



## The Study of Structural and Magnetization Properties of NiO Nanoparticles

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### **Abstract**

Magnetic properties of NiO nanoparticles with different sizes and at different temperatures are compared. We collected the experimental data reported in the literature, for the same conditions, and after fitting, extrapolating and doing some calculations, we obtained the magnetization and susceptibility as a function of the applied magnetic field. Although we obtained both linear and nonlinear terms, the main contribution due to the linear term is for magnetization. Of course, the nonlinear terms could help us to consider the nonlinear properties. The magnetization and susceptibility for smaller nanoparticles are bigger, for the samples we consider here. This difference could be explained by the difference of surface volume ratio of nanoparticle which shows the contribution of the paramagnetic surface is more important with respect to the anti-ferromagnetism of the core for smaller particles. Also the nanoparticle at lower temperatures shows bigger magnetization and susceptibility. Finally, the magnetic Helmholtz free energy is obtained as a functions of magnetic field. For smaller nanoparticle, the Helmholtz free energy is lower or the magnitude of the free energy is bigger. The comparison made here are helpful for computer simulation of magnetic properties of a sample containing nanoparticles.

**Keywords:** *Magnetization, Structural Properties; Nano particles, Nickel Oxide*

### **Introduction**

As we know there is a fairly big difference between the physical properties of the bulk and nanoparticles, and also among nanoparticle themselves, for the same matter [1]. Here we concentrate on the magnetic properties of NiO. It is anti-ferromagnetism up to 329 degree Kelvin and paramagnetic higher than this temperature [2,3]. Latacz and Baster [4] have considered the change of some magnetic properties of NiO in the vicinity of  $T_N$  for the paramagnetic state. The parallel magnetic and electric field dependence of the Neel temperature in NiO is considered by Latacz [5] using the modified Oguche method. Baster and Latacz [6] show the growth of parallel

magnetic susceptibility above  $T_N$  up to 378 K due to the change of crystal Lattice parameters with temperature and change of the exchange parameter. Their discussion is based on the modified Oguchi theory [7]. Nanoparticles of NiO with different sizes shows a variety of magnetic behaviors[8].

We produced NiO nanoparticles with particle diameters 30-100 nm. We observed a phase transition at 42 and a coercivity as high as 708 Oe at 5 K, although the bulk is anti-ferromagnetism. Lopez and co-workers [9] prepared nanoparticles of NiO with a diameter size of 20-200nm. The magnetic properties of these nanoparticles show the presence of a net magnetic moment at the surface, due to the large surface volume ratio. Magnetization

measurement of 150 Angstroms size  $NiO$  were reported by Makhlouf [10]. The structure and magnetic properties of  $NiO$  nanoparticles are investigated by Zhang et al. [11] too. As mentioned above many researchers produced  $NiO$  nanoparticles and investigated their magnetic properties separately. Here we are interested to compare the magnetic behavior of the various size of  $NiO$  nanoparticles with each other and also with the bulk one. Therefore we collected the experimental data from the articles mentioned in the References, although we could not find enough data with the same conditions. Then we fitted and extrapolated the data and did some calculations to plot the magnetization and susceptibility of the nanoparticles and we compared them. We also calculated the magnetic Helmholtz free energy of the nanoparticles and compared them. We were aware of this point that when we compare the magnetic behavior of a sample containing nanoparticles with a different size, some difficulties will arise, e.g. the change in the density of a sample with changing the particle size, the change of the particle size with the temperature and the change of the structural properties inside the particles

with their size. Of course, in the experimental data we used here the interaction between nanoparticles is also included. According to the variety of Physical and Chemical behaviors of 3 nanoparticles, and because the nanoparticles are small, it is better to study these systems, using computer simulation techniques. Therefore, our discussion here could help consider the computer simulation of the magnetic properties [13-15].

In the next section we present the figures and do the required calculations and finally discuss the results.

### Result and Discussion

Figure 1 and figure 2 shows the XRD patterns of the precursor Ni and  $NiO$  nanoparticles products after calcinations.

The XRD patterns of the calcined sample exhibited sharpened reflection peaks which indicate that a growth in the crystallite sizes of  $NiO$  has occurred. The peak positions appearing at  $2\theta=36.92$ ,  $43.9$ ,  $63.1$ ,  $75.9$  and  $79.8$  can be readily indexed as (111), (200), (220), (311), and (222) crystal planes of the bulk  $NiO$ , respectively.

