A DATABASE FOR NANOMAGNETIC MATERIALS – IT IS REALLY A NECESSITY★

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For a long time basic data and information on science and technology have been edited in some classical forms, such as dictionaries, encyclopedia, handbooks, manuals, data books and they have been in general use for now. The possibility of digitizing massive quantities of scientific and technical data was considered in a different way. Since then, a wide variety of databases have been constructed as information processing equipment has progressed. At the macroscopic scale the structure-properties relation for the magnetic materials is usually determined by microstructure and composition. For nanomagnetic materials this type of relation can be found on the atomic level. Commonly, what is known and valid in the macroscopic world does not automatically also hold true in the nano-world. As the scale changes, the ways physical phenomena manifest themselves, also change. This opens the chance of understanding and later for designing nanomaterials by means of computer simulations. The size, shape and other features are related to the expected or targeted properties. A great amount of scientific and technical data on this subject was accumulated. New techniques to find magnetic nanomaterials with optimum properties, including data minig, neural networks, genetic algorithms was considered. So, data must be stored.

Key words: Database, nano-magnetic, nano-materials, neural network.

1. INTRODUCTION

From the basic scientific data to the expert information commonly used, the data was usually edited in well known different forms such as dictionaries, encyclopedia, handbooks, manuals, data books. This type of data storage was of general use for a very long time. At the present, the fast increase of the computer speed and power makes possible to store data in a database and to perform large and more accurate simulations. When large general purpose computers became widespread in the 1990s, the possibility of digitizing huge quantities of data was studied. A wide variety of databases have been constructed as information processing equipment has progressed. Since the 1990s, people around the world

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have been able to share data and information over the Internet, thanks to the rapid dispersion of the world wide web. Generally, *materials data* can be classified into the following two categories:

1. *High-quality basic data* whose universality is high, such as physical constants, spectrum information, nuclear data, structure-independent characteristics, crystal structures, and phase diagrams, and

2. *Fundamental physical, chemical* and *engineering data* that give various characteristics on practical materials which are the basis of design and safety assessment.

High-quality basic data is made useful data by linking it with engineering data. As an example of *high-quality basic data*, basic physical constants were greatly revised and officially announced toward the end of 1999 after a lapse of over ten years by the *Task Group on Fundamental Constants* which was founded under the *Committee on Data for Science and Technology of the International Council for Science* (CODATA) of the *International Council of Scientific Unions* (ICSU) [1]. *Fundamental engineering data and information* are indispensable not only for researchers and technical experts but also for designers of equipment. Such data is used for materials design and various simulations. It is also used for selecting materials for equipment design and optimum use of materials. There are two ways of gathering physical, chemical and engineering fundamental data. One is to collect brochures of materials manufacturers, make a database of the data, and distribute it. The other is to accumulate measured data obtained by various research institutes by carrying out materials tests or data collected from scientific reference materials and compile them into a database. Therefore, a database containing characteristic values as well as information on the manufacturing process of a material, measuring equipment, shape, size and test conditions of a test sample, and test organizations needs to be constructed to enable physical, chemical and engineering fundamental data to be used in industry. However, there is no research institute in the world that collects data systematically, compiles databases therefrom and makes the databases widely available. Concerning such database-making activity, it is important to construct databases efficiently through international tie-ups while avoiding the duplication of similar work, and to establish databases as public goods to be used all over the world.

Magnetic materials have become controllable on the nanometric scale. Nano-magnetic structures exhibit a wide range of interesting magnetic and magnetic correlated phenomena. We recently introduce a new method [2, 3] Artificial Neural Networks (ANN) based, for the design and the characterization of some nano-magnetic materials and to explain several of unique magnetic and non-magnetic phenomena in two-, one- and zero-dimensional nano-structures.

Nanopowders, nanowires, thin films, {Fe, Co, NiCo, CoFeSiB}-based magnetic nano-materials recently prepared in our laboratories, needs now our theoretical consideration. The mechanism of this new ANN method requests massive data processing. First, we need to collect, and accumulate a large amount of physical data on magnetic nano-materials. So, we construct a database containing the main fields for data records as follows: general substantial, structural and chemical data, mechanical data, thermodynamic, electric and magnetic data.

For nano-scaled magnetic materials design it is extremely important to analyze and predict the physical properties and their functionalities [4], and to clarify the relationship between the structure, composition and this functionalities [5]. This seems to be the key for the real progress in the nanotechnologies. In this paper we advance an outline for a magnetic database for the nano-magnetic materials.

