Series in Condensed Matter Physics

MAGNETIC ANISOTROPIES IN NANOSTRUCTURED MATTER

Peter Weinberger

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Biography

Peter Weinberger was for many years (1972 - October 2008) professor at the Vienna Institute of Technology, Austria, and consultant to the Los Alamos National Laboratory, Los Alamos, New Mexico, USA (1982 - 1998), and the Lawrence Livermore National Laboratory (1987 - 1995), Livermore, California, USA. For about 15 years, until 2007, he headed the Center for Computational Materials Science, Vienna.

He is a fellow of the American Physical Society and a receiver of the Ernst Mach medal of the Czech Academy of Sciences (1998). In 2004 he acted as coordinator of a team of scientists that became finalists in the Descartes Prize of the European Union.

He (frequently) spent time as guest professor or guest scientist at the H. H. Wills Physics Laboratory, University of Bristol, UK, the Laboratorium für Festkörperphysik, ETH Zürich, Switzerland, the Department of Physics, New York University, New York, USA, and the Laboratoire de Physique des Solides, Université de Paris-Sud, France.

Besides some 330 publications (about 150 from the *Physical Review B*), he is author or coauthor of three textbooks (Oxford University Press, Kluwer, Springer). He is also author of 4 non-scientific books (novels and short stories, in German).

Presently he heads the Center for Computational Nanoscience Vienna, an Internet institution with the purpose of facilitating scientific collaborations between Austria, the Czech Republic, France, Germany, Hungary, Spain, the UK and the USA in the field of theoretical spintronics and/or nanomagnetism.

Acknowledgments

This book is dedicated to all my former or present students and/or collaborators in the past 10 years:

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From each of them I learned a lot and profited considerably. In particular I am indebted to **Laszlo Szunyogh** for a long lasting scientific partnership concerning the fully relativistic Screened Korringa-Kohn-Rostoker project.

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Rolf Allenspach, Klaus Baberschke, Bret Heinrich, Jürgen Kirschner, Ivan Schuller and Roland Wiesendanger.

Last, but not least: books are never written without indoctrinations by others. Definitely **Simon Altmann** (Oxford) and **Walter Kohn** (S. Barbara) did (and still do) have a substantial share in this kind of intellectual "pushing".

Contents

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Introduction

In here the key words in the title of the book, namely nanostructured matter and magnetic anisotropies, are critically examined and defined.

Nanosystems and *nanostructured matter* are terms that presently are very much *en vogue*, although at best semi-qualitative definitions of these expressions seem to exist. The prefix *nano* only makes sense when used in connection with physical units such as meters or seconds, usually then abbreviated by nm (nanometer) or ns (nanosecond):

$$1\ \text{Å} = 10^{-8}\text{cm} = 0.1\ \text{nm}$$
$$1\ \text{nm} = 10^{-9}\text{m}$$

Quite clearly the macroscopic pre-Columbian statue in Fig. 1.1 made from pure gold nobody would call a nanostructured system because in "bulk" gold the atoms are separated only by few tenths of a nanometer. Therefore, in

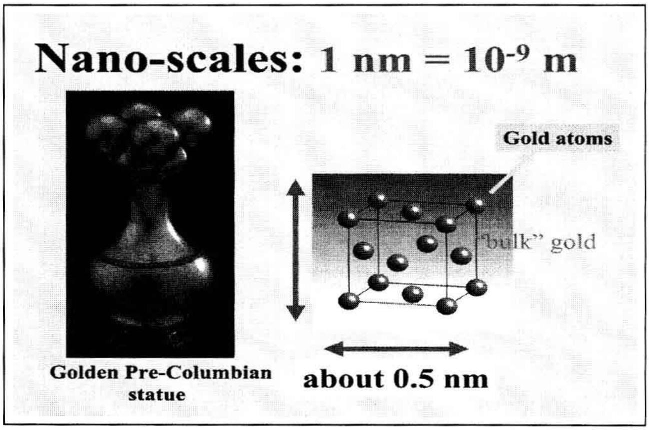

FIGURE 1.1: Left: *macroscopic golden artifact,* right: *microscopic structure of fcc Au.*

order to define nanosystems somehow satisfactorily the concept of functional units or functional parts of a solid system has to be introduced. *Functional* in this context means that particular physical properties of the total system are mostly determined by such a unit or part. In principle two kinds of nanosystems can be defined, namely solid systems in which the functional part is confined in one dimension by less than about 100 nm and those where the confinement is two-dimensional and restricted by about 10 - 20 nm. For matters of simplicity in the following, nanosystems confined in one dimension will be termed *1d-nanosystems*, those confined in two dimensions *2d-nanosystems*. Confinement in three dimensions by some length in a few nm does not make sense, because this is the realm of molecules (in the gas phase). In soft matter physics qualitative definitions of nanosystems can be quite different: so-called nanosized pharmaceutical drugs usually contain functional parts confined in length in all three directions, which in turn are part of some much larger carrier molecule. Since soft matter physics is not dealt with in this book, in the following a distinction between *1d-* and *2d-nanosystems* will be sufficient.