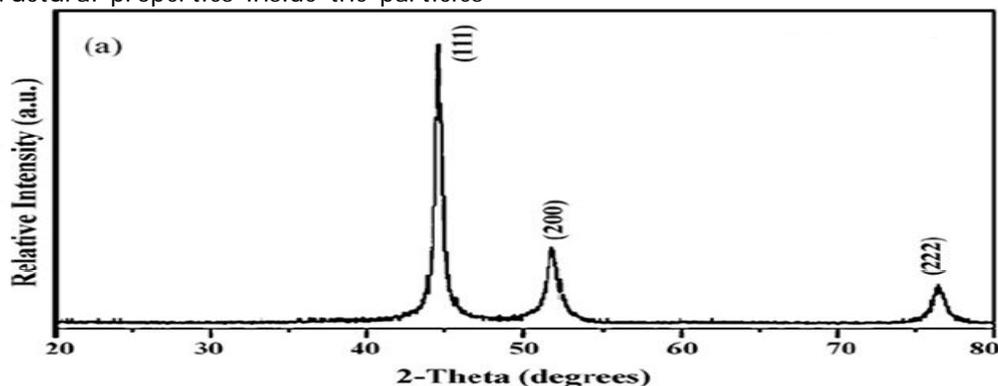


FIG. 1: XRD of the precursor Ni nanoparticles.

All the reflections can be indexed to face-centered cubic (fcc)  $NiO$  phase with

lattice constant (a):  $4.17 \text{ \AA}$  which agrees well with the standard data (JCPDS card

No. 47-1049)[16]. The sharpness and the intensity of the peaks indicate the well crystalline nature of the prepared sample.

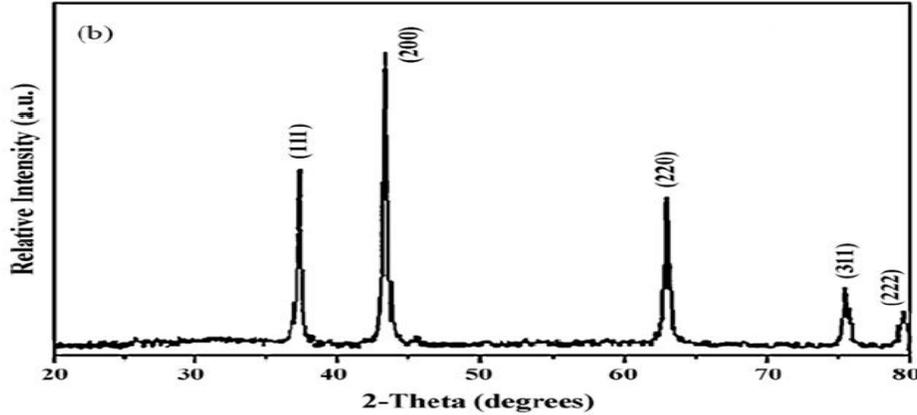


FIG. 2: XRD of the (A) precursor NiO nanoparticles.

As we know the nonlinear properties of nanoparticles show some behaviors which are far from that of the bulk. Here we are interested to find the nonlinear terms in the magnetic properties of *NiO* nanoparticles. We use the experimental data to find magnetization and susceptibility as a function of applied magnetic field and temperature. First, we compare the amounts of magnetization and then the susceptibility of the nanoparticles.

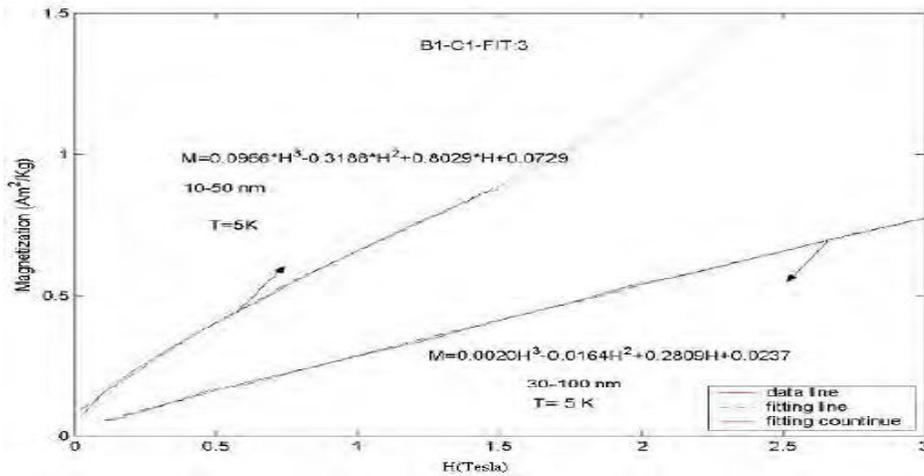


FIG. 3: Magnetization as a function of magnetic field for 10-50 nm and 30-100 nm *NiO* nanoparticles at T = 300 K.

