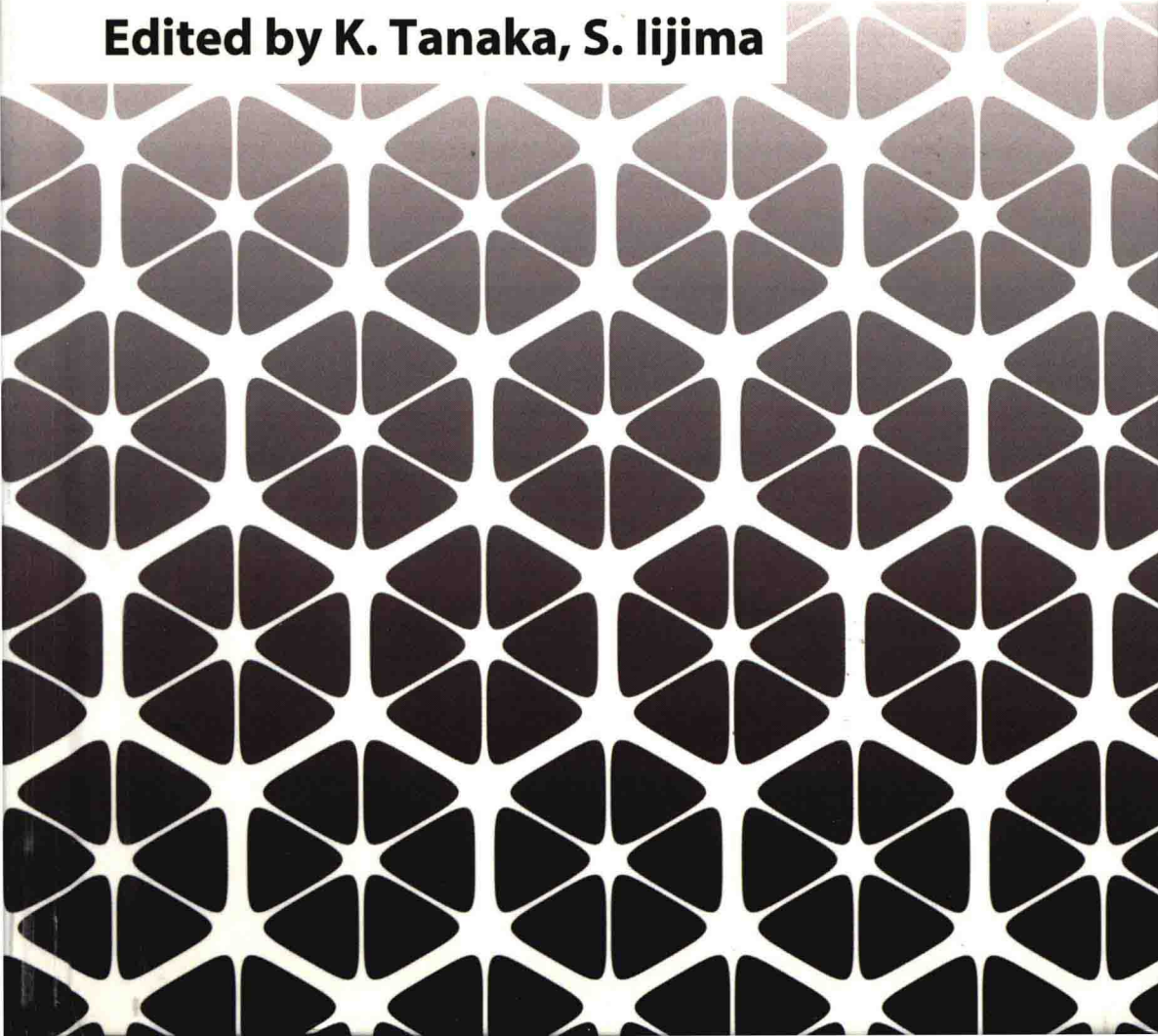
Edition 2

Carbon Nanotubes and Graphene

Edited by K. Tanaka, S. Iijima



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K. Tanaka
Department of Molecular Engineering,
Kyoto University, Nishikyo-ku,
Kyoto 615-8510, Japan

S. Iijima
Department of Materials Science and Technology,
Meijo University, Tempaku-ku, Nagoya 468-8502, Japan
and
Nanotube Research Center,
National Institute of Advanced Industrial Science
and Technology (AIST), Tsukuba 305-8565, Japan

