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A new simulation method based on artificial neural networks for a special class of nanomagnetic materials design

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A method for the simulation of some new advanced nanomagnetic materials with the Artificial Neural Network (ANN) is given. A Neural Network is an adaptable system that learn relationships through repeated presentation of data and is capable of generalizing to new, previously unseen data. Neural networks are used here for both, regression and classification. Since ANN's learn from the data, the data must be valid for the results to be meaningful. A successful neural network simulation requires the specification of many parameters. This is a hard condition and we show that our work give an important contribution. The performance is highly dependent on the choice of these parameters. By adapting its weights, the neural network works towards the optimal solution based on a measurement of its performance. In our model we intend to use for the input data the following: the chemical composition, the thermal treatments and possibly some structure data. As output data we chose: Hall Effect, and the magnetoresistance effect for FeCrCuNbSiB class nanomaterials.

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1. Introduction

The designing and manufacture of the new nanocrystalline and amorphous alloys with targeted properties is still an actual problem [1,2]. Controlling and manipulating matter down to the length of only one nanometer, which is the size domain of atoms and molecules, has been the dream of scientists and engineers for many years. With the achievements made over the past few decades in increasing the resolving power of the characterisation techniques used to look at atoms and molecules (e.g. microscopy, spectroscopy, diffraction) and the development of new tools to pick up and manipulate individual atoms (e.g. atomic force microscopy) or very small objects (nano-tweezers), new nanostructures have become a reality. At the atomic level forces and interactions are fundamentally different from the macro-world that in the near past led sometimes to confusing scientific concepts. Nanomagnetism includes the artificial structuring of magnetic materials on a sub micron level and natural occurring magnetic entities such as molecules and clusters. Here the emphasis will be on the macroscopic behaviour found in single domains of quantum spins, quantum coherence, dissipation and tunneling of magnetization, disorder and frustration effects. However, nanometer-sized magnetic particles are situated at the frontier between classical and quantum magnetism. In this context the solution to the problem of targeted design for nanomagnetic materials is extremely elaborated and may be so complex that we do not have analytical ways to solve it. So, we introduce here as a new tool the Artificial Neural Network (ANN) method [3]. Once we have a crisp definition, the next step is to select the input variables and the desired responses. We first use common sense to select the variables that are relevant for the problem. One should seek variables and conditions that appear relevant to the problem being analyzed. One should also seek data that covers a wide spectrum of cases. Our model is planed to enhance some new properties of special nanomagnetic materials (FeCrCuNbSiB – at this phase) [4] we have studied.

At this time the main objective of our team efforts is to establish an interdisciplinary research and training team focussed on two ways activities [5-8]. The first is the foundation of a new theoretical model meant for the structure-properties relation for nanomagnetic materials. The second is for directed synthesis of nanophase magnetic particulate materials whose magnetic properties are tailored by the size and composition of the particles, and by their assembly into mono- and multi-component two-dimensional ordered arrays. The broad goals of this program are to create new magnetic materials whose component constituents are magnetic clusters that can be tightly tailored in size and magnetic composition and whose mesoscopic magnetic properties (individual cluster moment, anisotropy, etc.) can be independently varied over a broad range. The synthesis and characterization program will elucidate correlations between physical and magnetic properties of the materials and thus will set a foundation for chemical design of magnetic nanomaterials. As an instrument for the solution of the first way activity is the new development taken by the exploit of the Artificial Neural Networks (ANN) method.

