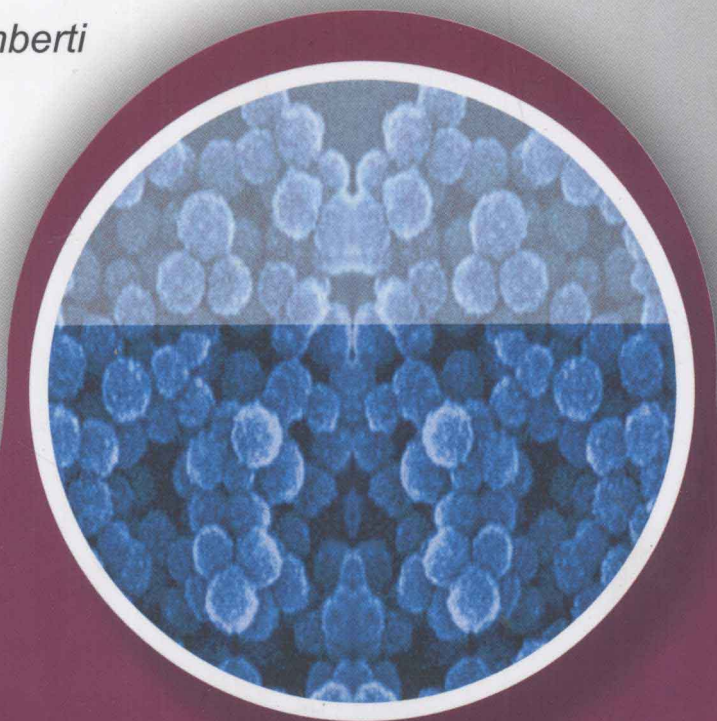


纳|米|科|学|进|展|系|列

半导体异质结构与 与纳米结构表征

Characterization of Semiconductor Heterostructures and Nanostructures

Carlo Lamberti



Characterization of Semiconductor Heterostructures and Nanostructures

半导体异质结构与纳米结构表征

Carlo Lamberti



科学出版社

北 京

图字:01-2010-1282 号

This is an annotated version of

Characterization of Semiconductor Heterostructures and Nanostructures

by Carlo Lamberti

Copyright © 2008 Elsevier Inc.

ISBN 13:978-0-444-53099-8

Authorized English language reprint edition published by the Proprietor.

ISBN 13:978-9-81-272613-1

Copyright © 2009 by Elsevier(Singapore)Pte Ltd. All rights reserved.

Elsevier(Singapore)Pte Ltd.

3 Killiney Road

#08-01 Winsland House 1

Singapore 239519

Tel: (65)6349-0200

Fax: (65)6733-1817

First Published 2010

(2010)年初版

Printed in China by Science Press under special arrangement with Elsevier(Singapore)Pte Ltd. This edition is authorized for sale in China only, excluding Hong Kong SAR, Macao SAR and Taiwan. Unauthorized export of this edition is a violation of the Copyright Act. Violation of this Law is subject to Civil and Criminal Penalties.

本书英文影印版由 Elsevier(Singapore)Pte Ltd. 授权科学出版社在中国大陆境内独家发行。本版权在中国境内(不包括香港和澳门特别行政区以及台湾)出版及标价销售。未经许可之出口,视为违反著作权法,将受法律之制裁。

图书在版编目(CIP)数据

半导体异质结构与纳米结构表征 = Characterization of Semiconductor Heterostructures and Nanostructures; 英文/(意)兰伯蒂 (Lamberti, C.) 著. —北京: 科学出版社, 2010

ISBN 978-7-03-026969-0

I. ①半… II. ①兰… III. ①半导体材料-异质结-英文 ②半导体材料: 纳米材料-结构-英文 IV. ①TN304

中国版本图书馆 CIP 数据核字(2010)第 040653 号

责任编辑: 霍志国/责任印制: 钱玉芬

封面设计: 耕者设计工作室

科学出版社 出版

北京东黄城根北街 16 号

邮政编码: 100717

<http://www.sciencep.com>

双青印刷厂 印刷

科学出版社发行 各地新华书店经销

*

2010 年 3 月第 1 版 开本: B5(720×1000)

