

A NEW IT STRATEGY ANN BASED FOR SPECIAL
NANOMAGNETIC MATERIALS DESIGN AND CHARACTERISATION*

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Modelling has played a very important role in the development and improvement of new materials for applications. Our knowledge of nanomaterials such as quantum dots, nanostructures, molecular assembly, proteins or DNA molecules, is still at a very beginning stage. Modelling and simulation techniques affect all stages in the development and improvement of new materials, from the initial formation of concepts to synthesis, characterization and properties. We think new modelling strategies for complex material systems are needed. At present time it still seems unlikely that we will be able to treat all of the interesting problems by *ab initio* methods. Even if this were to become possible, the analysis of the enormous amount of data generated from computer simulations would itself require massive computing power and a comprehensive modelling strategy. Such modelling strategies should focus on the multi-scale and multiphysics nature of emergent problem in area. We gently introduce here the Artificial Neural Network (ANN). In our first model we intend to use for the input data *e.g.* the chemical composition, thermal treatments and some structure data. As output data: AHE, and magneto-resistance effect of some of our new magnetic Co-based alloys.

Key words: nanostructures, IT strategy, ANN, nanomagnetic materials, characterization, design, computer modelling.

1. INTRODUCTION

Beside the exciting new capabilities and opportunities, nanostructured materials cause some challenges that were not present in the field of *traditional* materials. While trial-and-error engineering was a successful approach for most of the traditional materials, one can show why this is difficult in the nanoscale materials domain, where fundamental understanding on the atomic level is required for the successful materials design [1–5]. In this area, computer modeling poses new chances, for targeted design – when developing new magnetic nanomaterials.

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Characterization. For **traditional materials**, the microstructure and the composition – weight fractions of the different elements in the mixture, determine their properties. For **nanostructured materials**, the exact composition (what atomic species are present), and the configuration (where the atoms and sometimes even electrons are exactly located on the atomic scale), determine the materials properties[6]. Conventional tools such as light microscopes, X-ray diffraction, mass spectrometers etc., cannot provide such information. Combinations of atomic-level modeling and atomic-resolution characterization [7, 8] *e.g.* analytical electron microscopy gave us hopes in this area so far.

Fabrication – process modeling. For **traditional materials** average properties such as concentrations in continuum or phase-field modeling and mostly equilibrium thermodynamics – phase diagrams, diffusivities are sufficient to model the evolution of a material during processing. For **nanostructured materials**, single atoms need to be traced during the processing in order to predict the final structure and its properties. However, traditional atomic-level techniques such as molecular dynamics are only capable of following a few atoms reliably for few nanoseconds, not long enough for most processing steps. The recent development of new techniques such as transition-state-theory based methods, accelerated dynamics and physics-based Monte Carlo methods get around this problem and enable nanoscale process modeling.

Structure-property relationship. For **traditional materials**, the properties are determined by microstructure and composition. The structure-property relationships are in many cases still poorly understood from a fundamental point of view, but vast experience and theory exists which tells us how to change the structure in order to improve the properties. For **nanostructured materials**, the structure-property relationships can only be found on the atomic level and experience is missing. As examples there are the scaling relationships between dimensions and electron transport in nanoelectronics devices, which strongly differ from those of the conventional devices. The theory that is currently being developed is less heuristic and more fundamental than for traditional materials, which opens the chance of designing and understanding materials more reliably by using computer simulations.

Nanomagnetic Materials Design. For **traditional materials**, revolutionary new materials are in most cases discovered by accident. Most of the *design* time is spent on incremental improvement of a known type of materials, *e.g.* alloying it with small amounts of impurities. For **nanostructured materials**, computational design of hypothetical new materials is possible, including the study of stability and the prediction of properties. In combination with a mature materials synthesis facility completely new materials can be virtually designed and made-up.

Nanomagnetism research involves investigating the basic magnetic, magneto-optical, galvanomagnetic, magnetotransport phenomena associated with reduced dimensionality [9]. It has long been known that confinement and

finite-size effects alter magnetic properties. Recently, it has been shown that these finite-size effects can be connected for new magnetic applications [10, 11]. Thus, it is vital to understand the magnetic behavior of individual building blocks, which eventually will be combined into more complex structures for new functionalities. In addition to technological relevance, other exciting basic science questions remain to be answered, which arise from the interplay of finite size and shape-induced modifications of magnetic behavior combined with interactions across interfaces between magnetically different materials. Nanopowders, nanowires, thin films, (Fe, Co, NiCo, CoFeSiB) and magnetic nanomaterials recently prepared in our laboratories, now need our theoretical consideration. Our research is focused on a large extent on developing a robust IT method to solve the *prediction problem* for a *nice* relationship structure-property concerning our magnetic nanostructures.