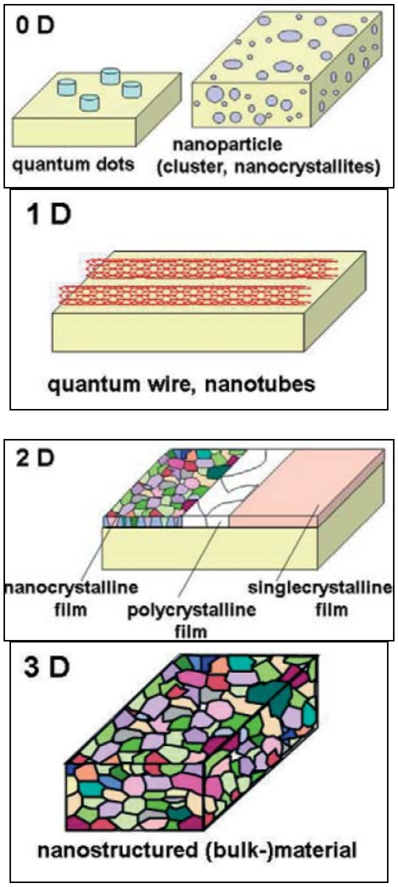

Fig. 1. Nanomaterials and nanostructures classified by their reduced dimensionality.

Almost any effect used in the nano/micro assimilation field depends on the material properties [9-11]. The ability to synthesise 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 revolutionise segments of the materials manufacture industry. In Fig. 1 we illustrate nanomaterials and nanostructures classified by their reduced dimensionality. 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. For example, the wave like properties of electrons inside condensed matter are strongly influenced by structural variations on the nanometre scale. Furthermore, by patterning matter on the nanometer length scale, it is possible to vary fundamental properties of materials, for instance melting temperature, magnetization, colour without changing the chemical composition. Consequently, macroscopic materials and structures with fundamentally new properties can be developed following new design rules. For nanocomposites, the addition of nanoparticles to an otherwise homogenous material can further lead to a fundamental change in the macroscopic material behaviour. Thus, most material properties may be changed and engineered dramatically through the controlled size-selective synthesis and assembly of nano-scale building blocks.

On the other part the manipulation of spin-polarized currents in structures with dimensions in the nanometer range offer new opportunities for device design. First-generation spin electronics has been based on magnetoresistors -spin valves and tunnel junctions used as field sensors and nonvolatile computer memory. The next generation will be very probably built on multi-terminal devices, and perhaps exploit magneto-optics to generate novel technology. Spin-transport across ferromagnetic interfaces or nanocontacts is a poorly-understood process, but it plays a central role in many device structures. High-frequency magnetic response of nano-objects, and the transport of electrons through regions of intense electric fields or magnetic field gradients have to be explored in the near future. Our experimental team efforts is now focussed on the physics of charge transport phenomena in nanomagnetic materials too.

2. Experimental

a) Theoretical aspects. This new brand of approach used in our work recommends the use of software simulation using Neural Network combined with clustering analysis in order to determine the *hidden* relations between different parameters. This is the point and the purpose of the work described in this paper. The frequently used models of statistical mechanics lead often to analytical solutions, although these are not so close to reality; these models are important in the testing of a new theory. In order to build realistic models for a large number of the present nanomaterials we have to do better than these analytical solutions. Some theories like the kinetic Ising model, the classic Heisenberg model, the micromagnetic Langevin model were studied using a Monte Carlo simulator i.e [12-16]. The new method proposed here wants to replace the traditional methods of finding out new properties with a new model based on a better understanding of the vague information offered by the experiment, but also on re-analysing the already existent and checked models. A new theory can be conceived after its basic results are proved and then new hypothesis can be made.

This new instrument can extend, in most cases, laws or relations directly just by “looking” at the given data. It is structured and based onto a massive Data Base. The major actions made would be: the analysis of the results, the conception of a raw model and later the characterisation of the nanomagnetic materials obtained. As we already illustrate nano-metric substance one can distinguish nanoparticles, thin films of nano-metric thickness, columns with nano-metric diameters on a massive support, nano-metric magnetic ribbons and wires, nanocomposites and nanostructured materials. The magnetism of nanomaterials has been studied for a long time, but there always was a difficult task – the characterisation of these nanomaterials. Magnetism, as a cooperative phenomena, includes the handeling of small structures, in which the atoms can be easily replaced with other atoms that have more or less magnetic strength in order to control the magnetic field created. It is well known that the wave function of electrons changes when it is mandatory that they remain in a space that has the dimensions comparable with their wave function. At usual temperature e.g. for metals $E = kT = 0.026$ eV and de Broglie wavelength