2010 年 3 月第一次印刷 印张: 31 1/2

印数: 1—1 500 字数: 635 000

定价: 135.00 元

(如有印装质量问题, 我社负责调换)

导 读

本书是由意大利 Torino 大学材料系 Carlo Lamberti 教授主编的, 以意大利的大学教授为主体, 包括欧洲其他国家: 英国 (第 8 章)、法国 (第 10、11 章)、西班牙 (第 11 章)、瑞士 (第 12 章) 及比利时 (第 13 章) 学者共同编写的。全书共 13 章, 内容是介绍表征异质结构, 包括半导体异质结、超晶格, 以及低维结构如 III-V 族化合物纳米线、量子点等——的结构性质与电子性质的分析手段和方法。这些性质主要是指在衬底上生长的异质表面层或异质材料间的界面、界面层 (interlayer) 特性。

具体来说, 结构参数包括生长出来的层中的材料组分、掺杂及应变等; 界面特性则有材料跨越界面的原子互混 (inter-mixing)、共价键的键长变化等。固体的电子结构则是指 $E-k$ 关系 (即能带、能级), 包括通常在异质结能带图中最为关注的导带底与价带顶的偏差。另一类与载流子 (电子、空穴) 在异质结构中输运十分有关的晶格振动模式 (用声子描述), 其表征方法在书中也有介绍。

该书十分全面地描述了对上述异质/纳米尺度结构性质进行表征的手段与方法, 包括

- ◆ 高分辨率 X 射线衍射技术 (XRD) (第 4 章)
- ◆ 透射电子显微镜 (TEM) (第 5 章)
- ◆ 光致发光技术 (PL) (第 6 章)
- ◆ 与功率大小有关的阴极发光 (第 7 章)
- ◆ 拉曼谱技术 (第 8 章)
- ◆ X 射线吸收精细结构 (XAFS) 方法 (第 9 章)
- ◆ 采用同步辐射的对表面敏感的 X 射线技术: 包括掠入射 (GI) 及异常散射 (第 10 章)
- ◆ 掠入射衍射异常精细结构 (GIDAFS) (第 11 章)
- ◆ 光发射谱 (第 12 章)
- ◆ 电子自旋谐振 (ESR) 谱分析 (第 13 章)

这种对表征手段的全方位介绍 (基本上都是基于各种谱分析原理, 包括固体实空间与晶体倒格子空间的变换), 可以帮助读者在进行结构的体材料特性、表面特性或界面特性分析时做适当的选择。

除了实验手段,本书的另一个显著特点是用了大量篇幅介绍了计算机分析与辅助设计在异质结构的表征上起到的日益重要的作用。这种计算机模拟方法包括用第一原理(ab initio,也称从头开始)对器件电子结构的计算。本书第3章专门讨论了采用第一原理计算方法来研究材料的结构与电子性质,以及相应模型的建立。该书提供的这种实验与理论计算相结合的方法是研究与设计高性能的异质结构和纳米结构的强有力的工具,也是目前科学界发展的趋势。

该书在叙述结构安排上也颇具匠心。在每一章的起头都对所叙述的表征与实验方法的物理原理进行了简要而清晰的介绍,使得初学者能很快地掌握与熟悉该方法的历史背景与应用范围、特点,然后介绍使用该方法的具体步骤。各章的后一部分则给出了所描述的方法的具有代表性与当前的应用实例。

需要指出的是,书中介绍的参考文献十分全面(近期与经典的)与准确,这是因为各章的作者都是从事该方面测试方法与技术研究有长的专门学者,对本领域的发展状况与动态十分熟悉。从这个意义上说,本书提供了一个深入了解晶体、异质结构表征研究的捷径或入门向导。

该书对于从事硅 CMOS 大规模集成电路研究与开发的科研、工程人员也有很好的参考价值。

(1) 书中多处讨论了应变对晶体晶格与界面结构的影响,也介绍了多孔(porous)材料(如多孔硅)的原子排列与物理性质。这两个技术(应变硅与多孔介质)都是目前 CMOS 技术进入纳米尺度(即 90nm 及以下工艺节点)后,工业与学术界广泛使用以改善集成电路性能(前端晶体管与后端互连)的主要方法。