We try to obtain at the beginning, a new model for the characterization of some materials in the class: FeCrSiBMo and CoFeSiB alloys. They were studied with other methods for some interesting properties like: Hall Effect, magneto-resistance effect on the influence of the composition and of the thermal treatments for the magnetic properties of this alloys [12–14].

Now we don't have analytical solution for them. Once we have a crisp definition, the next step is to select the input variables and the desired responses. So we introduce the new strategy, we bring in the *Artificial Neural Network* (ANN). The IT method used is based on an adapted Neural Network with the *Neuro Dimension* platform. We notice some major applications of ANN's as follow: **Pattern classifiers:** The necessity of a data set in classes is a very common problem in information processing. We find it in quality control, financial forecasting, laboratory research, targeted marketing, bankruptcy prediction, optical character recognition, etc. ANNs of the feedforward type, normally called multilayer perceptrons (MLPs) have been applied in these areas because they are excellent functional mappers – these problems can be formulated as finding a good input-output map. **Associative memories:** Human memory principles seem to be of this type. In an associative memory, inputs are grouped by common characteristics, or facts are related. Networks implementing associative memory belong generally to the recurrent topology type, such as the Hopfield network or the bidirectional associative memory. However, there are simpler associative memories such as the linear or nonlinear feedforward associative memories [15]. **Feature extractors:** This is also an important building block for intelligent systems. An important aspect of information processing is simply to use relevant information, and discard the rest. ANNs can be used as principal component analyzers, vector quantizers, or clustering networks. They are based on the idea of competition, and normally have very simple one-layer topologies. **Dynamic networks:** A number of important engineering applications require the processing of time-varying information, such as speech recognition, adaptive

control, time series prediction, financial forecasting, radar/sonar signature recognition and nonlinear dynamic modeling.

The field of neural networks has been studied for almost five decades but has found solid application only in the past fifteen years, and this field is still developing quickly. Today neural networks can be trained to solve problems that are difficult for conventional computers or human beings.

2. THEORY ON NANOMAGNETIC MATERIALS AND EXPERIMENTAL ASPECTS

2.1. NANOMAGNETIC MATERIALS. WHAT WENT BEFORE AND THE PRESENT

One knows that in a very simplified atomic orbital model, the moment is created by interaction between electrons on the same atom and the coupling between electrons on different atoms. Spins are aligned antiparallel at the smallest distances or volumes, since Pauli's exclusion principle prevents equal spins from occupying the same status. This reduces the moment of an individual atom and produces antiferromagnetic coupling between atoms. The interaction changes its sign as soon as the wavefunctions cease to overlap strongly. The moment increases and the coupling becomes ferromagnetic. At larger distances the magnetic coupling becomes indirect, using conduction electrons as mediators. It oscillates with a period determined by Fermi wave-vectors, thereby bringing orientation-dependent Fermi surface parameters into the model [16]. More sophisticated treatments, such as local density theory, take the band-like nature of the 3d wavefunctions in metallic ferromagnets into account, which distort the simple atomic picture. Magnetism reflects the essential band structure. The magnetic moment is given by the difference between the filling of majority and minority spin bands [17], which is directly related to the ferromagnetic exchange splitting between the bands. Total energy minimization over all occupied band states yields crystal structure and magnetic ordering. Magnetic coupling and magnetic moment are sensitive functions of the interatomic spacing and the atomic volume respectively. Both are dominated by the Coulomb and, or exchange interactions at small distances. Magnetic domains provide a large-scale texture that adds enormous complexity. As a consequence, there are many more magnetic properties than band-structure parameters, and a large number of techniques to measure them. The variability of an H(M) hysteresis loop reflects a complex domain structure. The situation becomes simpler in **nanostructures**, which are smaller than the typical extension of a domain wall (0.1–1 μ m). They often exhibit a square hysteresis loop. Magnetic anisotropy and magnetostriction in thin films demonstrate that magnetic ordering is sensitive to small energy changes that are induced by the presence of an interface and by strain. Magnetization and magnetic coupling are calculable from first principles by band