2. THEORY AND SOME EXPERIMENTAL ASPECTS

The simulation with a neural network requires the orchestration of many pieces. One of this, very important is the linked *DataBase*. Because this new method requires a large amount of data – some of them measurable, some other not, colected from experiences, made using many different substances and materials with magnetic properties – we will use both data from our laboratory and data already published in other papers. Unlike more analytically based information processing methods, neural computation effectively explores the information contained within input data, without further assumptions. The methods are based on assumptions about input data ensembles.

Almost any effect used in the nano/micro assimilation field depends on the material properties [6–8]. The ability to synthesize nano-scale building blocks with precisely controlled size and composition and then to assemble them into larger structures with unique properties and functions will possibly revolutionize segments of the materials manufacture industry. The most important feature relies on the fact that the nano-scale building blocks offer improved properties and functionalities which are unavailable in conventional materials and devices, since materials in the size range of few nanometres generally exhibit fundamentally new behaviour when their size falls below the critical length scale associated with any given property. Due to rapid progress in the fabrication and processing of nanostructures, it is now possible to realize a broad variety of geometries, crystalline textures and chemistries. Magnetism as a cooperative phenomenon lends itself to manipulation in small structures, where neighbors atoms can be replaced systematically by species with stronger or weaker magnetism. Magnetic nano-structures can be produced in a wide range of geometries. In combination with specific choices of magnetic materials for the structures – or for parts of the structures – this versatility is a major reason for interest in magnetic nano-structures. The structural length scales of nano-magnetics are intermediate between interatomic and macroscopic distances, but nano-magnetism cannot be reduced to a mixture of atomic-scale and macroscopic phenomena. A dynamic aspect of this interplay between atomic (intrinsic) and hysteretic (extrinsic) phenomena is that equilibration times may take values from less than *1 ns* to *millions of years.* This is related to the fact that the thermal instability of the magnetization, occurs in very small magnetic particles and is strongly temperature dependent.

In the following we briefly characterize typical geometries, and mention some systems of practical or scientific interest.

A) NANOPARTICLES, CLUSTERS

Small magnetic particles exist in nature or are artificially produced. Nano particles have sizes ranging from few nanometers to submicron dimensions. Clusters are intermediate structures with less-defined atomic environments but exhibiting atomic features such as facets.

B) GRANULAR NANOSTRUCTURES

Embedded clusters, granular materials, other bulk nanostructures. The structural correlation length of typical nanocomposite materials range about *1 nm* to several *100 nanometers* in submicron structures. A well-known soft-magnetic nano-composite is the “Yoshizawa” alloy $Fe_{73.5}Si_{13.5}B_9Cu_1Nb_3$ – which consist of a DO_3 – structured Fe_3Si grains embedded in an amorphous matrix.

C) PARTICLE ARRAYS AND FUNCTIONAL COMPONENTS

Two-dimensional array of nanoparticles are of interest as scientific model system and have many present or future applications. *Dots* made from iron-series transition metals (Ni), but also from alloys such as Permalloy – with size to less than *100 nm*. *Antidots* – holes in thin films.

D) NANOWIRES

Magnetic nanowires have present or potential applications in advanced nanotechnology: patterned magnetic media, magnetic devices, materials for microwave technology. Problems: establishing an easy axis for typical preparation conditions (shape anizotropy).

E) MAGNETIC THIN FILMS AND MULTILAYERS

Magnetic thin films and multilayers are intermediate between nano-magnetism and surface magnetism. There is a variety of interesting thin-film effects, such as vicinal and interface anisotropies, moment modification at surfaces and interfaces, thickness-coupling, and finite-temperature magnetic ordering. Nanostructures open new possibilities to tailor the mechanical, chemical, optical, magnetic and electronic properties of materials and at present there is strong demand basic understanding of new phenomena that they exhibit. Nanomagnetic objects are different from both atoms and bulk materials, thereby providing an interface between physics, chemistry, material science, engineering and biology.

Magnetic properties. Here we briefly state some magnetic properties used in the design of present *DataBase*: magnetization, thermal stability, coercive force, magnetic remanence; magnetic moment, anisotropy, magnetostriction. Traditionally, magnetic materials are classified by their magnetic coercitivity. That is reflected in the *DataBase* construction also.

3. RESULTS AND DISCUSSIONS

A *DataBase* for nanomagnetic materials was created in March 2007.