(2) 书中涉及的电子自旋效应讨论(第 10 章)也对日趋活跃的半导体自旋电子学研究有很好的回顾与分析。

(3) 全书的讨论多处提及氮化物半导体或合金材料的表征方法。这也十分适合目前研究的热点。以 GaN 为例,其宽禁带与良好的热导率与化学稳定性,使其在光学与电学器件中的应用极有价值。

以上三方面的内容都反映了本书写作有很好的时效性与实际意义。

最后可以提及的是,尽管本书是编著而成的,但依然提供了索引(index),这对检索众多纷繁的表征方法与现象提供了极大的方便。

诚如编著者指出,本书可供从事基于异质结构的器件设计、材料生长,表征

与测试的研究人员与大学研究生（包括本科高年级学生）阅读。笔者更认为，对从事微电子（包括集成电路工艺、器件）与纳电子材料、器件研究的科学、工程人员也极具参考价值。谨此推荐。

余志平

清华大学微电子学研究所

为了那些年代久远的树木，因为它们是我们的起源；但是更重要的是，为了年轻的树木，因为未来属于它们。

7

在我的内心里，我愿意将知识的传播视为一棵其根深深扎入土地的老树，它的种子被可爱的风吹散在四周。让土地紧裹着老树的根，让微风轻抚它的枝条，直到年轻的树木成长起来并最终取代老树，越长越壮……

（余志平 译）

前 言

在 C. Lamberti 的“采用同步辐射技术对应变半导体异质结构与薄膜的表征”综述文章发表之后，Elsevier 出版社与我联系来协调编写一本有关用于研究半导体异质结构和纳米结构的最常用的表征技术的新书。在最开始的拖延之后，我接受了这个任务。我所接触过的大多数章节作者的迅即又热情的回复使我的工作比起预期的要容易得多。我要对所有这些同事们表示衷心感谢。我也要对那些章节进行校验的能干的同事表示感激，因为他们的辛勤工作对章节的作者和我在改进最后的定稿质量方面帮助极大。在结束这项任务时，回顾最终的成果，我能自豪地在章节作者中数出不少我的好朋友以及在各自领域中的杰出科学家。在这些杰出的科学家中，我更为女科学家在其中起的作用而骄傲：她们共编写了 4 章。

《半导体异质结构与纳米结构表征》一书章节是这样组织的：每个章节介绍了一种用于了解半导体量子阱和超晶格的性质（结构、物理、化学、电磁等）中表征技术。有一章专门介绍了用第一原理进行模拟的建模方法。本书有两个基本目的。第一个是基于教学的考虑。本书提供了可被物理、化学、材料、科学、工程和纳米技术领域的硕士和博士生理解的某一特定技术的基本概念。第二个目的是从最新文献中选择一些例子，它们能代表应用某一专门技术来理解半导体异质结构与纳米结构性质的前沿结果。因此每一章有双重结构：第一部分是用来解释基本概念以服务于最大限度的读者；第二部分则用来讨论特别与新颖的例子，使得本书可以在书架上寿命可以更长些。如果发现理解每个章节的第二部分有困难时，不用沮丧。我的建议是集中精力在第一部分：当经验增加时，总是可以在随后几年里回过头来再看第二部分。当然，本书也对学术和工业界中对基于异质结构的器件的设计、生长、表征和测试领域中工作的科学家适用。这些读者可以跳过每个章节的第一部分，直接专注于第二部分。

除了上面谈到的之外，本书还有一个更长远，甚至可以说是雄心勃勃的目的。这是指，本书中有关量子阱、量子线和量子点的内容应该被看作是一个将先进表征技术应用到理解纳米（甚至亚纳米）尺度物质的结构、电子等性质一个前奏。可以这么说，本书的目的是作为更为广阔和极其活跃的纳米技术领域的参考书。

（余志平 译）

To the older trees, because that's from them that we came from but most importantly, to the young trees, because to them belongs the future.

