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SIMULATIONS ON DILUTE MAGNETIC SEMICONDUCTOR PROPERTIES

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Abstract. We have computed some magnetic properties of several substances by adding to the basic matrix of semiconductor like GaAs, ZnO, GaN some magnetic particles of Mn, Fe, Co to create new substances with novel magnetic properties. From simulations we have concluded that they act as anti-ferromagnets when doped with Mn and as ferromagnets doped with Fe.

Analyzing the magnetization as function of magnetic impurity concentration there can be seen a maximum magnetization for about 30–40 % concentration of magnetic impurities, distributed randomly in the semiconductor matrix.

Key words: modeling, magnetic properties, diluted magnetic semiconductors, spintronics.

1. INTRODUCTION

As technology has allowed evolution, the need of knowledge of man kind permitted the investigation of smaller and smaller dimensions in order to respond to questions about human existence. This inside in material structure enabled the development of new materials with properties not known until then, that lead to the next step in technological evolution. The fact that the level of atoms and molecules could be reached opened the path to new materials with specific properties obtained by manipulating individual atoms.

Due to reduced size of nanostructured magnetic materials they are especially studied for implementation in quantum computers where the information is carried by the spin. Spin is used as bit of information in multilayer structures, in read heads of hard-disks and magnetic memory MRAM. Since the first computers were build on semiconductor devices, the best structures to be implemented are semiconductors because they are compatible with the technology, but in order to use the magnetic spin there were created new materials where the basic matrix is a semiconductor having dispersed magnetic particles types 4f or 3d.

In a world where everything is constantly changing and technology represents the evolution of this world, we often wonder how electronic devices will simplify our life. Electronics have an increased storage capacity due to technologies that offer us new materials. These materials are multilayer systems that present giant magneto-resistive effect, so when electrons are crossing through such a multilayer, there will be noticed a resistance depending on the material used [1], due to the scattering on the separation surface between two layers and to the orientation of the magnetic field in layers. Common denominator of all these materials is the spin. This property is used in making quantum computers to reduce dimensions and to maintain or even increase the speed and capacity of data storage. Physical characteristics of spin in metals and semiconductors studied from the viewpoint of theoretical physics, in particular solid state physics, have already showed potential paths for electronic technologies. Thus, advanced countries have prototypes of electronic devices where giant magnetoresistive [1] properties are tested in cells for information storage named “active memories”.

2. MODELS

Nanomaterials magnetism is for a long time in the attention of researchers but there was always difficult to characterize these materials. The magnetism is a cooperative phenomenon that involves handling small structures, where neighbor atoms are systematically replaced with atoms from other elements with greater or smaller magnetic weight so that the order is somewhat controllable.

It is known that the electron wave function changes when they confine to dimensions comparable with it. There is expected that the order imposed by the magnetic forces to contribute to the nanometer structure. Magnetic properties are very sensitive to local order. The discovery of magnetism in nanostructures is somehow a consequence of correlations between the mechanisms of growth and their magnetic properties. The ordering degree may be changed by adjusting the conditions for obtaining the nanostructure. Even the magneto-crystalline anisotropy may be connected to the structure degree of order. Another way to study such systems is to correlate electronic properties with the material’s degree of order.

The study of nanocomposites hard magnetic materials occurred when it was demonstrated that a mixture of hard and soft magnetic nanograins coupled by exchange interactions may lead to high energy products [2]. The low residual magnetization of isotropic magnets can be improved by exchange as a result of the coupling at nanometer scale of a soft magnetic phase with a hard one [3]. By associating the coercivity of hard magnetic phase with high magnetization of soft phase is obtained a new class of hard magnetic materials with high energy product.

Diluted magnetic semiconductors are compounds based on typical semiconductors for which a fraction has been replaced by magnetic ions (transition metal ions like Mn, Fe or rare earth metal ions) [4]. The most relevant feature is the coexistence and interaction of two different electronic subsystems: delocalized conduction (s-type) and valence (p-type) band electrons and localized (d or f-type) electrons of magnetic ions [4]. In particular the spd exchange interaction leads to strong band splitting, which result in giant magneto-optical effects [4]. The d-d interaction of randomly distributed magnetic ions, triggers formation of spin-glass and anti-ferromagnetic phases, depending on magnetic concentration and temperature [4-7].