theory. Actually, the most common approach uses the local density formalism, where the spin-dependent part of the total energy is approximated by an expression derived from an electron gas. Different magnetic structures, such as paramagnetic, ferromagnetic and various antiferromagnetic configurations, exhibit different total energies, and the lowest-energy configuration obtained by local density theory represents the observed magnetic state in most cases. Ferromagnetism occurs in rather few elements, Fe, Co, Ni, Gd and a few rare earths with low Curie temperatures. The stability of ferromagnetism in these elements can be explained by the Stoner criterion, which takes the density of states at the Fermi level and an atomic exchange integral as input. Stoner criterion explains why Fe, Co and Ni are single for ferromagnetism, several other elements, close to accomplish the criterion, for example Pd. In some thin-film structures these elements are transformed into ferromagnets, *i.e.* V, Cr, Mn, Mo, Ru, Rh, Pd, Pt. Magnetism can either be induced by exchange coupling to a ferromagnetic substrate or occur spontaneously owing to a higher density of states in a monolayer. *Magnetic anisotropy* is a magnetic variable that becomes rather changeable as the bulk symmetry is reduced in small nanostructures [18]. The magnetic energy density E varies quadratically with the angle θ of the magnetization with respect to a symmetry axis in a crystal or thin film: $E = K \cos^2\theta$, the anisotropy constant, K can be negative or positive. The source of crystalline bulk anisotropy is the spin-orbit interaction. In nanostructures the symmetry of the system is lowered by the existence of a surface or interface, where orbitals perpendicular and parallel to the interface become inequivalent. This symmetry breaking, drive the anisotropy from a fourth-order effect to a second-order effect *i.e.* in Fe and Ni.

Micromagnetic modelling typically includes a minimization over several energy terms, such as the exchange energy, crystalline anisotropy, the magnetostatic energy of the magnetic moment in the demagnetizing field, and the Zeeman energy of the magnetic moment in an external field. To see what might happen to particle-particle interactions at sublithographic dimensions one can look at the magnetic behaviour of random arrays of magnetic islands. They exhibit distinct magnetic phases, such as perpendicularly magnetized random antiferromagnet (island diameters, less than 3 nm), in-plane superparamagnet (diameters, 3–6 nm) and in-plane ferromagnet (diameters, greater than 6 nm). Many properties of thin films can be described by three dimensional bands, or by magnetic energies that are proportional to the volume of the film, they are dramatically modified by the influence of the substrate. As the film thickness is reduced, one can ask the question when, and how the transition to two-dimensional behaviour takes place. As the thickness of a thin film decreases, one expects to make a transition from three to two-dimensional behaviour. To quantify this transition, for example to see whether it is abrupt or continuous, we have to find characteristics of three- and two-dimensional magnetism. Near a

magnetic phase transition there exist characteristic power laws for magnetic quantities, such as the magnetization [19–21]. The Curie temperature is thickness dependent because the reduced number of neighbours in a thin film reduces the overall magnetic coupling. Another signature of two-dimensional behaviour is the transition from *parallel to perpendicular anisotropy* in a thin film. Most of the concepts developed for surface states in planar structures can be extended to one-dimensional wire or stripe structures. Magnetic domain-wall motion in soft magnetic thin films was observed in response to a varying in-plane magnetic field. Domain walls became trapped [22] at nanoscale defects and were then studied using standard TEM imaging. Several different types of films were studied, including Ni-Fe alloys, Ni-Fe-Co-Si-B amorphous films, and Co-Fe-B amorphous films.

Concentrated efforts are now focused in our labs finding innovative and modern solutions to obtain soft and hard nanostructured magnetic materials – **magnetic nanocomposites**, and also to understand the intrinsic mechanisms governing their specific magnetic behavior. Fe, Co, NiCo and CoFeSiB magnetic nanopowders of 20–200 nm have been prepared by chemical reduction. Due to their specific magnetic behavior, very different compared with their bulk counterparts, the magnetic nanopowders might be successfully used as soft or permanent magnets. Ni, Co, NiCo, and amorphous $\text{Ni}_{100-x}\text{Fe}_x$, $\text{Co}_{100-x}\text{Fe}_x$ nanowire arrays of 20 to 200 nm in diameter and 1 to 10 μm in length were prepared by electrodeposition. Their magnetic characteristics [23, 24]: coercive field, magnetic hysteresis loops, magnetic domains structure, gavanomagnetic properties, magnetic interactions between nanowires was comparatively studied [25–35]. Magnetic nanostructures have been also obtained. Moreover, the nanostructures have been obtained directly during the preparation process, in Fe-(Au, Cu)-B and (Fe, Co, Ni)-Nb-B systems, without any intermediate treatments, in the *as-cast state* in a few families of permanent magnets. Nanocrystalline regions of 10 to 20 nm randomly distributed in the amorphous matrix have been revealed in Fe-(Au, Cu)-B melt-spun ribbons and (Fe, Co, Ni)-(Zr, Nb, Ti, Ta, Mo)-B bulk shaped samples (torroids, bars) prepared by conventional mould-casting techniques.