In my naïve mind I like to think of knowledge dissemination as an old tree, with its roots strongly and deeply set in the ground, and with its seeds gently taken by a lovely wind that spreads them all around. Let the ground stick close to the old tree's roots and let the wind caress its branches, as long as possible . . . till new young trees grow up from the ground and become stronger and stronger and can finally replace the old one.

Preface

After the publication of the review “C. Lamberti, The use of synchrotron radiation techniques in the characterization of strained semiconductor heterostructures and thin films, *Surf. Sci. Rep.*, **53** (2004) 1–197”, Elsevier contacted me for the coordination of a new book collecting the most used characterization techniques for the investigation of semiconductor heterostructures and nanostructures. After an initial inertia from my part, I accepted the task. The immediate enthusiastic replay of most of the contacted chapter coordinators has made my work easier than expected. I would like to express my gratitude to all these colleagues, as well as to all colleagues who have kindly acted as competent reviewers, as their hard work has importantly helped the chapter coordinators and myself to improve the quality of the final product. At the end of the task, looking to the final result, I am proud to count within the chapter coordinators dear friends and eminent scientists that are in the top positions in the ranking lists of the corresponding disciplines. I am even more proud to underline that, among such list of eminent scientists, women play an important role, leading four chapters.

“Characterization of Semiconductor Heterostructures and Nanostructures” is structured in chapters, each one devoted to a specific characterization technique used in the understanding of the properties (structural, physical, chemical, electrical, etc.) of semiconductor quantum wells and superlattices. A chapter is devoted to the *ab initio* modeling. The book has basically a double aim. The first one lies on the educational ground. The book provides the basic concept of each of the selected techniques with an approach understandable by master and Ph.D. students in Physics, Chemistry, Material Science, Engineering, and Nanotechnology. The second aim is to provide a selected set of examples from the recent literature of the TOP results obtained with the specific technique in understanding the properties of semiconductor heterostructures and nanostructures. Each chapter has consequently this double structure: a first part devoted to explain the basic concepts, serving the largest possible audience, and a second one to the discussion of the most peculiar and innovative examples, allowing the book to have the longest possible shelf life. So students should not get frustrated if they find more difficulties in the understanding of the second part of the chapters. My advice is to focus on the first parts; they can always come back to the second parts in the ensuing years, when their experience will be improved. Of course, the book is devoted also to the specialized community of scientists working in the fields of design, growth, characterization, and testing of heterostructures-based devices in both academic and industrial laboratories. Such readers should skip the first parts of the chapters, focusing on the final ones.

On top of this, the book has a further and somewhat even more ambitious goal. In this regard, the topic of quantum wells, wires, and dots should be seen as a pretext of applying top level characterization techniques in understanding the structural, electronic, etc. properties of matter at the nanometer (even sub-nanometer) scale. In this way, it is aimed to become a reference book in the much broader, and extremely hot, field of Nanotechnology.

目 录

前言	ix
第 1 章 导论：纳米技术的多学科性质与探索前沿表征技术的必要性 <i>Carlo Lamberti</i>	1
第 2 章 结构性质与电子性质的第一原理（从头算起）模拟研究 <i>Maria Peressi, Alfonso Baldereschi, Stefano Baroni</i>	17
第 3 章 纳米结构的电学性质表征 <i>Anna Cavallini, Laura Polenta</i>	55
第 4 章 采用高分辨率 X 射线衍射技术（XRD）的半导体异质结构的应变与组分确定 <i>Claudio Ferrari, Claudio Bocchi</i>	93
第 5 章 透射电子显微镜（TEM）技术用于成像与半导体异质结构的组分确定 <i>Laura Lazzarini, Lucia Nasi, Vincenzo Grillo</i>	133
第 6 章 通过光致发光技术（PL）以了解半导体纳米结构的结构性质与电子性质 <i>Stefano Sanguinetti, Mario Guzzi, Massimo Gurioli</i>	175
第 7 章 III 族元素氮化物（III-nitride）的异质结构中的与功率大小有关的阴极发光：从内部场屏蔽到可控能带带隙调制 <i>Giancarlo Salviati, Francesca Rossi, Nicola Armani, Vincenzo Grillo, Laura Lazzarini</i>	209
第 8 章 拉曼谱技术 <i>Daniel Wolverson</i>	249
第 9 章 用于半导体异质结构与纳米结构研究的 X 射线吸收精细结构（XAFS）方法 <i>Federico Boscherini</i>	289
第 10 章 受同步辐射光照的纳米结构：对表面敏感的 X 射线技术及异常散射 <i>Till Metzger, Vincent Favre-Nicolin, Gilles Renaud, Hubert Renevier, Tobias Schilli</i>	331
第 11 章 用于研究纳米结构的结构性质的掠入射衍射异常精细结构（GIDAFS）方法 <i>Maria Grazia Proietti, Johann Coraux, Hubert Renevier</i>	371

