Magnetic and thermodynamic properties of nanodisks by Monte Carlo simulations

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Abstract. The idea that the properties of nano materials depend on their crystalline structure and the form and geometric sizes of them is discussed in this paper. The progress in the growth area of nano magnetic devices attracts the interest from both experimental and theoretical study of the nano structures for potential applications in industry. In various fields of electronics there is need to have nano materials with a wide range of magnetic properties. In this case theoretical research could provide a way to get the nano compounds with the required characteristics. In this paper we present the results of Monte Carlo simulations of magnetic nanodisks, which are based on simple cubic and body-centered cubic unit cell. The magnetization of spin, magnetic susceptibility and specific heat are investigated for nanodisks with the different diameters, thicknesses and for different values of the ratio of the correlation constants. The combination of dipolar and Heisenberg model interaction are considered for ferromagnetic case and are show that the magnetic and thermodynamic properties of the nanostructures are strongly dependent on their geometry. The structures with body-centered cubic unit cell demonstrate stronger dependences on the thickness of the disks and also higher critical temperature and wider hysteresis loop.

1. Introduction
The miniaturization of semiconductor devices creates strong interest in production of different nano magnetic structures. It explains that in recent years there has been significant progress in the creating of nano magnetic devices and extensive study of the magnetic properties of new nano compounds (see, e.g., [1-5] and references therein). Some recent works are already dealing with new practical designs for hard discs based on the new technologies. These experimental works were devoting to create nanostructures which are capable of maintaining their magnetic properties under changing temperature or external magnetic fields. Consequently, there is a growing interest in theoretical studies of magnetic nanostructures, in particular by means of the Monte Carlo simulations [1,6-12]. The investigations in this area should be focused on the prediction of magnetic properties of the new prospective compounds that can be important for electronics. Interests of new technologies require magnetic materials with a wide range of magnetic properties. In particular, there are requests for materials with maximal permeability (rectangular hysteresis loop), materials with low losses in the reversal, materials with high initial permeability, and materials with constant permeability over a wide range of magnetic fields (slope of the hysteresis loop). The importance to obtain alloys that guarantee an acceptable thermal stability of the permanent magnetization in very small volumes due to the need scale reduction of the memory bits in the recording media [1,2]. It is expected that the geometric structure of magnetic nano materials may significantly affect their magnetic properties. In the present paper we start an analysis of some magnetic and thermodynamic
properties of nanodisks with different geometries. Some of the most common magnetic compounds are based on a simple cubic unit cell or body-centered cubic cell [3,5] of ferromagnetic type. In the present work we explore the properties of the nanodisks with these types of internal structures. As a first step, we perform theoretical simulations of various properties of the model magnetic nanodisks based on the simple cubic (sc) and body-centered cubic (bcc) unit cells. The main target of our study is the dependence of the thermodynamic and magnetic properties of studied structures from their geometry and from the values of the ratio of the correlation constants. In particular, we explore the difference between the nanodisks of three different thicknesses, two different diameters and also the dependence on the type of the unit cell.

2. Method of calculations

In this work we consider the possible influence of the type of the unit cell, such as simple cubic and body-centered cubic cells, on thermodynamic and magnetic properties of the nanodisks with different thickness. The structures under consideration are listed in Table 1 and their geometry is illustrated in Figure 1, where we present a bcc-disk with three layers. The procedure of fitting a crystalline structure into a circular disk was defined as follows: the starting 3D structure is cut by a disk of a given radius, with center in one of the atoms. The axis of the disk is parallel to the axis of the initial cubic structure.

| Structure | sc1-l2 | sc1-l3 | sc2-l2 | sc2-l3 | bcc1-l2 | bcc1-l3 | bcc2-l2 | bcc2-l3 |
|-----------|--------|--------|--------|--------|---------|---------|---------|---------|
| Number of spins | 138    | 207    | 276    | 290    | 435     | 580     | 218     | 367     | 516     | 446     | 747     | 1048    |

Table 1. The numbers of the sites in the studied structures. In the names of the structures, the letters mean the type of the unit cell, and the number 1 indicates 11 sites in diameter, the number 2 indicates 15 sites in diameter and the abbreviation l with number is the thickness of the disk (layer’s number).

Fig. 1. Body-centered cubic disk with 15 sites in diameter and three layers (bcc2-l3).

The spin configurations can be obtained using the numerical calculations within the Monte Carlo (MC) method. We take into account the combinations of dipolar and Heisenberg model interactions simultaneously, because the effect of dipolar interaction component is stronger for the small sizes of nanostructures, while for the larger sizes of the nanostructures the Heisenberg interaction is dominating (the discussion of this issue has been presented earlier in [7]). We will study the nanodisks with diameter of 11 and 15 sites in each frame, and with the thickness of two, three and four layers. We report on the thermal equilibrium magnetization, the susceptibility and the specific heat for these structures. As a result of this study one can observe how the spin configurations depend on the type of the unit cell and on the thickness of the nanodisks.