2.2. THE IT BASED ON ANN METHOD

We introduce here the use of Artificial Neural Network (ANN) method [36]. We always 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 cover a wide spectrum of cases. If the ANN does not see an equilibrated set of cases, its output will be ‘biased’. The designing and performing of the new nanocrystalline and amorphous alloys with targeted properties is an actual problem for the ferromagnetic

materials. Our model is intended to enhance some new properties of these materials. Because this new method requires a large amount of data – some of them measurable, some other not, collected 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 reviews.

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 [37]. Neural networks, *discover* relationships in the input data sets through the iterative presentation of the data and the intrinsic mapping characteristics of neural topologies – *learning*. There are two basic phases in neural network operation. The *training* or learning 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 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. We notice that a lot of real world problems fall in this category, ranging from classification of irregular patterns, forecasting, noise reduction and control applications. Humans solve problems in a similar way. They observe events to extract patterns and then make generalizations based on their observations.

Neural networks were 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 Multilayer Perceptron (MLP) can learn any desired continuous input-output mapping if there are sufficient numbers of axons in the hidden layer(s). 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. Neural networks have been trained to perform this complex functions for identification and classification.

3. RESULTS AND DISCUSSION

We advance a new method to characterize the magnetic properties of nanomagnetic materials.

Our work purposes: 1) To develop the underlying theory and a general simulation approach to handle nanomagnetic materials; 2) To develop the large-scale computing approach necessary to simulate nano scale magnetic materials and the distributed infrastructure to make easy the rapid development of new simulation programs and their use directly by experimentalists; 3) To work closely with experimentalists in order to verify models and to explore new nanoscale magnetic materials; 4) High-performance computing aspects of physics-based modeling of nanomagnetic materials.

The simulation of a neural network requires the orchestration of many pieces [38]. When we run the simulation we start by checking if the data was correctly fed into the network by placing probes on the input sources. Another important aspect is to check if the learning rates are sufficiently low to avoid divergence. Divergence will usually occur during the beginning of the training. We place a matrix viewer on the first synapse to see if the weights are changing (see Fig. 1). Observing a steady decrease of the cost is the best overall indicator that everything is progressing well. Most of the time, the first check is to see if the cost is within what we think is appropriate for the application. All the information gathered by the network from the input data is contained in the weights. So, we should save the weights, along with the topology.

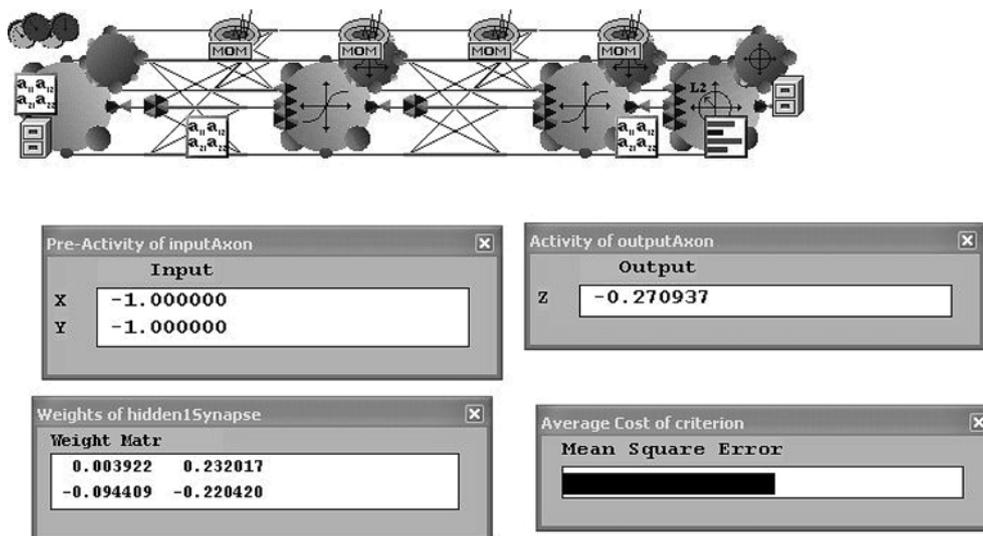


Fig. 1 – Example of a breadboard for Neural Network with matrix viewer.

