety of forms, as has already been shown in fullerene and nanotube geometries.

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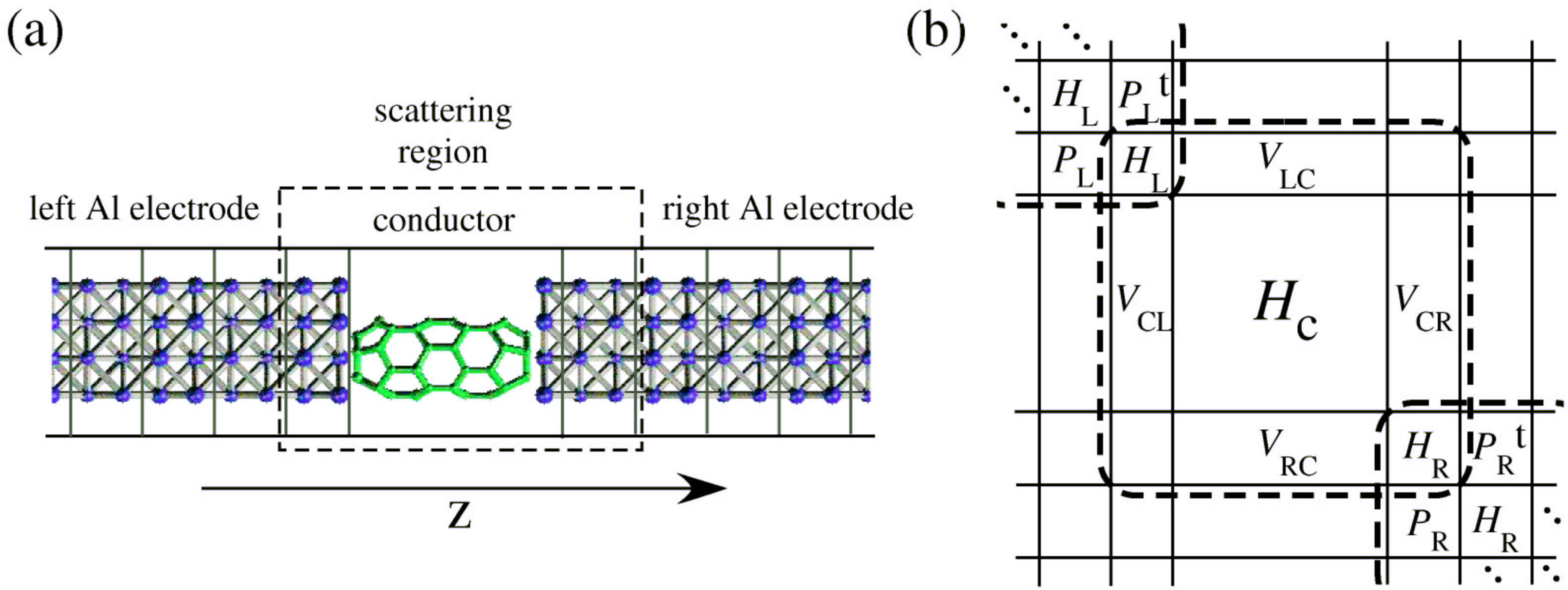
Not only C_{60} but also many kinds of large fullerenes (6) and endohedral metallofullerenes (7) have been produced in a macroscopic amount, and macroscopic production of size-controlled nanotubes is now in progress (8). The technology for manipulation of these nanostructural units and the quantum-mechanical material design will be the keys to realizing carbon-nanostructure electronics in the next century.

References

1. S. Saito and A. Oshiyama, *Phys. Rev. Lett.* **66**, 2637 (1991).
2. N. Hamada, S. Sawada, A. Oshiyama, *ibid.* **68**, 1579 (1992); R. Saito, M. Fujita, G. Dresselhaus, M. S. Dresselhaus, *Appl. Phys. Lett.* **60**, 2204 (1992).
3. See, for example, L. Chico *et al.*, *Phys. Rev. Lett.* **76**, 971 (1996).
4. P. G. Collins, A. Zehl, H. Bando, A. Thess, R. E. Smalley, *Science* **278**, 100 (1997).
5. N. Hamada, *Mater. Sci. Eng. B* **19**, 181 (1993).
6. K. Kikuchi *et al.*, *Nature* **357**, 142 (1992).
7. M. Takata *et al.*, *Phys. Rev. Lett.* **78**, 3330 (1997).
8. A. Thess *et al.*, *Science* **273**, 483 (1996); H. Kataura *et al.*, in preparation.

SiからCへ:

「ミクロな系・マクロな物性」から「ミクロな系・ミクロな物性」へ


(a)
scattering
region
left Al electrode
conductor
right Al electrode
Z
(b)
H_L
P_L^t
P_L
H_L
V_LC
V_CL
H_c
V_CR
V_RC
H_R
P_R^t
P_R
H_R

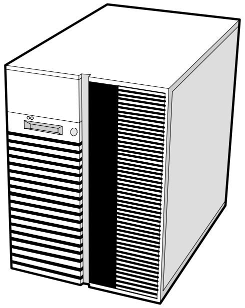
20th Century

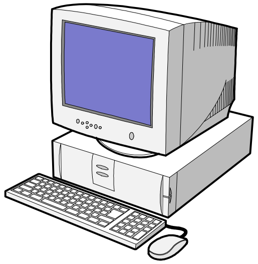
Century of Physics

21st Century

Century of

Nanoscience and Quantum Physics





ナノサイエンス無くしてナノテク無し！