Data structuring principle. Two fundamental criteria were taken into account for the data structure:

A) From general to particular: It results a vertical structure on three layers:

a) **Layer 1** Nanomaterials classes:
   - i. Nanomaterial type
   - ii. Specific size
   - iii. Shape
   - iv. Provenience

b) **Layer 2** General information on magnetic nanomaterials:
   - a. Internal codification
   - b. Name
   - c. Commercial denomination

c) **Layer 3** The principal properties of magnetic nanomaterials (as shown, for example in Fig. 1 and Fig. 2).

B) Data structuring as function of their nature, with 8 tables for properties:
   - – Physical (general)
   - – Magnetic
   - – Electric
   - – Thermal
   - – Mechanical
   - – Structural, Composition
   - – Investigation method
   - – The method used to obtain.

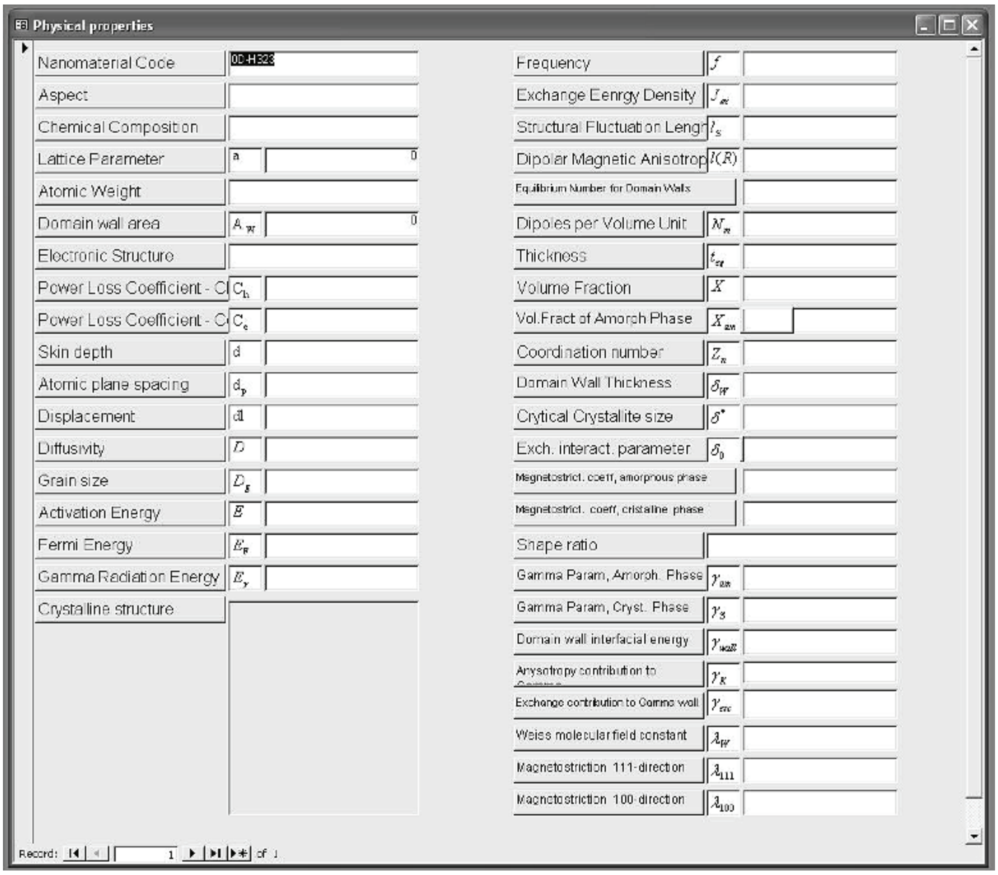

Fig. 1 – Physical properties Form.