3. SIMULATIONS AND RESULTS

We have started our model taking into account the interaction between first and second degree neighbors and considering the spin interaction. In our simulations we have considered that a magnetic particle substitutes the entire semiconductor molecule. In order to calculate the magnetization, we have calculated the energy of the entire system (the contribution is given by the exchange interaction). The magnetization is obtained by deriving the energy reported to the temperature.

$$E(\{s_N\}) = -\varepsilon \sum_{\substack{i,j=1 \\ i \neq j}}^{N} s_i s_j - H \sum_{i=1}^{N} s_i \,, \tag{1}$$

$$M = -\frac{\partial}{\partial \beta}(\beta Q) = \left\langle \sum_{i=1}^{N} s_i \right\rangle, \tag{2}$$

where ε is the exchange constant, $s_{i,j}$ the spin of the molecules, H the Hamiltonian of the system and $\beta=kT$, where k is the Boltzmann constant and T the temperature at witch the process is measured.

From the simulation data we have extracted the magnetization curve *versus* the number of magnetic particles. We can notice that there is an optimum concentration on witch the magnetization has a maximum value, than it decreases back to zero for a concentration of 100% magnetic particles. This is according to experimental data because a ferromagnet has zero magnetization at room temperature when it is not inside a magnetic field.

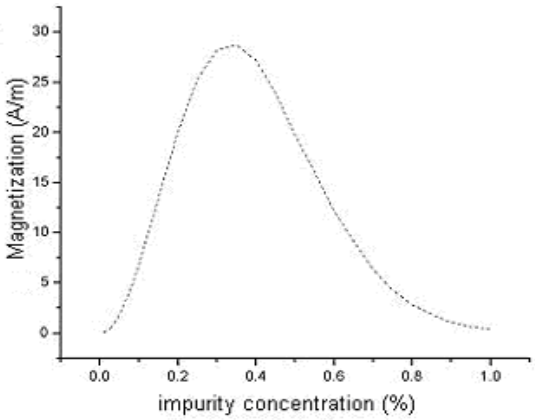


Fig 1 – The dependence of magnetization as function of magnetic particle's concentration (Fe).

For semiconductors such as InSb, GaN, InN, GaP, GaAs doped with Mn we can observe an anti-ferromagnetic behavior because the plot inverse of susceptibility *versus* temperature in Celsius degrees, when extrapolated, intersects the temperature axis in a value lower than zero degrees. For other semiconductors such as ZnO, CdTe, ZnS doped with Fe we can observe a ferromagnetic behavior from the graphic of the inverse of susceptibility as function of temperature.

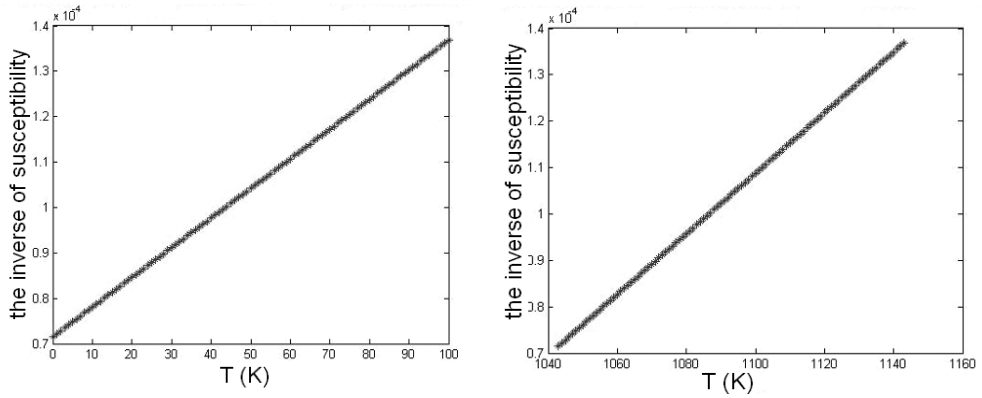
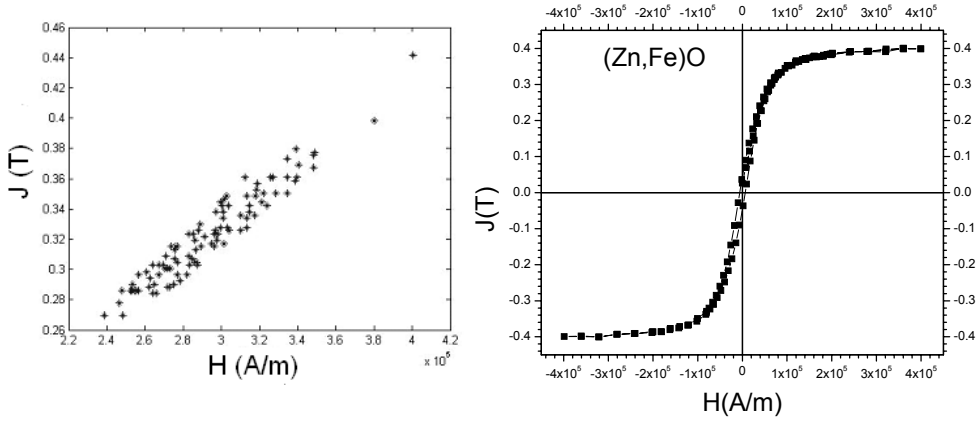