A diagram of a typical *1d-nanosystem* is displayed in Fig. 1.2 reflecting the situation, for example, of a magnetically coated metal substrate such as a few monolayers of Co on Cu(111). Systems of this kind are presently very much studied in the context of perpendicular magnetism. Very prominent examples

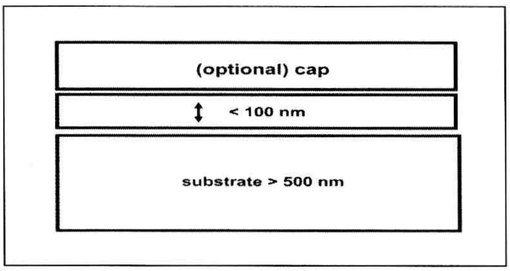

FIGURE 1.2: *Solid system, nanostructured in one dimension.*

of *1d-nanosystems* are magnetoresistive spin-valve systems, see Fig. 1.3, that consist essentially of two magnetic layers separated by a non-magnetic spacer. As can be seen from this figure the functional part refers to a set of buried slabs of different thicknesses. It should be noted that in principle any interdiffused interface between two different materials is also a *1d-nanosystem*, since usually the interdiffusion profile extends only over a few monolayers, i.e., is confined to about 10 nm or even less.

Fig. 1.4 shows a sketch of a *2d-nanosystem* in terms of (separated) clusters of atoms on top of or embedded in a substrate. These clusters can be either small islands, (nano-) pillars or (nano-) wires. "Separated" was put cau-

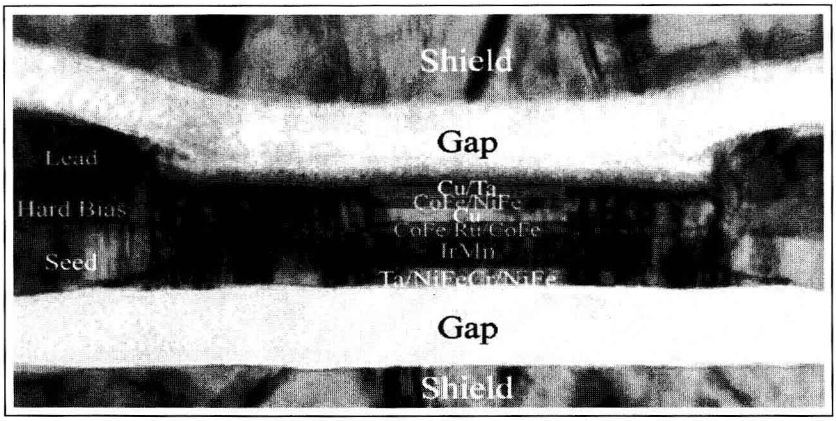

FIGURE 1.3: *Transition electron micrograph of a giant magnetoresistive spin-valve read head. By courtesy of the MRS Bulletin, Ref. [1].*

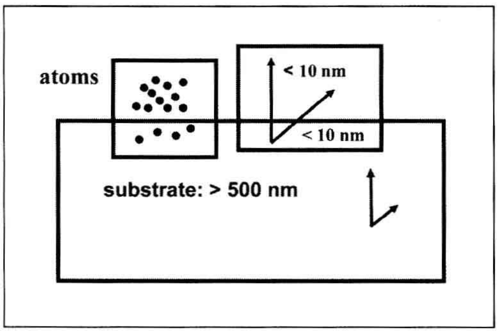

FIGURE 1.4: *Solid system, nanostructured in two dimension.*

tiously in parentheses since although such clusters appear as distinct features in Scanning Tunnelling Microscopy (STM) pictures, see Fig. 1.5, in the case of magnetic atoms forming these clusters they are connected to each other, e.g., by long range magnetic interactions.

It was already said that a classification of nanosystems can be made only in a kind of semi-qualitative manner using typical length scales in one or two dimensions. There are of course cases in which the usual scales seemingly don't apply. Quantum corrals for example, see Fig. 1.5, can have diameters exceeding the usual confinement length of *2d-nanosystems*. Another, very prominent case is that of magnetic domain walls, which usually in bulk systems have a thickness of several hundred nanometers. However, since in nanowires domain walls are thought to be considerably shorter, but also because domain walls

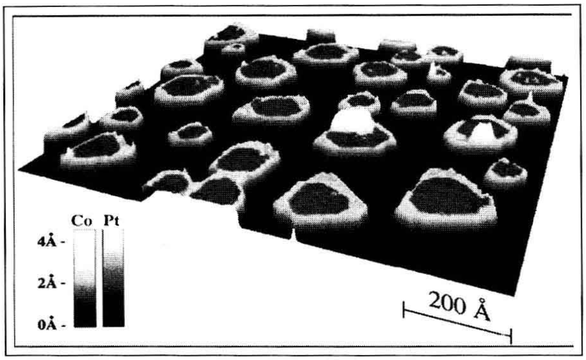

FIGURE 1.5: *Three-dimensional view of a STM image of one-monolayer-high islands with a Pt core and an approximately 3-atom-wide Co shell. By courtesy of the authors of Ref. [2].*

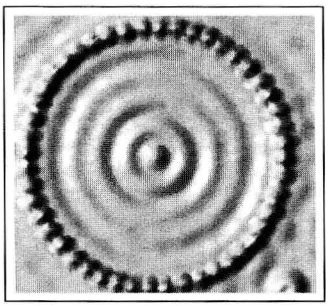

FIGURE 1.6: *Theoretical image of a quantum corral consisting of 48 Fe atoms on top of Cu(111). From Ref. [3].*

are a kind of upper limit for nanostructures, in here they will be considered as such.

Theoretically *1d-* and *2d-nanosystems* require different types of description. While *1d-nanosystems* can be considered as two-dimensional translational invariant layered systems, *2d-nanosystems* have to be viewed in "real space", i.e., with the exception of infinite one-dimensional wires (one dimensional translational invariance) no kind of translational symmetry any longer applies.

It should be very clear right from the beginning that without the concept of nano-sized "functional parts" of a system one cannot speak about nanoscience, since – as the name implies – they are part of a system that of course is not nano-sized. In the case of GMR devices, e.g., there are "macro-sized" leads, while for *2d-nanosystems* the substrate or carrier material is large as compared

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