$$\lambda = h/p = h/(2mE)^{1/2} < 1.23\,nm,$$

it's nano-metric. So, the order imposed by the magnetic forces will contribute to the structure of the substance at the nano-metric size. The magnetic properties of a material are sensitive regarding to the local structure. Nanostructure magnetism is in this manner related to the study of other methods and materials. The order of the nanostructure can be modified by adjusting the conditions under which the materials are produced. Another possibility is to correlate the electronic properties with the structure of the nano-material.

b) Modelling What is ANN, and how it works? A neural network is an adaptable system that can learn relationships through repeated presentation of data and is capable of generalizing to new, previously unseen data. Some networks are supervised, and a human determines what the network should learn from the presented data. In this case, you give to the network a set of inputs and corresponding desired outputs, and the network tries to learn the input-output relationship by adapting its free parameters.

Neural networks are used for both regression and classification. In regression, the outputs represent some desired, continuously valued transformation of the input patterns. In classification, the objective is to assign the input patterns to one of several categories or classes, usually represented by outputs restricted to lie in the range from 0 to 1, so that they represent the probability of class membership. For regression, it can be shown that a single hidden layer **M**ulti**l**ayer **P**erceptron (MLP) can learn any desired continuous input-output mapping if there are sufficient numbers of axons in the hidden layers. For classification, Multilayer Perceptrons can learn the Bayesian posterior probability of correct classification. This means that the neural network takes into account the relative frequency of occurrence of the classes, giving more weight to frequently occurring classes. Our neural networks have been trained to perform complex functions in this field including pattern recognition, identification, classification.

The neural networks domain has a history of five decades but has found solid application only in the past fifteen years and the field is still developing rapidly [17-19]. Today neural networks can be trained to solve problems that are difficult for conventional computers or human beings.

c) Experiment. The important objective for this work is the relation between the structure of the material and its magnetic properties. This material structure through its order or disorder can be understand using ANN methods as a theoretical instrument. The relations between the structure and the properties are then easily exploited and finally lead to the new material characterization.

These are the steps:

1. gathering data referring to different categories of nanomagnetic materials;
2. storage and the organizing of the data in a massive data base;
3. the modelling of a pattern for a category of magnetic nanostructures;
4. testing the instrument using the neural networks for the given pattern;
5. the use of the instrument in order to characterize a new nanomagnetic material;
6. the construction of the model for simulating neural networks that will be useful in the future experiments to make;

We can use for example, to feed the instrument constructed with ANN as input - data extracted from the typical MFM images with "dark and bright contrast" depending on direction and strength of the magnetic stray fields. Fig. 2 [20] shows an MFM image of microstructured Fe(110) ellipsoid-shaped elements with lateral dimensions of 1.5 μm 500 nm. Starting with a 25 nm thick iron film with (110) orientation these elements have been fabricated by using electron beam lithography and argon ion etching [21]. After applying a magnetic field of 1 Tesla perpendicular to the long axis of the elements - i.e. along the magnetic hard axis - the MFM image exhibits three different remanent magnetic states for zero magnetic field (see white frame in Figure 2). If the bright contrast represents an attractive interaction between the tip and the stray fields the upper element in the white frame shows a single domain state (or dipole state) with the magnetization pointing to the right side as illustrated in the upper left inset in Fig. 2. According to this the magnetization of the lower element in the white frame is pointing to the right. The element in the middle shows a less pronounced magnetic contrast. This is an evidence for a multi domain state (or demagnetized state). By forming such a state the stray fields are minimized by closing the magnetic flux within the element (see the upper right inset in Fig. 2). All the details extracted from this image may be taken as input data for the ANN simulation.

