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Computational Research in the Investigation of New Nanomagnetic Materials

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1. Introduction

Our Institute NIRDTP Iasi for almost 30 years has researched magnetism and magnetic materials. The way these materials are created, their characterization and the study of their magnetic properties in relation with the factors that influence these properties was concentrated during the last years on micro and **nano materials** that we will name thereafter **nanomagnetic materials.**

Over the last decade : **computer modeling** – evolved to become **a third pillar of research** alongside ***experiment*** and ***theory !***

Reasons for this emergence :

•An exponential increase in processing speed;
•Relatively inexpensive platforms for parallel computing and data storage;
•New visualization capabilities;
•The development of powerful algorithms with full advantage of this in hardware;

ADVANCES in simulation methodologies :

– Have made results in atomic-level computer modeling : simulation can replace expensive and difficult experiments;
– Enable atomistic dynamics using full electronic energie – now allow processes involving up to several thousand atoms to be accurately modeled;
– The ability for *computer modeling* and *computer experiment* to characterize phenomena on a common scale, and now at micro and through our work at nano scale.

As a consequence of using such a results :
- We can now explore and predict new phenomena that can be probed experimentally, to suggest new materials and structures with unique and desirable properties;
-We can provide insight into the results of experiments;
-We may generate data for larger-scale analysis;
-We can test scaling laws and analytic theories.

Magnetism is a very complex and intriguing phenomenon. Early experiments to elucidate magnetic phenomena and magnetic materials behavior were based on the measurement of forces and torques exerted on “samples” placed into magnetic fields produced by current flow through wires. Our modern understanding of electronic structure is based on the concepts of charge and spin.

As a remember here are some of the most notorious **modeling methods** in domain:
-**Molecular Dynamics and Monte Carlo Modeling;**
-**Atomic Potential Energies and Forces;**
-**Multiscale Modeling**

Our method is a new one. Extracting valuable information from data using the distributed computer processing and storage technologies, as well the Artificial Neural Network (ANN) and the development of advanced algorithms for **knowledge discovery** are the purpose of our work. Our new methods allows that, by searching on the correlations for the most recent material properties to enhance the actually known magnetic properties.

Modeling and simulation techniques can be used in all stages in the development and improvement of new materials, from the initial formation of concepts to synthesis and characterization of properties. We describe how a Simulation and Design Method (**SDM**) attempt, based on our last results [1-4], is applied on some new type nanomaterials.

Our new ANN and the SVM (Support Vector Machines) technique is intended to contribute on the effort to improve some properties of the new nanomagnetic materials. It implements and uses the basic building blocks of neural computation, such as multi-layer perceptrons. Support Vector Machines are systems for eficiently training the linear learning machines in the kernel-induced feature spaces exploiting the optimization theory.

Our IT simulation results are now proposed to be checked in labs with the experimental data and we expect a good agreement. *This work presents the last results in the investigation of the structure-properties relationship and the size effect for some nanomagnetic materials using some new IT research instruments. The study allow the discovery of some new nanomagnetic materials.*

2. Theoretical aspects

Currently **nanomagnetism research** involves investigating the basic magnetic, magneto-optical, galvanomagnetic, magnetotransport phenomena associated with reduced dimensionality.

It seems that today's magnetic materials are not only the **bulk materials**, but mainly atomically engineered **wires**, **particles** or **thin film** and also **multi layer structures** that often have one, two or three dimensions on the nanometric scale (as shown in figure 1).

The growth of magnetic technologies is due to scientific and technological developments in four key areas:
(1) the development for the research of the new magnetic materials,
(2) the progress in theoretical developments,
(3) the developments of new experimental techniques,
(4) the developments in simulation techniques

The idea of extracting valuable information from data [5] [OLD3], *data mining*, is not new. It is new the distributed computer processing and storage technologies, which allow *gigabytes*, even *terabytes* of data to remain on-line, available for processing by client/server applications. It's new as well, the Artificial Neural Network (ANN) use and the development of advanced algorithms for knowledge discovery.

On the global framework of computational nanotechnology [6] [OLD4] the software required for the modeling and to design complex molecular structures becomes progressively available.

Our new ANN based model, is intended to contribute to this effort and to improve some properties of the new magnetic materials. This new method, requires a large amount of data, some of them directly colected from experiences made using different substances and materials with known magnetic properties.

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. Artificial intelligence encodes a priori human knowledge with simple *if-then* rules, performing inference on these rules to reach a conclusion [7] [OLD5].

With Neural networks, **we notice that *we can discover* relationships in the input data sets** through the iterative presentation of the data using the intrinsic mapping characteristics of neural topologies - *learning*. There are two basic phases in a neural network operation : the *training* phase, where data is repeatedly presented to the network, while its weights are updated to obtain a desired response and the recall or *retrieval phase*, where the trained network with frozen weights is applied to new data, which were never seen. The learning phase is time consuming due to the iterative nature of searching for the best performance. Once the network was trained, the retrieval phase can be very fast, because processing can be distributed. In our recent attempt Neural Networks were used for both, regression and classification.