Another aim of this work was to investigate advanced neural online parameter estimation procedures for non-linear modelling structures such as Multilayer Layer Perceptrons (MLPs), Radial Basis Functions (RBFs) and Local Model Networks (LMNs) [39].

The research is intended to set the foundation for more long-term work on on-line learning and construction techniques for modelling. Training is central to the use of neural networks for modelling since this is still a computationally intensive and time-consuming task, particularly for large-scale problems. Very often the success or failure of a neural network based control strategy depends on whether or not an acceptable model can be found in a reasonable amount of time. It was therefore vital for us to chose a fast, efficient and reliable training method applying this technology in our practical purpose [40].

Data Structures. The format of input data structures affects the simulation of networks. For concurrent vectors, the order is not important, and if we have 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 use for the input data the following: the chemical composition, the thermal treatments and some structure data. As output data Hall Effect (AHE), (as an example see Fig. 2, and Table 1), or magneto-resistance effect of one of our nanomagnetic alloys.

Table 1

$H (\times 10^{-3} \text{ Oe})$	$\rho_H (\times 10^8 \Omega \text{ m})$
0.000	0
0.697	0.395
1.393	0.715
2.090	1.025
2.787	1.355
5.573	2.325
8.360	2.575
11.146	2.615
13.933	2.615
16.720	2.625
19.506	2.635
22.292	2.64
25.080	2.645
26.473	2.65

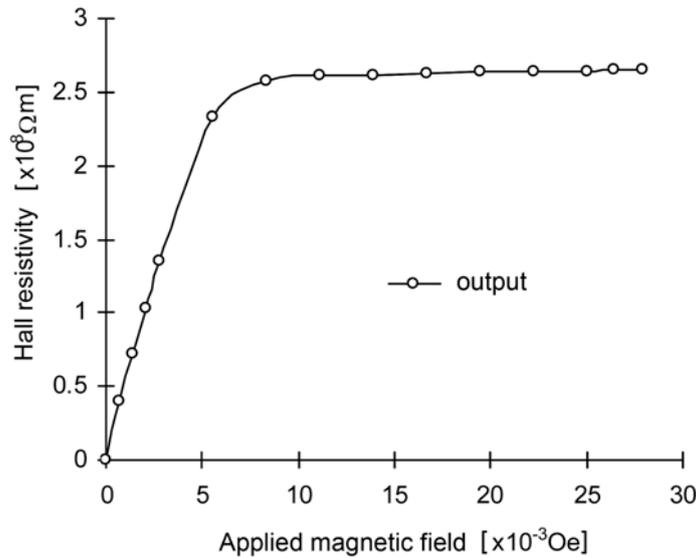


Fig. 2 – Dependence of Hall resistivity on applied magnetic field, used as output data (as given in Table 1).

Training Styles. In incremental training the weights and biases of the network are updated each time an input was presented to the network.

Learning Rules. We define a learning rule as a procedure for modifying the weights and biases of a network. The learning rule is applied to train the network to perform a particular task. As the inputs are applied to the network, the network outputs are compared to the targets. The used algorithm performs clustering operations. They categorize the input patterns into a finite number of classes.