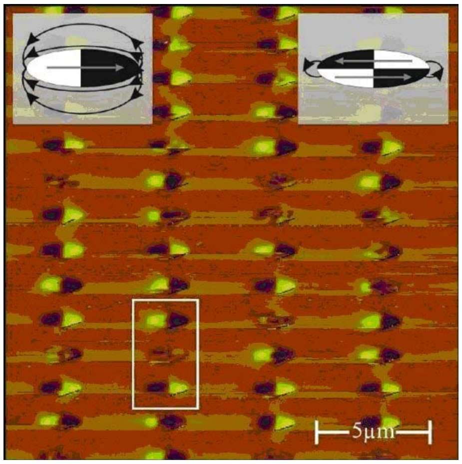

Fig. 2 MFM image of microstructured ellipsoid shaped Fe(110) elements [20].

The current stage. We obtain for the beginning a new model for the design and the characterization of some special nanomagnetic materials in the class: FeCrSiBMo and CoFeSiB alloys. In the present this nanomagnetic alloys are studied with other methods some interesting properties like: Anomalous Hall Effect (AHE), Magnetoresistance Effect, the influence of the composition and of the thermal treatments on their magnetic properties [22-24].

3. Results

At the core of neural computation are the concepts of distributed, adaptive and nonlinear computing. Neural networks perform computation in a different way than conventional computers, where a single central processing unit sequentially dictates every piece of the action. Neural networks are built from a large number of very simple processing elements that individually deal with pieces of a big problem. A processing element (PE) simply multiplies an input by a set of weights, and nonlinearly transforms the result into an output value. The principles of computation at the PE level are deceptively simple.

Data Structures How the format of input data structures affects the simulation of networks. For concurrent vectors, the order is not important, and if we had a number of networks running in parallel, we could present one input vector to each of the networks. For sequential vectors, the order in which the vectors appear is important. In our model we used as input data the following: the chemical composition which has been coded, the thermal treatments and possibly some structure data which was coded. As output data the Hall Effect, the magnetoresistance effect of this alloys.

Training Styles We use two different styles of training. In incremental training the weights and biases of the network are updated each time an input is presented to the network. In batch training the weights and biases are only updated after all of the inputs are presented.

Learning Rules The learning rule is applied to train the network to perform particular task. As the inputs are applied to the network, the network outputs are compared to the targets. The learning rule is then used to adjust the weights and biases of the network in order to move the network outputs closer to the targets. Most of these algorithms perform clustering operations. They categorize the input patterns into a finite number of classes.

Using of neural networks in order to predict the solution of this complex practical problem is one of the improvements suggested by this paper. While applying the neural network methods we follow several steps like: gathering data; correlate the input data with the structural analysis data; determining how good the newly model with neural networks are, and so on.

We must also establish the optimal architecture, the number of intermediate layers and the number of neurons in each layer. We also must compare the new model with the ones obtained before. This new model will provide information in the later studies. The optimization of the processes may use an inverse neural modelling: the input will be the former output and vice-versa – the result are the conditions for a new experiment. In order to improve the neural network performances we will use different network types and techniques: multilayer neural networks – type forward, recurrent networks that are able to predict how the system will evolve, stacks of networks, which are able to memorize different other aspects; and also different algorithms for grouping and classifying of the date we obtain. Hibrid shaping combines phenomenological modelling with neural modelling – used for the hard part. Using the instruments of artificial intelligence in a design process is a complex research but once the work techniques are understood and used, they can be used in a lot of other physical or chemical processes.