Fig. 2 – The inverse of susceptibility as function of temperature for semiconductors doped with: a) Mn that present an anti-ferromagnetic behavior; b) Fe presenting a ferromagnetic behavior.

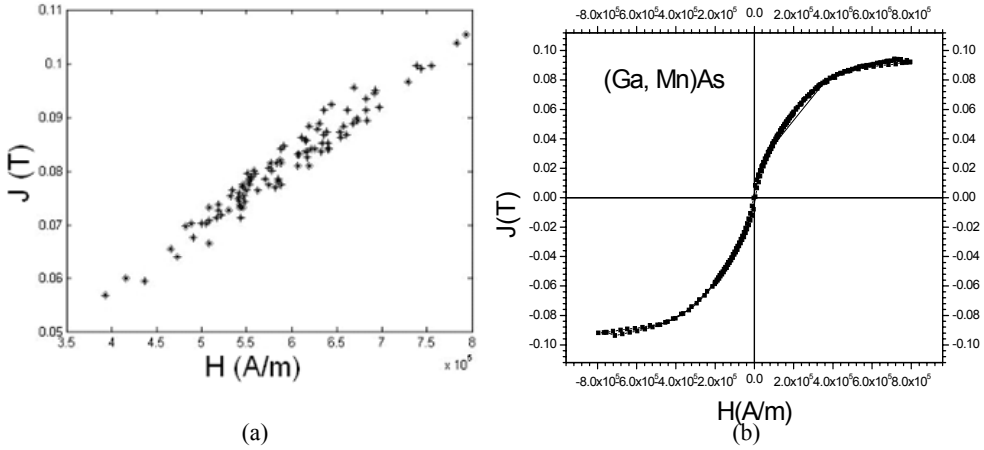
For ferromagnetic materials we have computed the first curve of magnetization for a ZnO semiconductor doped with Fe. We have compared our results with measured data.



(a) (b)

Fig 3 – Hysteresis behavior for a ferromagnet (Zn, Fe)O: a) simulations (first curve); b) experimental data.

And also for semiconductors doped with Mn witch presents an anti-ferromagnetic behavior.



(a) (b)

Fig. 4 – Hysteresis behavior for a antiferromagnet (Ga,Mn)As: a) simulations (first curve); b) experimental data.

4. CONCLUSIONS

Among the deficiencies of this model the most important one is that it neglects the intersite Coulomb repulsion. This assumption is justified based on the low concentration of carriers since in this latest case the probability of double occupancy is small. To this reason one may add the fact that a small or

intermediate value of the exchange integral also suppresses the double occupancy. Another deficiency is that the anti-ferromagnetic coupling among Mn ions is not included, but as long as density of Mn atoms is small the probability of finding two neighboring magnetic sites is proportional to the square of the density of Mn atoms. Moreover, Mn placement disorder is neglected. Finally, the Coulomb attraction by acceptors is not considered in the Hamiltonian. Nevertheless, the model is reliable and its prediction agrees at least qualitatively with the experiment.

This paper presents the confirmation of experimental results by a simulation model, where it was observed that semiconductors doped with Mn present an anti-ferromagnetic behavior due to the coupling between the Mn atoms while those doped with Fe present a ferromagnetic behavior.

Here is described the coupling between magnetic particles. There can be seen three regimes: the first one of less than 20% in magnetic particle concentration, when there are only a few magnetic particles and the magnetization is not significant, the second one where the magnetic particle percentage is between 20% and 50% where the magnetization achieves a maximum due to the coupling over a certain distance. The material acts as a magnetized one due to the influence of the neighbors. The third regime presents a decrease in the magnetization due to the arrangements of the magnetic particles in domains in order to minimize the internal energy of the material. This is according to the reality because a magnetic material like iron, when is not put in a magnetic field has a null magnetization.

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