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List of Contributors

Elena Bekyarova
Departments of Chemistry and Chemical & Environmental Engineering, Center for Nanoscale Science and Engineering, University of California, Riverside, CA 92521-0403, USA

Alexey Cherevan
Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstrasse 28-30, 48149 Münster, Germany

Daniela Dragoman
Physics Department, University of Bucharest, P.O. Box MG-11, 077125 Bucharest, Romania

Mircea Dragoman
National Institute for Research and Development in Microtechnology (IMT), P.O. Box 38-160, 023573 Bucharest, Romania

Mildred S. Dresselhaus
Department of Physics; Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA

Dominik Eder
Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstrasse 28-30, 48149 Münster, Germany

Caitlin Fisher
CSIRO Materials Science and Engineering, Bradfield Road, Lindfield, New South Wales 2070; School of Physics, The University of Sydney, Sydney, New South Wales 2006, Australia

Robert C. Haddon
Departments of Chemistry and Chemical & Environmental Engineering, Center for Nanoscale Science and Engineering, University of California, Riverside, CA 92521-0403, USA

Zhao Jun Han
CSIRO Materials Science and Engineering, Bradfield Road, Lindfield, New South Wales 2070, Australia

Zhong Hu
Department of Mechanical Engineering, South Dakota State University, Brookings, South Dakota 57007, USA

Jiaxing Huang
Department of Materials Science and Engineering, Northwestern University, 2220 Campus Drive, Evanston, IL 60208, USA

Akihiro Ito
Department of Molecular Engineering, Kyoto University, Nishikyo-ku, Kyoto 615-8510, Japan

Jing Kong
Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA

Shailesh Kumar
CSIRO Materials Science and Engineering, Bradfield Road, Lindfield, New South Wales 2070, Australia

Hans Kuzmany
Universität Wien, Fakultät für Physik, Strudlhofgasse 4, A-1090 Wien, Austria

Igor Levchenko
CSIRO Materials Science and Engineering, Bradfield Road, Lindfield, New South Wales 2070; School of Physics, The University of Sydney, Sydney, New South Wales 2006, Australia

Xiaoxing Lu
Department of Materials Science and Engineering, University of California, Los Angeles, California 90095, USA

Brendan Meany
Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742, USA

Toshiya Okazaki
Nanotube Research Center, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, 305-8565, Japan

Kostya (Ken) Ostrikov
CSIRO Materials Science and Engineering, Bradfield Road, Lindfield, New South Wales 2070; School of Physics, The University of Sydney, Sydney, New South Wales 2006; Australian Institute for Innovative Materials, The University of Wollongong, New South Wales 2522; Faculty of Science, University of Technology, Sydney, New South Wales 2007; School of Chemistry, Physics, and Mechanical Engineering, Queensland University of Technology, Brisbane, QLD 4000, Australia

Amanda E. Rider
CSIRO Materials Science and Engineering, Bradfield Road, Lindfield, New South Wales 2070, Australia

Kalyan Raidongia
Department of Materials Science and Engineering, Northwestern University, 2220 Campus Drive, Evanston, IL 60208, USA

Riichiro Saito
Department of Physics, Tohoku University, Sendai 980-8578, Japan

Takeshi Saito
Nanotube Research Center, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8565, Japan

Santanu Sarkar
Departments of Chemistry and Chemical & Environmental Engineering, Center for Nanoscale Science and Engineering, University of California, Riverside, CA 92521-0403, USA

Cameron J. Shearer
Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstrasse 28-30, 48149 Münster, Germany

Yong Cheol Shin
Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA

Chuan-Fu Sun
Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742, USA

Alvin T.L. Tan
Department of Materials Science and Engineering, Northwestern University, 2220 Campus Drive, Evanston, IL 60208, USA

Kazuyoshi Tanaka
Department of Molecular Engineering, Kyoto University, Nishikyo-ku, Kyoto 615-8510, Japan

Timothy van der Laan
CSIRO Materials Science and Engineering, Bradfield Road, Lindfield, New South Wales 2070; School of Physics, The University of Sydney, Sydney, New South Wales 2006, Australia

YuHuang Wang
Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742, USA

Kazuhiro Yanagi
Department of Physics, Tokyo Metropolitan University, Hachioji, Tokyo, 192-0397, Japan

Preface

Novel carbon allotropes often mentioned as nanocarbon materials due to their size dimension have been giving a ceaseless impact to carbon science and technology. At the same time, these materials, without doubt, construct main core of nanoscience and nanotechnology as well.