The general learning problem for a neural networks is refering at the finding of parameters of a particular architecture. All the components can be totally or partially unknown: the number of hidden layers, the number of neurons, the connection mode, the activation function, the weight values. The difficulty of the learning problem is closely related to the parameters that must be determined by the learning algorithm. In the context of nanomagnetic structures field, will be developed and applied both the hypostasis of learning corresponding to the finding of weights (using gradient algorithms with the backpropagation of the error, methods of level two and various techniques of acceleration) and the most comprehensive, but complex case, corresponding to the finding (during the learning process) of the network graph and weights that are producing the minimization of a complexity function. For this task will be developed hybrid methods based on genetic algorithms and optimisation techniques with multiple objectives. In the context, the neural networks is used for the modelling of the dependencies that exist in the nanomagnetic structures. One of the approaches used to solve this problem is based on genetic algorithms, combined with Newton type methods.

4. Discussion

Fundamental concepts that are valid in the macroscopic world cannot easily be transferred to the nanoworld and opposite. However, this opens up new possibilities to assimilate nanostructures in new application and to benefit from the physical, chemical or biologically material properties at the nano-scale. The integration of nanomagnetic materials covers a broad range from technologies and applications like gas sensors with nanostructured gas sensitive films, GMR sensors, high-resolution spectroscopic measurement techniques, packaging and interconnection technologies, to name a few topics. Most integrated nanostructures in sensors today are ultra-thin or nanostructured films and multilayers. This is sometimes sufficient to improve important properties or the sensitivity of the sensor by orders of magnitude.

The power of neural computation comes from the massive interconnection among the PEs, which share the load of the overall processing task, and from the adaptive nature of the parameters – weights, that interconnect the PEs. Normally, a neural network will have several layers of PEs. The most basic feed forward architecture is the multilayer perceptron (MLP). By adapting its weights, the neural network works towards an optimal solution based on a measurement of its performance. For supervised learning, the performance is explicitly measured in terms of a desired signal and an error criterion. Artificial neural networks permit us the almost perfect approximation of the systems on which we don't have enough information and therefore we cannot apply the classical methods. A neural network is a general model, based on the information received from a set of data without any need of rules or explicit equations. They are used in applications were precision is an obstacle while using traditional methods, e.g. applications that need the recognition of shapes or simulating a too complex physical system.

5. Conclusions

Designing and manufacture of new magnetic nanomaterials with targeted properties is an actual problem. Controlling and manipulating matter to the nanometer length, the size domain of atoms and molecules, is an important activity. Neural networks have been applied successfully in the new simulation method for the magnetic nanomaterials. The universal approximation capabilities of the multilayer perceptron make it a useful choice for modelling nonlinear systems and for implementing general-purpose controllers and magnetic characteristics extractor from wide data amount. Neural networks are used for both, regression and classification. ANN's learn from the data, so the data must be valid for the results to be meaningful. A successful neural network simulation requires the specification of many parameters. The chemical composition has been coded, the thermal treatments and some structure data which was coded. As output data was taken the Hall Effect parameters , the magnetoresistance effect parameters of this alloys.

The model and the method presented allow to find new magnetic materials with enhanced Hall and magnetoresistive properties.

References

[1] Interagency Working Group on Nanoscience, Engineering and Technology of the National Science and Technology Council's Committee on Technology, "National Nanotechnology Initiative: Leading to the Next Industrial Revolution," Washington D.C., 2000.

[2] National Science and Technology Council (NSTC) Committee on Technology and the Interagency Working Group on NanoScience, Engineering and Technology (IWGN), edited by R.W. Siegel, E. Hu, M.C. Roco, WTEC, Loyola College in Maryland, "Nanostructure Science and Technology A Worldwide Study,“ 2000.

[3] Wasserman, P. D., Advanced Methods in Neural Computing, New York: Van Nostrand Reinhold, 1993

[4] C. M. Hurd, Hall Effect in Metals and Alloys, Plenum Press, New York, 1972.

[5] H. Chiriac, M. Lozovan, Maria Neagu and Cornelia Hison, J. Magn. Magn. Mater. **215-216**, 378 (2000).

[6] H. Chiriac, M. Lozovan, M. Neagu, Romanian Reports in Physics **46**(2-3), 215 (1994).