第 12 章	光发射谱在异质结研究中的作用	
	<i>Giorgio Margaritondo</i>	407
第 13 章	半导体异质结构界面与界面层的电子自旋谐振 (ESR) 谱分析方法	
	<i>Andre Stesmans, Valery V. Afanas'ev</i>	435
名称索引	483

(余志平 译)

Table of Contents

<i>Preface</i>	<i>ix</i>
Chapter 1: Introduction: the interdisciplinary nature of nanotechnology and its need to exploit frontier characterization techniques <i>Carlo Lamberti</i>	<i>1</i>
Chapter 2: Ab initio studies of structural and electronic properties <i>Maria Peressi, Alfonso Baldereschi, and Stefano Baroni</i>	<i>17</i>
Chapter 3: Electrical characterization of nanostructures <i>Anna Cavallini and Laura Polenta</i>	<i>55</i>
Chapter 4: Strain and composition determination in semiconducting heterostructures by high-resolution X-ray diffraction <i>Claudio Ferrari and Claudio Bocchi</i>	<i>93</i>
Chapter 5: Transmission electron microscopy techniques for imaging and compositional evaluation in semiconductor heterostructures <i>Laura Lazzarini, Lucia Nasi, and Vincenzo Grillo</i>	<i>133</i>
Chapter 6: Accessing structural and electronic properties of semiconductor nanostructures via photoluminescence <i>Stefano Sanguinetti, Mario Guzzi, and Massimo Gurioli</i>	<i>175</i>
Chapter 7: Power-dependent cathodoluminescence in III-nitrides heterostructures: from internal field screening to controlled band-gap modulation <i>Giancarlo Salviati, Francesca Rossi, Nicola Armani, Vincenzo Grillo and Laura Lazzarini</i>	<i>209</i>
Chapter 8: Raman spectroscopy <i>Daniel Wolverson</i>	<i>249</i>
Chapter 9: X-ray absorption fine structure in the study of semiconductor heterostructures and nanostructures <i>Federico Boscherini</i>	<i>289</i>
Chapter 10: Nanostructures in the light of synchrotron radiation: surface-sensitive X-ray techniques and anomalous scattering <i>Till Metzger, Vincent Favre-Nicolin, Gilles Renaud, Hubert Renevier, and Tobias Schüllli</i>	<i>331</i>

Chapter 11: Grazing incidence diffraction anomalous fine structure
in the study of structural properties of nanostructures
Maria Grazia Proietti, Johann Coraux, and Hubert Renevier371

Chapter 12: The role of photoemission spectroscopies in heterojunction research
Giorgio Margaritondo407

Chapter 13: ESR of interfaces and nanolayers in semiconductor heterostructures
Andre Stesmans and Valery V. Afanas'ev435

Subject Index.483

1

Introduction: the interdisciplinary nature of nanotechnology and its need to exploit frontier characterization techniques

Carlo Lamberti

Department of Inorganic, Physical, and Materials Chemistry and NIS Centre of Excellence, Università di Torino, Via P. Giuria 7, 10125 Torino, Italy and INSTM Centro di Riferimento, Torino, Italy