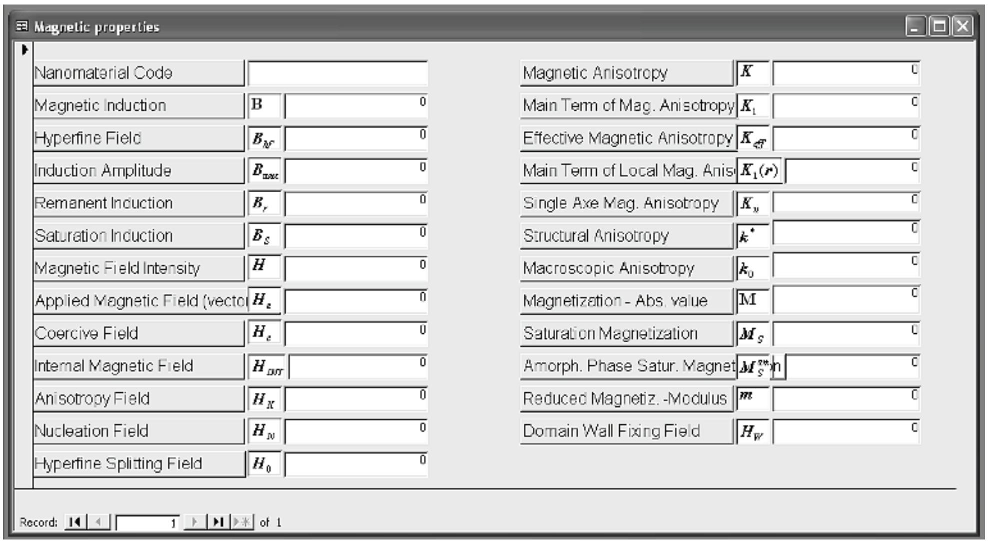

Fig. 2 – Magnetic properties Form.

DataBase was constructed for the beginning in the *MS Office Access* environment, for the *PC Windows XP Operating System*. A special care to avoid redundancies was taken. The relationship between Data-Tables is specified (as show in Fig. 3).

Of course, all of known operation with a DataBase elements may be done.

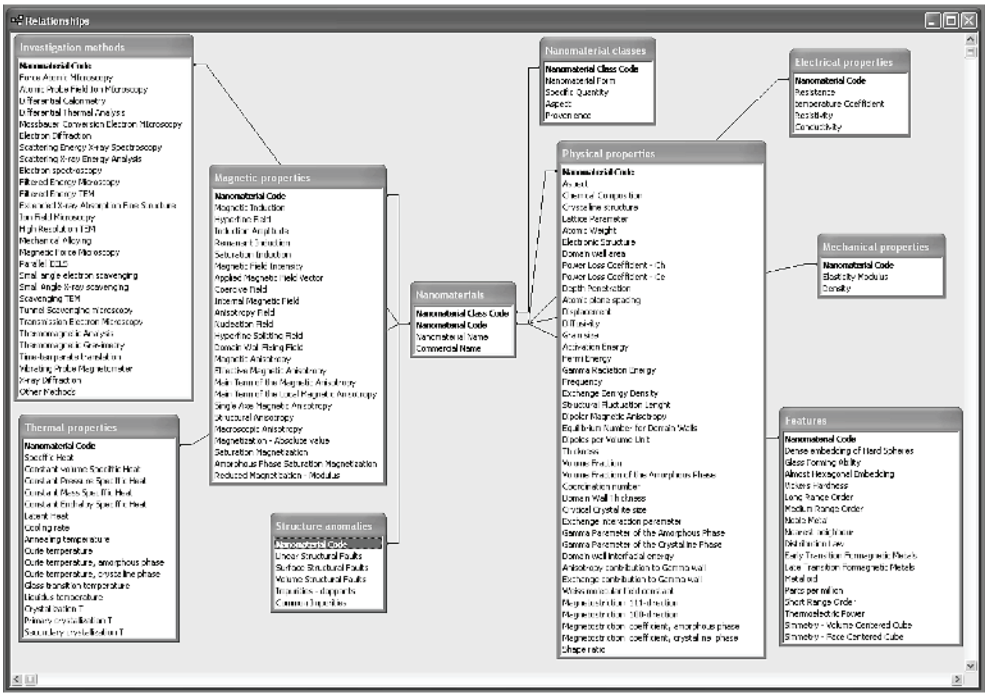

Fig. 3 – Database Relationship.

4. CONCLUSIONS

Past databases were used only by groups engaged in development, and many of them disappeared as the development budget was curtailed and no data was added when the R&D period came to an end. Databases must be continuously accumulated by grasping the needs of users and “usable databases” must be constructed.

A nano-magnetic database was constructed and tested. The database has the main fields for data records as follows: general - physical substantial, structural and chemical data, mechanical data, thermodynamic, electric and magnetic data. The database items contain results of a compilation on data from various sources concerning a given magnetic compound. Mainly published papers with experimental determination of the magnetic structure were used, and some of ours and our main collaborators are also included.

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