Carbon nanotube (CNT) is one of the main members of nanocarbon family, and the initial stage of the development for CNT was mostly established in the 1990s. In 1999 we launched a monograph 'The Science and Technology of Carbon Nanotubes' from Elsevier (herein called the 1st edition), which covered most of the themes researched on CNT by that time.

Researches on CNT have further been carried out in many ways thereafter from the fundamental aspects to the applied field including the improvement of synthesis, modification of its structure, detailed characterization of properties and making miscellaneous devices. In particular, more advanced developments have been made including a large scale of its production, effective fractioning of CNT with different chiralities and various aspects such as its incorporation into organic reactions, biological interaction with protein or DNA, utilization of the functionalized hybrids towards miscellaneous catalysis and so on. Based on these we have come to an idea to review the 'second-phase' developments of CNT researches after 2000. In this sense, we rather suppress the same old subjects that have already been described in the 1st edition.

Meanwhile, in 2004, graphene was explicitly introduced to nanocarbon material group. This material is very thin by itself with atomic-size thickness and, hence, has purely two-dimensional (2D) structure. In this sense, specific 2D electronic properties of graphene were explicitly checked in its early stage. It is of interest to note that the electronic property such as the band structure of graphene had been quite familiar to the researchers since the 1940s, for graphene was taken as the simplest model for graphite when neglecting the interlayer interaction therein.

After 2004, researches on applications of graphene and its fragments (nanographene and graphene nanoribbon) have been conducted. Moreover, large-area production of graphene using the chemical vapour deposition (CVD) technique is being intensely performed towards its actual application, for instance, touch panel of the electronic devices and so on.

The situations mentioned above make us consider that it is time to unify the new aspects and developments of these two materials together so as to offer a concrete viewpoint to overlook these in a parallel sense. The editors hope this

unification results in preferable interaction and exchange of knowledge and information between the researchers dealing with CNT and/or graphene.

On this occasion we would like to thank Sharmila Vadivelan, Christine McElvenny, Jessica Vaughan, Louisa Hutchins, Graham Nisbet and Adrian Shell in the Editorial Office of Elsevier for their management and incessant encouragement.

Spring, 2014
The Editors

Contents

Chapter 1

Classification of Carbon

Kazuyoshi Tanaka
Department of Molecular Engineering, Kyoto University, Nishikyo-ku, Kyoto 615-8510, Japan

One of the reasons of fertile chemical nature of carbon materials comes from its hybridization state, which also basically determines the features of the variety of organic compounds. In association with this fact, classification of carbon materials would be of importance, which can be simply seen in terms of a certain domain map as shown in Figure 1.1. In this map there are two axes: one is the degree of sp^n hybridization with taking n as variable and the other [H]/[C] atomic ratio of the material. Typical carbon materials and the relatives occupying specific points on this domain map are shown in Figure 1.2.

Since graphene has complete sp^2 hybridization at every carbon atom and hydrogen atoms are ideally not involved in the skeleton, it occupies the point (2, 0) on the map, being the same for graphite when neglecting the small interlayer interaction. On the other hand, the point (2, 1) for polyacetylene and benzene has complete sp^2 hybridization with the [H]/[C] ratio of unity. On the line between the points (2, 1) and (2, 0) exists the graphene-fragments group including graphene nanoribbon and nanographene. Hence, the members belonging to this group also consist of sp^2 hybridization but their [H]/[C] ratios are between 1 and 0 (mostly between 0.5 and 0) along with the development of carbon skeleton.

Fullerenes and carbon nanotubes (CNTs), moreover, belong to an interesting family without any hydrogen atoms but not have genuine sp^2 hybridization due to the curved surfaces. In other words, they have the hybridization of $sp^{2+\delta}$, a bit closer to sp^3 (between $n = 2$ and 3) and, hence, they are on the broken line on the horizontal axis at the right to the point for graphene and graphite. It is, however, generally considered that these two materials are of π conjugation system in actuality. In this sense, π conjugation on the carbon atoms is rather robust even on the curved surface. This feature has been mentioned as σ-bond hybridization due to more mixing of 2s atomic orbital of carbon atom into the original $2p\pi$ orbital [1].