[7] C. Chiriac, M. Lozovan, S. Mohorianu, H.Chiriac,V. M. Cosma, Conferința Internațională TMCM′96, Iaşi, vol.III, 1996, 279-282

[8] H. Chiriac, M. Lozovan, Maria Neagu and Cornelia Hison, J. Magn. Magn. Mater. **215-216**, 378 (2000).

[9] M. Grimsditch, G. K. Leaf, H. G. Kaper, D. A. Karpeev, R. E. Camley, Normal modes of spin excitations in magnetic nanoparticles, Phys. Rev. B**69**, 174428 (2004).

[10] K. L. Metlov, K. Yu. Guslienko, K. Yu., Quasi-uniform magnetization state in soft ferromagnetic nano-cylinders, Phys. Rev. **B70**, 052406 (2004).

[11] K. Yu. Guslienko, V. Novosad, Vortex state stability in soft magnetic cylindrical nano-dots, J. Appl. Phys. **96**, 4451 (2004).

[12] M. Grimsditch, L. Giovannini, F. Montoncello, F. Nizzoli, G. Leaf, H. Kaper, and D. Karpeev, Magnetic normal modes in nanoparticles, Proc. Workshop Frontiers of Condensed Matter: Magnetism, Magnetic Materials, and Their Applications, Physica B **354**, 266-270 (2004).

[13] A. Hoffmann, Symmetry driven irreversibilities at ferromagnetic-antiferromagnetic interfaces, Phys. Rev. Lett. **93**, 097203 (2004).

[14] K. Yu. Guslienko, O. Chubykalo, O. Mryasov, R. W. Chantrell, D. Weller, Magnetization reversal via perpendicular exchange spring in FePt/FeRh bi-layer films, Phys. Rev. B **70**, 104405 (2004).

[15] G. Gubbiotti, K. Yu. Guslienko, A. Andre, C. Bayer, and A.N. Slavin, Magnetic Field Dependence of Quantized, and Localized Spin Wave Modes in Thin Rectangular Magnetic Dots, J. Phys.: Cond. Mat., **16**, 7709 (2004).

[16] M.R. Fitzsimmons, S. D. Bader, J. A. Borchers, G. P. Felcher, J. K. Furdyna, A. Hoffmann, J. B. Kortright, I. K. Schuller, T. C. Schulthess, S. K. Sinha, M. F. Toney, D. Weller, and S. Wolf, Neutron Scattering Studies of Nanomagnetism, and Artificially Structured Materials - Topical Review, J. Magn. Magn. Mater., **271**, 103 (2004).

[17] Lippman, R. P., "An introduction to computing with neural nets," IEEE ASSP Magazine, pp. 4-22, 1987
[18] Kohonen, T., Self-Organizing Maps, Second Edition, Berlin: Springer-Verlag, 1997.
[19] Lippman, R. P., "An introduction to computing with neural nets," IEEE ASSP Magazine, pp. 4-22, 1987
[20] C. König, M. Sperlich, R. Heinesch, R. Calarco, J. O. Hauch, U. Rüdiger, S. Kirsch, B. Özyilmaz, A. D. Kent, and G. Güntherodt, Appl. Phys. Lett. **79**, 3648 (2001).
[21] J. Yu, U. Rüdiger, A. D. Kent, L. Thomas, S. P. Parkin, Phys. Rev. B **60**, 7352 (1999).
[22] H. K. Lachowicz, R. Zuberek, M. Kuzminski, A. Slawska-Waniewska, J. Magn. Magn. Mater. **196-197,** 151 (1999).
[23] J. Gonzalez, N. Murillo, J. M. Blanco, P. Quintana, E. Amano and R. Velenzuela, IEEE Trans. Magn. **30**, 4812 (1994).
[24] G. Bordin, G. Buttino, A. Cecchetti and M. Poppi, J. Magn. Magn. Mater. **172**, 291 (1997).

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