In figure 3 and figure 4 the magnetization are plotted against magnetic field for 10-50 nm and 30-100 nm for T=300 K and T=5 K respectively. As it is shown in the figures, the main contribution in the polynomial is due to



the linear part, which means the relation between M and H is almost linear but at H=0.3-0.5 Tesla We have two values for the slope of lines. Therefore when the magnetic field is increasing the relation between M and H is linear. As the figures show the amount of magnetization for 10-50 nm is bigger than 30-100nm nanoparticles.

contribution of the paramagnetic or the effect of spines on the surface (it means; the spins increase as the particle size decreased) is more important with respect to the anti-ferromagnetism of the core for smaller particles.

These differences could be explained by the difference surface volume ratio of nanoparticles which means the

In figure 5 and figure 6 the magnetization is plotted and compared for two different temperatures. As it is seen from the figures for given magnetic field, the magnetization at 5 K is bigger than 300 K which shows more ordering, particularly on the surface.

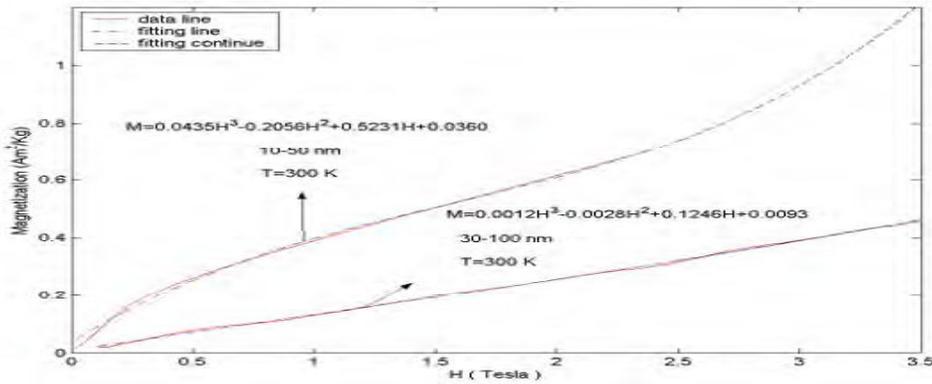


FIG. 4: Magnetization as a function of magnetic field for 10-50 nm and 30-100 nm *NiO* nanoparticles at T=5 K.

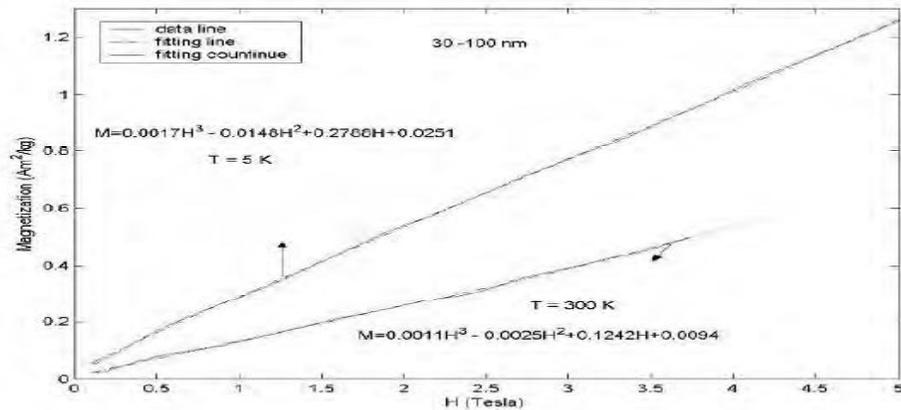


FIG. 5: Magnetization as a function of magnetic field for 30-100nm *NiO* nanoparticles at T=5 and T=300K.