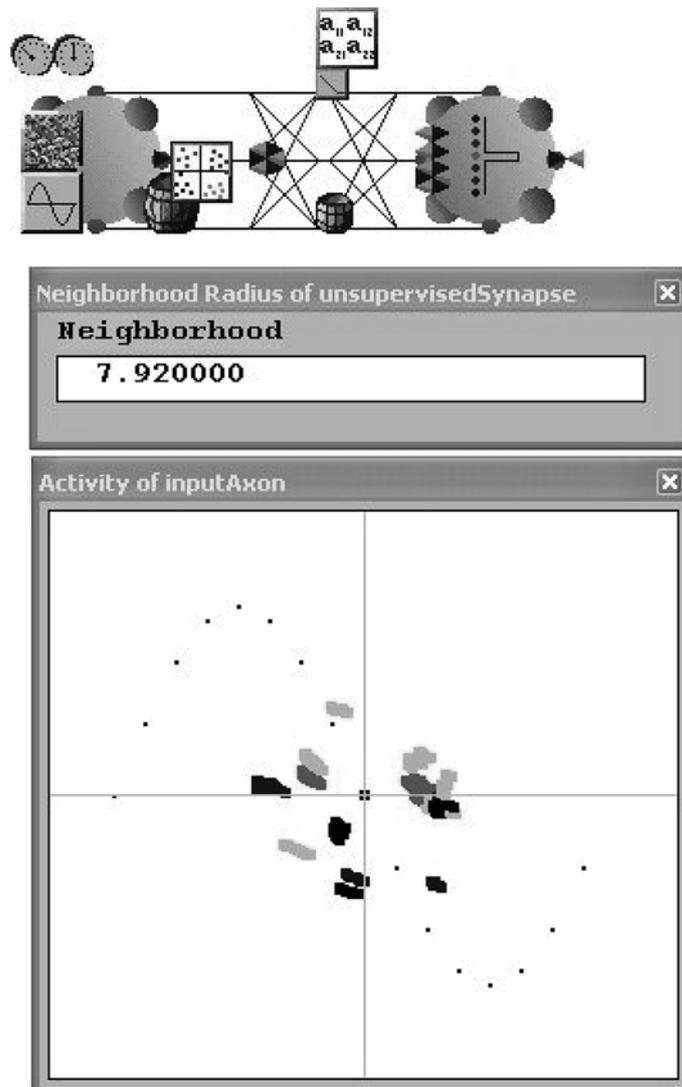


Fig. 3 – Kohonen type Neural Network.

What we expect from our new method?

Since ANNs learn from the data, the data must be valid for the results to be meaningful. Sometimes the desired response is unknown. Our model implements and uses the basic building blocks of neural computation, such as multi-layer perceptrons, Kohonen (see Fig. 3), Jordan and Elman networks, radial basis function, also called probabilistic networks, principal component analysis networks, self-organizing feature map networks and time-lagged recurrent networks. In our work we usually use **NeuroSolutions**, a *Neuro Dimension Inc. product* (Fig. 4). A successful neural network simulation requires the specification of many parameters. The performance is highly dependent on the choice of these parameters. A productive way to assess the adequacy of the chosen parameters is to observe the signals that flow inside the network. One can observe signals flowing in the network, weights changing, errors being propagated, and most importantly the cost, all while the network is working. This means that we do not need to wait until the end of training to find out that the learning rate was set too high. All probes within **NeuroSolutions** belong to one of two categories – static probes and temporal probes. The big difference is that the first kind access instantaneous data, while the second access the data over a window in time. By generating the code for the network, we can compile this code on a high-end workstation and train the network there. The resulting weights can then be saved to a file and imported back into your breadboard within **NeuroSolutions**.

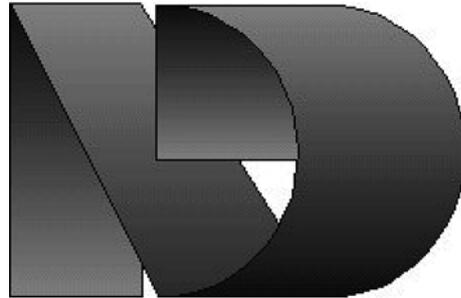


Fig. 4 – The Neuro Dimension Incorporated;
<http://www.nd.com>.

NeuroDimension, Inc.
1800 N. Main Street, Suite D4
Gainesville, FL 32609
www.nd.com

4. CONCLUSIONS

Concentrated efforts are now focused in our labs in order to find original and modern solutions to obtain soft and hard nanostructured magnetic materials,

and also to understand the intrinsic mechanisms governing their specific magnetic behavior. Modelling has now a very important position in the development and improvement of new materials for applications. Our knowledge of nanomaterials such as quantum dots, nanostructures, molecular assembly, is still at a very beginning stage. Modelling 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. We think new modelling strategies for complex material systems are needed.

A new IT strategy ANN based for the nanomagnetic materials was given. Neural networks have been applied successfully in the identification and classification of some nanomagnetic characteristics from large amounts of data. Neural networks was used for both regression and classification. 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. Our model will permit the search of new materials with enhanced Hall effect – AHE and other magnetoresistive properties. The research is intended to set the foundation for more long-term work on on-line learning and construction techniques for the magnetic nanomaterials modelling.

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