In our simulations we used a Hamiltonian model given by [12]:

\[
H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - B \cdot \sum_i \mathbf{S}_i - D \sum_{i \neq j} 3 \left( \mathbf{S}_i \cdot \mathbf{e}_y \right) \left( \mathbf{S}_j \cdot \mathbf{e}_y \right) - \frac{\mathbf{S}_i \cdot \mathbf{S}_j}{r_{ij}}.
\]
In this expression the first sum represents the ferromagnetic exchange between the nearest neighbors with a coupling constant $J$, the second sum stands for the coupling of the spins to an external magnetic field $B$ and the last sum is the dipolar interaction term, where the coupling $\omega$ describes the strength of the dipole-dipole interaction. The $\mathbf{S}_i$ are three-dimensional magnetic moments of unit length, $\mathbf{e}_{ij}$ are unit vectors pointed from lattice site $i$ to the lattice site $j$ and $r_{ij}$ are the distances between these lattice sites. We considered three different values for the ratio between correlation constants $\frac{\omega}{J}$, which are equal as 0.001 (in accordance to [12]), 0.01 and 0.1.

For the numerical analysis of the magnetic and thermodynamic properties of nanodisks we have used the MC simulations with the Metropolis algorithm [13,14]. The Metropolis Monte Carlo algorithm enables one to obtain the macro-state equilibrium for a physical system at the given temperature $T$, starting from some randomly chosen initial micro-state and then proceed by performing a very large number of random transformations of the micro-states, until we arrive at the equilibrium macro-state. One spin is chosen at random and gains a new direction in a random way (note that there is no discretization of orientations in the Heisenberg model which we use here). As a result, the energy of the system changes by the value $\Delta E$. If $\Delta E < 0$, the temporary direction of the spin becomes permanent. If $\Delta E > 0$, the temporary direction becomes permanent with the probability $\exp(-\Delta E/k_bT)$. The preliminary calculations have shown that with $10^4$ Monte Carlo steps per is sufficient for our system to "forget" the initial randomly chosen configuration and arrive at the state of equilibrium.

The external magnetic field was directed along the axis $z$, which was also the axis of the nanodisk. The simulations for magnetization and magnetic susceptibility were performed for the values $B=-20, -18, \ldots, -4, -2, -1.5, -1, -0.5, 0, 0.5, 1, 1.5, 2, 4, \ldots, 18, 20$. Here the energy and the applied magnetic field are expressed in the units of $J$. In all these cases the value for the temperature was chosen to be $T=0.15$. In order to study the magnetic properties in low-temperature, all simulations have been performed for temperatures smaller than the critical temperature. The temperature is expressed in units of $J/k_b$, where $J$ is the magnitude of the coupling constant and $k_b$ is Boltzmann’s constant.

We obtain the susceptibility $\chi$ along the $z$ axis by MC data, given by

$$\chi = N^{-1} \frac{1}{k_bT} \left( \frac{\langle m_z^2 \rangle}{\langle m_z \rangle} - \frac{\langle m_z^2 \rangle}{\langle m_z \rangle} \right),$$

where $N$ is the number of spins in the system, $k_b$ is Boltzmann’s constant, $T$ is temperature and $\langle m_z \rangle$ is the mean magnetization per spin in direction $z$. The susceptibility was also calculated as a function of applied magnetic field with constant temperature. The specific heat $C$ we obtain from the energy fluctuations relation

$$C = N^{-1} \frac{1}{k_bT^2} \left( \frac{\langle E^2 \rangle}{\langle E \rangle} - \frac{\langle E \rangle^2}{\langle E \rangle} \right),$$

where $\langle E \rangle$ is the mean energy per spin. For calculating the specific heat we used $B=0$ and the values $T=4.05, 3.95, 3.85, \ldots, 0.15$.

3. Results and discussions

Let us start the description of the results from spin orientations obtained by Monte Carlo simulations for different types of disks (sc and bcc) with two diameters and three different thicknesses for different values of the ratio between correlation constants. As we have already mentioned above, the simulations have been performed for the longitudinal external magnetic field with the twenty seven different values of $B$ between -20 and +20. If the external field is sufficiently strong, one can observe that the spins are oriented along the field direction. This picture does change when one weakens the
external field. Let us consider the magnetic properties. The plots of magnetization versus applied magnetic field are presented in Figures 2(a,b,c).