Abstract High-performance electronic and optoelectronic devices based on semiconductor heterostructures are required to obtain increasingly strict and well-defined performances, needing a detailed control, at the atomic level, of the structural composition of the buried interfaces. This goal has been achieved by an improvement in the epitaxial growth techniques and by the parallel use of increasingly sophisticated characterization techniques and of increasingly accurate ab initio calculations. This chapter, introducing the book *Characterization of Semi-conductor Heterostructures and Nanostructures*, is divided into five sections. In Section 1, the impact of nanoscience and nanotechnology in our society is described, using the point of view of the articles, the citations and the journals devoted to the field. The multidisciplinary nature of nanotechnology is reported in Section 2, while the dynamic interplay among growth/synthesis techniques, theoretical modeling, and characterization techniques in the design and improvement of semiconductor heterostructure-based devices is discussed in Section 3. Section 4 reports the purposes of the book and the layout of the chapters. Finally, in Section 5, the strength of combined experimental and theoretical investigation of a selected nanomaterial is underlined by an example.

Keywords nanotechnology, nanoscience, heterostructures, nanostructures, characterization techniques, ab initio calculations

1. The scientific and editorial blow up of nanotechnology in the new millennium

The term nanotechnology refers to a branch of applied science and technology whose unifying theme is the control of matter at the atomic and molecular scale, normally 1–100 nm (1 nm = 10^{-9} m), and the fabrication of devices within that size range. The appeal in such approach lies in the fact that the structural, physical, chemical, electronic, optical, etc. properties of nanometer-dimensioned materials differ markedly from those of the corresponding bulk (unconfined) materials. Nanotechnology, among the most advanced frontiers of Science, is certainly showing the higher degree of multidisciplinary, generated from the well-accorded interplay among different fields such as materials science, applied physics, interface and colloid science, device

physics, supramolecular chemistry, surface science, and engineering. Nanotechnology results from a combined extension of such sciences into the nanoscale.

Scientists, politicians, media, and industries have much expectation concerning what new science, technology, and application may result from these lines of research. Such expectations have strongly stimulated the effort made in the previous years by university and industrial laboratories in the field of nanoscience and nanotechnology. A simple way to evaluate such effort is to look to the number of papers published per year that are found using *nanochemistry* OR *nanophysics* OR *nanotechnology* OR *nanoscience* as search keys (Fig. 1(a)), and to the number of citations that such papers have received (Fig. 1(b)). It is evident that such simple and superficial statistical study is far to be comprehensive, as most of the papers that actually report results in this field do not necessarily used one of those four keywords. It is evident from the last row of Table 1 that the 32 journals belonging to the *Subject Category*¹ named “Nanoscience & Nanotechnology” have published 8939 papers in 2006, while only 1125 have been found using those four keywords (Fig. 1(a)). So, the data reported in Fig. 1 are not important as absolute values, which are underestimated by a factor of about 10, but for the trend they are showing. It is evident that this trend shows an impressive acceleration starting from the new millennium.