Around the line of the graphene fragments is an ambiguous area surrounded by broken line called amorphous carbon (a-C) including coal, charcoal, coke, soot, carbon black and so on. These members are sometimes of importance in the industrial field and often consist of not only carbon and hydrogen atoms but

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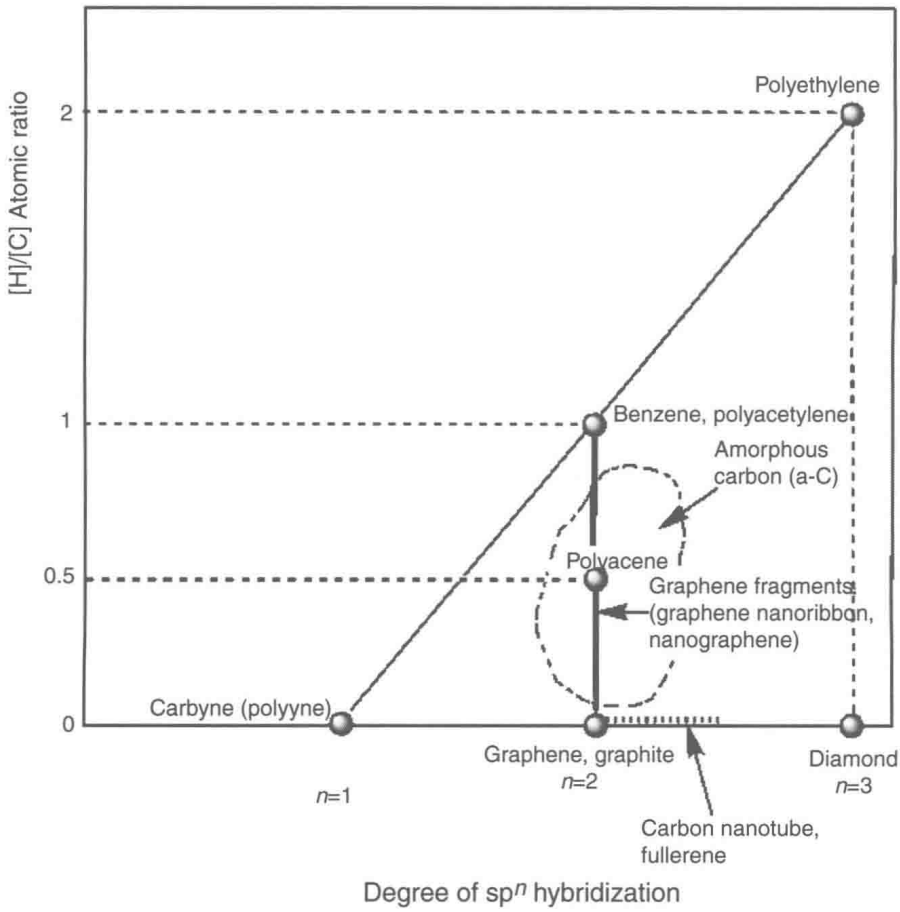

FIGURE 1.1 Domain map of carbon-material family.

also heteroatoms, such as oxygen, nitrogen or sulfur. Carbon fibres also belong to this group although they are rather near to graphite from the viewpoints of atomic arrangement. It is of interest to note that the precursor of vapour-grown carbon fibre (VGCF) quite looks like CNT [2].

On the other hand, the sp^3 hybridization members are paraffinic including polyethylene and diamond with the [H]/[C] ratio values of two and zero, respectively. The materials of this group have no π conjugation but only chemical bonds of σ type. Note that diamond is less energetically stable than graphite by 1.895 kJ mol^{-1} (the standard heat of formation) at 298.15 K. In this sense, the phase diagram of carbon material in Figure 1.3 shows that graphite is the most thermodynamically stable morph at ambient condition. On the contrary, for both silicon and germanium the most energetically stable morph is the diamond structure as is well known.

An sp hybridization should be seen in carbyne (or polyyne) at the point (1, 0), which has a typical linear structure with two orthogonal π conjugations.