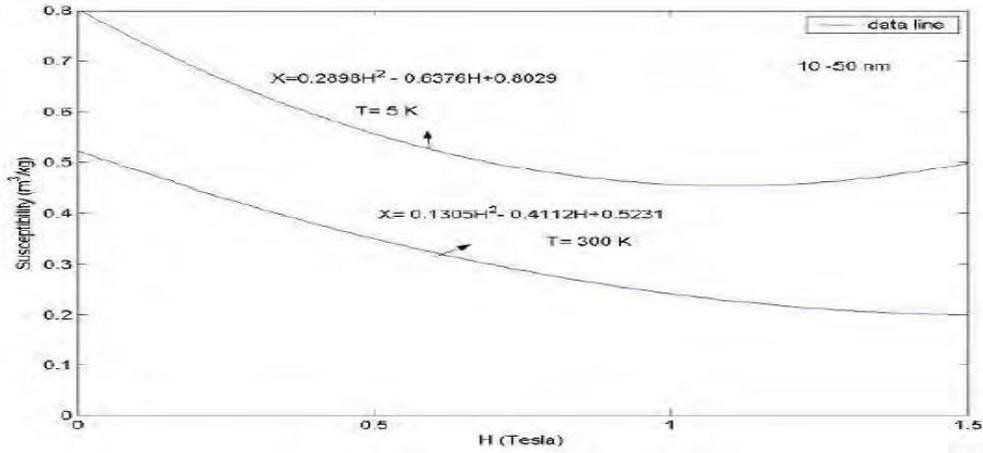


FIG. 6: As Fig. 5 but for 10-50 nanoparticles.

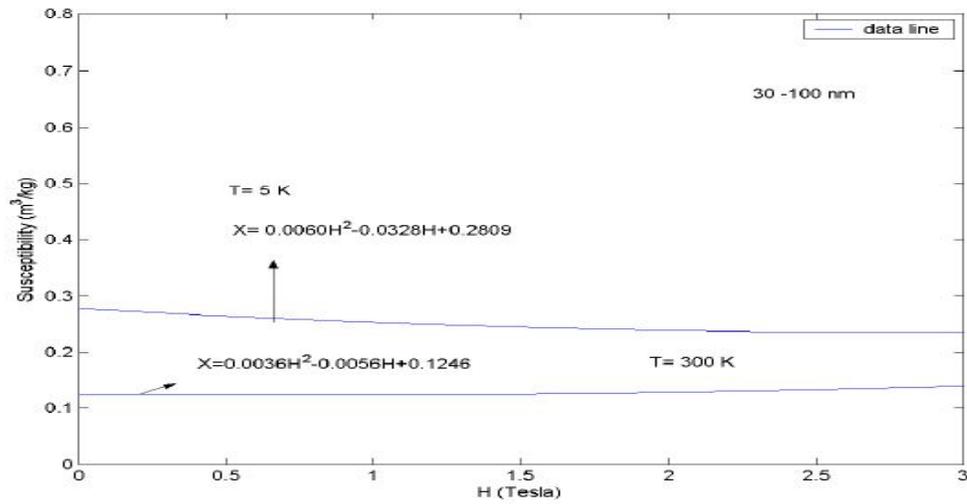


FIG. 7: Susceptibility as a function of magnetic field for 10-50 nm  $\text{NiO}$  nanoparticles at  $T = 5$  and 300 K.

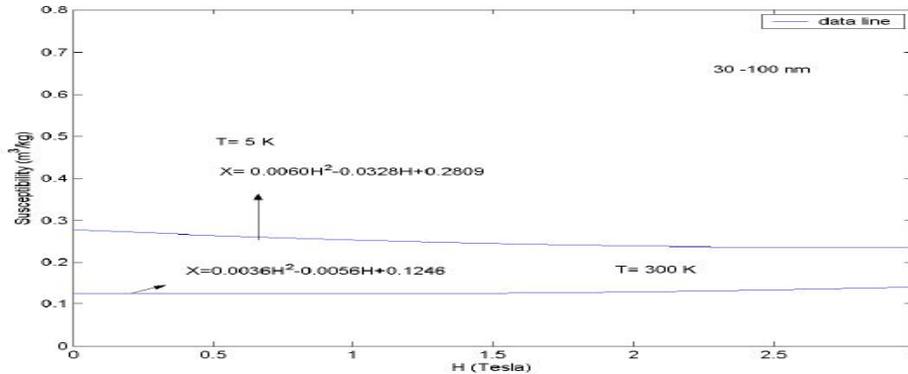


FIG. 8: Susceptibility as a function of magnetic field for 30-100 nm *NiO* nanoparticles at T=5 and 300 K.

The susceptibility at 5 K and 300 K is shown in Figure 7 and Figure 8.

Finally, according to the expressions

$$M(H) = -\frac{1}{V} \frac{\partial F}{\partial H}$$

For zero magnetic field, the magnetization is zero, we can write

$$\frac{F}{V} = \int_0^H M(H) dH$$

We obtain the Helmholtz free energy *F* as a function of applied magnetic field, where *V* is the volume of the sample. In figure 7 the Helmholtz free energy as a function of magnetic field for a given nanoparticles at 5 K are plotted. As we can see from the figure, for a sample with smaller nanoparticles, the Helmholtz free energy is more negative or the magnitude of the free energy is bigger.

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