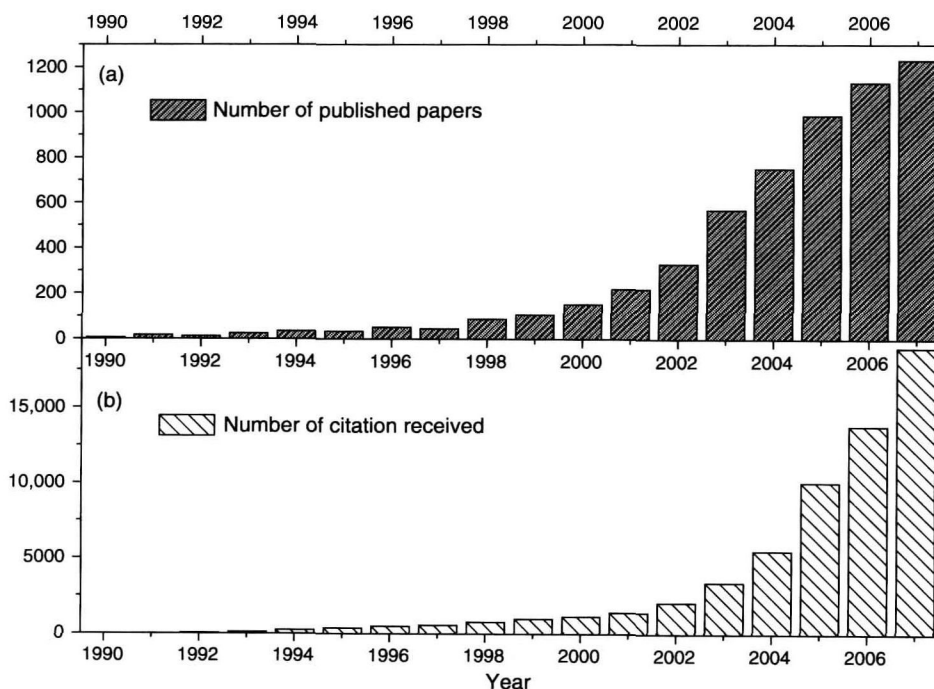


Fig. 1. (a) Number of paper published per year found using *nanochemistry* OR *nanophysics* OR *nanotechnology* OR *nanoscience* as search keys. Spanned period 1990 to 2007; total number of papers 5788 source ISI web of science. (b) Number of citations received per year by the papers reviewed in (a): total number of citations 59,747.

¹ *Subject Categories* are classes where journals are sorted according to the scientific topic of the published papers.

Table 1

List of a selection of scientific journals belonging to the Subject Category named “Nanoscience & Nanotechnology” sorted by publishing age. The last column refer to the aggregated values obtained by the 32 journals together. Data reported in this line allow to evaluate the impact of the Subject Category and to locate each single journal belonging to the category in a pondered ranking scale

Journal name	Publisher	Published since	Papers published in 2006	Impact factor 2006 ^a	Immediacy index 2006 ^b
<i>Nanotechnology</i>	IoP	1994	1042	3.037	0.534
<i>J. Nanopart. Res.</i>	Kluwer first, now Springer	1999	101	2.156	0.119
<i>Nano Lett.</i>	ACS	2001	555	9.960	1.485
<i>Lab Chip</i>	RSC	2001	190	5.821	1.111
<i>Physica E</i>	Elsevier	2001	503	1.084	0.163
<i>J. Nanosci. Nanotechnol.</i>	American Scientific Publishers	2001	586	2.194	0.309
<i>IEEE Trans. Nanotechnol.</i>	IEEE	2002	111	1.909	0.207
<i>Small</i>	Wiley-VCH	2005	210	6.024	1.152
<i>Curr. Nanosci.</i>	Bentham Science Publ. Ltd	2005	33	2.080	0.242
<i>Nano Today</i>	Elsevier	2006	14	—	1.357
<i>Nature Nanotechnol.</i>	Nature Publishing Group	2006	24	—	0.833
<i>ACS Nano</i>	ACS	2007	0	—	—
Subject Category: 32 journals	—	2005	8939	2.459	0.400

^aThe journal impact factor of year 2006 is the average number of times articles from the journal published in 2005 and 2004 have been cited in 2006. Journals published first in 2006 will have their first impact factor evaluation for year 2007, usually divulgated in spring 2008.

^bThe journal immediacy index of year 2006 is the average number of times an article published in 2006 is cited in 2006. The journal immediacy index indicates how quickly articles in a journal are cited.

This scientific and technological phenomenon has been so significant that the most important publishing companies have decided to create new journals specifically devoted to this topic (see Table 1 for a selection). The Institute of Physics (IoP) has been the first publisher in this field, founded in the early 1990s the journal *Nanotechnology* (impact factor 3.037), which has published more than 4000 papers so far. This number makes *Nanotechnology* the most important journal in the field in terms of published papers. In 1999 Kluwer Academic Publishers founded the journal *J. Nanopart. Res.* Then, in 2001 appeared *Nano Lett.*, from the American Chemical Society (ACS), which probably represents today the most prestigious journal in the field, with more than 2800 published papers and an impressive impact factor that, starting from 5.033 in 2002, progressively increased to almost 10 in 2006. Among the ACS journals, excluding the review journals (*Chem. Rev.* and *Accounts Chem. Res.*), *Nano Lett.* has become the highest impact factor journal, even exceeding the prestigious *J. Am. Chem. Soc.*, first published in 1879. In the same year 2001, the Elsevier journal *Physica E* changed its name into *Physica E-Low-Dimensional Systems & Nanostructures*, while the Royal Society of Chemistry (RSC) launched