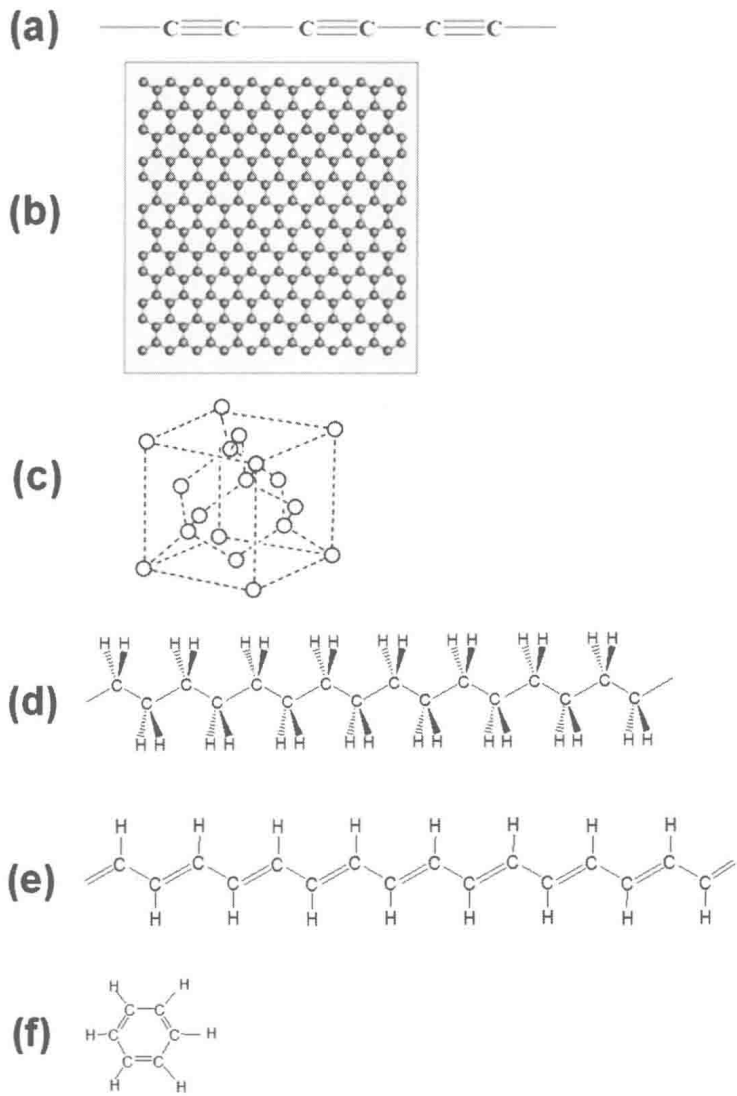

FIGURE 1.2 Various carbon materials and their relatives: (a) carbyne (polyyne), (b) graphene, (c) diamond, (d) polyethylene, (e) polyacetylene, (f) benzene,

(continued)

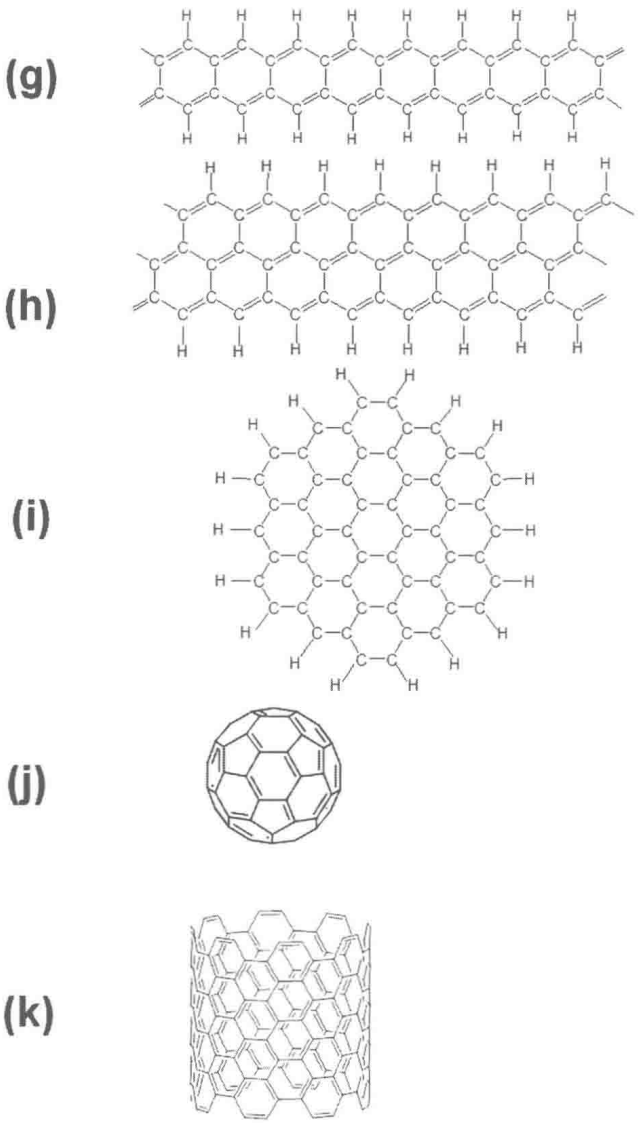

FIGURE 1.2 ***(cont.)*** (g) polyacene, (h) graphene nanoribbon, (i) nanographene, (j) fullerene and (k) CNT.