Fig. 2. The plots of magnetization versus applied field for (a) $\frac{\omega}{J}=0.001$, (b) $\frac{\omega}{J}=0.01$ and (c) $\frac{\omega}{J}=0.1$. 
One can see that the hysteresis loops has stronger dependence of the values of the ratio of the correlation constants. For $\omega J = 0.001$ the hysteresis loops (see Fig. 2a) are similar for all sc-disks and bcc-disks with two layers, which demonstrate rectangular form of loops with a width close to 1.5, when others bcc-disks have the loop close to 2.5. For $\omega J = 0.01$ the hysteresis loops (Fig. 2b) sc-disks and bcc-disks with two layers have the loop with a width close to 1.5, bcc-disks with three layers for both diameters have the loop close to 2.0 and bcc-disks with four layers for both diameters close to 2.5. For $\omega J = 0.1$ the hysteresis loops (Fig. 2c) bcc1-l2 disk has the loop with the width close to 0.5, sc1-l2 disk has the loop close to 1.0 and others close to 1.5. The lower value of the ratio between the correlation constants corresponds to a greater contribution of the dipole-dipole interaction. Thus we can note that the increase of the dipole-dipole interaction leads to a decrease in the width of the loop.

Let us consider the thermodynamic behavior of the studied nano-structures. Thermal equilibrium results obtained by Monte Carlo simulations enable us to obtain the dependence of the specific heat versus temperature. The plots of specific heat versus temperatures are presented in Figures 3(a,b,c).
Fig. 3. The plots of specific heat versus temperature without external magnetic field for (a) $\omega/J=0.001$, (b) $\omega/J=0.01$ and (c) $\omega/J=0.1$.

For all types of the unit cells the nanodisks with the smaller thickness have smaller value of specific heat. One can see that the result depend on the size of the structure and number of nearest neighbors (also called coordination number). It can be noted that there is also a strong dependence on the type of crystal lattice. The critical temperatures for the bcc structures are bigger than the one for sc structures. Moreover the dependence of the thickness is stronger for bcc disks compared with sc case. Let us present some explanation of why the critical temperature varies depending on the structure and thickness of the disks. The coordination number of sc structure is 6 and the same number for bcc is 8. For the nano-disk with the two layers almost all atoms are on the surface, while for the disk with three layers there are more internal atoms with a greater number of neighbors. In the calculation of interaction energy we take into account not only immediate neighbors, but also the next order neighbors, which prove to make an essential contribution. In order to illustrate this general situation, consider some particular examples. If one consider a sphere of radius $a$ around an internal atom in sc-disc, it is easy to see that the ball has six atoms, all of them are located at the distance $a$ from the center. In comparison, similar internal atom in bcc-structure has eight nearest neighbors, located at the distance equal to $0.86a$ and also 6 atoms which are located at the distance $a$. All in all, the difference in the thermodynamic properties of bcc-disks with two and three layers is definitely related to the influence of all interactions which are taken into account. The reduction of the value of the ratio between the correlation constants leads to a decrease in the spread between the values of the critical temperature for sc and bcc structures. It can be noted that difference in properties between the cases when the correlation constants are $\omega/J=0.001$ and $\omega/J=0.01$ is less, than between cases when the correlation constants are $\omega/J=0.01$ and $\omega/J=0.1$.

Very similar considerations can be done for the analysis of the Figures 4(a,b,c), which show the plots of magnetic susceptibility versus temperature. One can observe that bcc structures have a wider distance between peaks. Furthermore, we note that the magnitude of the peaks in Figures 4 depends on the type of the unit cell. The magnitude of susceptibility decreases with increasing number of sites in the structure. There is, once again, an increase of the critical temperature with increasing thickness for all types of the disks, a strong dependence on the thickness for the bcc-type of the disks and the same behavior of the ratio between the correlation constants.
Fig. 4. The plot of magnetic susceptibility versus temperature without external magnetic field for (a) $\omega/J = 0.001$, (b) $\omega/J = 0.01$ and (c) $\omega/J = 0.1$. 


4. Conclusions
In this article we presented the results of the Monte Carlo simulations of magnetic nanodisks with the simple cubic and body-centered cubic unit cells in the structures for three different values for the correlation between constants $J/\omega$. We have found that hysteresis form, magnetic susceptibility and specific heat of such structures manifest dependence on the type of the unit cell and on the thickness of the disk. In particular, one can note that the behavior of magnetic and thermodynamic properties for the structures with bcc type of unit cell show greater dependence on thickness of the disks, higher critical temperature and higher width of the hysteresis loop. The value of the ratio between the correlation constants corresponds to a greater contribution of the dipole-dipole interaction and it should be noted that this ratio affects the properties of studied structures. Thus we can note that the increase of the dipole-dipole interaction leads to a decrease in the width of the loop. The reduction of the value of the ratio between the correlation constants leads to a decrease in the spread between the values of the critical temperature for sc and bcc structures. Qualitatively similar dependence on the geometry of magnetic nanostructures can be seen in experimental works [1-5]. The MC calculations for the systems containing a large amount of spins permit to obtain a qualitative estimative of how some magnetic and thermodynamic properties of nanodisks depend on their unit cell, diameter, thickness and correlation constants. We expect to continue exploration the dependence of the magnetic properties of different nanostructures on their geometry.

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