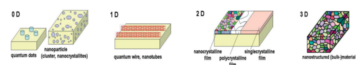


Figure 1 Nano-materials and nano-structures. Dominant dimension classification

3. Experimental

The basic idea is to obtain a fine correlation between the **material structure** and/or **composition** in one hand and **the magnetic material properties** on the other, using either ANN or SVM or RF as **Computational Research** (CR) instrument.

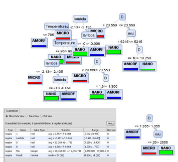
Here is a starting point for looking at the experimental objectives of this part of work we done, and we describe here. The analyst has a near-infinite number of approaches that can be taken in the course of an simulation/numerical experiment.

The approach that is used will depend on
(1) the kind of material to be analyzed,
(2) the form of the material,
(3) the problem that is required to be solved,
(4) the experimental or instrumental technique that can be employed,
(5) the known limitations of the instrumental/simulation method.
The 5 categories that may conduct the analyst's approach are detailed in [Granda].

Previous simulation experiments have been made using the ANNs. The results have already been published and acknowledged. Since it is know that the ANNs depend very much on the initial choice of weights we try to find a method that can overcome this disadvantage. Some methods we can mention are Support Vector Machine (SVMs) and Random Forest (RF).

Before applying any machine learning techniques we must understand how the data are described – we need to define the features that will help us learn the desired properties. The great step is understanding the data, (Fig. 2, Fig. 3) – so, we analyse the datasets using WEKA and Rapid Miner as techniques.

Fe_ZrHfNb_alloys	Total AMORF	True Amorf	Total NANO	True Nano	Total MICRO	True Micro	ACC	
Zr	5	4	18	17	5	4	0.892857	RF
HF	5	4	30	30	7	7	0.97619	
Nb	6	6	24	23	16	16	0.978261	
	Total AMORF	True Amorf	Total NANO	True Nano	Total MICRO	True Micro	ACC	
	5	5	18	18	5	5	1	SVM
	5	5	30	30	7	7	1	
	6	6	24	24	16	13	0.934783	
	Total AMORF	True Amorf	Total NANO	True Nano	Total MICRO	True Micro	ACC	
FeCoZrB alloys								
FeCoZrB	Total AMORF	True Amorf	Total NANO	True Nano	Total MICRO	True Micro	ACC	
	6	6	30	28	9	8	0.933333	RF
	6	6	30	28	9	9	0.955556	SVM
FeZrB	Total AMORF	True Amorf	Total NANO	True Nano	Total MICRO	True Micro	ACC	
	3	3	32	31	8	7	0.953488	RF
	3	0	32	32	8	7	0.906977	SVM



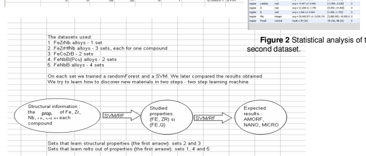


Figure 2 Statistical analysis of the second dataset.

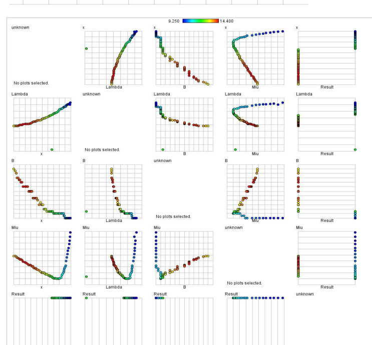


Figure 3 Graphical analysis of the second dataset.

4. Results

We prove that both on average and in the majority of the conducted studies the Random Forest method is comparable with the SVM method [8] and they both are more reliable than the ANN. We also developed a strategy of approaching this problem and a two step method which is usefull for the ***discovery*** of *new nanomagnetic materials.*

The artificial intelligence machine has the capability to discover new nanomagnetic materials by “learning”, and “predict”. The new found materials are represented as islands in a **INOUE-type diagram**, as one can see, figure 4.

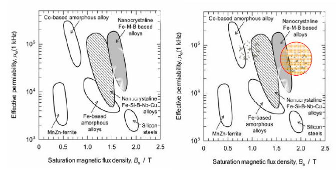


Figure 4 INOUE type diagram

a) original - known islands of materials
b) b) new islands from the simulation (marked areas)

5. Conclusions

Low dimensional magnetic systems, such as thin films, wires, multilayers, and surfaces exhibit many scientifically interesting and technologically useful properties. Modeling has now a very important position in the development and improvement of new materials for applications.

Modeling and simulation techniques affect all stages in the development and improvement of new materials, from the initial formation of concepts to synthesis and characterization of properties. Neural networks have been applied successfully in the identification and classification of some nanomagnetic characteristics from a large amount of data. The universal approximation capabilities of the multilayer perceptron make it a useful choice for modeling nonlinear systems and for implementing general-purpose controllers and magnetic characteristics extractor from wide data amount. Even better than the ANNs are the SVMs, which have a strong statistical backgorund and also the Random Forests, which are more intuitive. Both of these methods are used alternatly to ANN and prove themselves to be better candidates for the discovery of new magnetic nanomaterials.

The work presents the last results in the investigation of the structure-properties relationship and the size effect for some nanomagnetic materials using some new IT research instruments. The study allow the virtual discovery of new nanomagnetic materials.

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