ORIGINAL ARTICLE

Mean-field calculation of some magnetic properties of Ising thin-films

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Abstract

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In this work, the magnetic properties of Ising thin-films were investigated as a function of temperature and thickness by means of mean-field calculation. The magnetization and the magnetic susceptibility profiles, including layer variation, were investigated in detail. From the results, the magnetic behavior was found changing from a two-dimensional to a three-dimensional character with increasing the film thickness. In addition, the critical temperatures were calculated and a similar trend was found. The shift of the critical temperatures from a two-dimensional to a bulk value was in good agreement with previous theoretical prediction. This indicates the dimensional crossover of the magnetic critical behavior from thin-films to bulk limit when the films become thick.

Key words : magnetic properties, thin-films, mean-field, ising model

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บทคัดย่อ

ยงยุทธ เหล่าศิริถาวร

การคำนวณคุณสมบัติแม่เหล็กบางชนิดของฟิล์มบางไอซิงค์ด้วยวิธีสนามเฉลี่ย

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ในงานวิจัยนี้ได้ศึกษาคุณสมบัติเชิงแม่เหล็กของฟิล์มบางที่อธิบายด้วยโมเดลไอซิงค์เป็นฟังก์ชันของอุณหภูมิและความหนาของฟิล์มโดยการใช้การคำนวณวิธีสนามเฉลี่ย และได้คำนวณค่าสภาพแม่เหล็กและค่าสภาพรับไว้ได้เชิงแม่เหล็กโดยรวมและค่าสภาพแม่เหล็กและค่าสภาพรับไว้ได้เชิงแม่เหล็กของแต่ละชั้นของฟิล์มด้วยโดยละเอียด จากผลการคำนวณพบว่าพฤติกรรมของคุณสมบัติเชิงแม่เหล็กมีการเปลี่ยนแปลงจากคุณลักษณะในสองมิติไปยังสามมิติตามจำนวนชั้นของฟิล์มที่หนาขึ้น นอกจากนั้นได้มีการคำนวณอุณหภูมิวิกฤตและพบว่ามีการเปลี่ยนแปลงไปในทางเดียวกัน การเลื่อนของอุณหภูมิวิกฤตนี้จากค่าในสองมิติไปยังค่าในระดับเชิงปริมาตรสอดคล้องกับการทำนายเชิงทฤษฎีอันบ่งชี้ถึงการเปลี่ยนแปลงตามมิติของพฤติกรรมวิกฤตของแม่เหล็กจากฟิล์มบางไปยังสู่ระดับเชิงปริมาตรเมื่อฟิล์มมีขนาดหนา

ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ มหาวิทยาลัยเชียงใหม่ อำเภอเมือง จังหวัดเชียงใหม่ 50200

The magnetic property in a reduced geometry has recently gained much interest as a result of both technological and fundamental importance (Falicov *et al*., 1990; Johnson *et al*., 1996). Of a particular interest is the critical behavior of magnetic thin-films for which the dimensional crossover from two-dimension (2D) to three-dimension (3D) or bulk limit is not well established, especially when the surface effect is taken into account. Consequently, it is interesting to observe how magnetic properties such as the magnetization per spin m, the magnetic susceptibility per spin χ, and the critical temperature T_C depend on the temperature T and the thickness l of the films. Critical temperatures T_C in multilayered systems are known to change from 2D- to 3D-values with increasing numbers of layers; however, under the condition of the universality of the critical phenomena, a same convergence form of T_C from different lattice structures has not yet been analytically verified. Moreover, the variation of the magnetization and the susceptibility from surfaces to the inner layers of the films are also not well explained. Previous investigation of this layer-dependent of magnetic properties in thin-films was carried out by an extensive Monte Carlo simulation (Laosiritaworn *et al*., 2004). However, Monte Carlo method is prone to statistical errors arising from random number generators, number of configurations in making the average, the correlation time, the finite size effects, etc (Newman, 1999). Accordingly, it may be prudent if an analytic method, that is the mean-field method in this study, is carried out to verify such a phenomena. Therefore, to confirm this layer-variation behavior and the condition of universality between different structures, the Ising thin-films were considered for investigation by means of mean-field analysis of simple cubic (sc), body centered cubic (bcc), and face centered cubic (fcc) coordinated thin-films. Instead of using the more realistic Heisenberg model, the Ising model was chosen because both theoretical (Binder and Hohenberg, 1974; Bander and Mills, 1988) and experimental (Li and Baberschke, 1992; Elmer *et al*., 1994; Dunlavy and Venus, 2004) investigations have shown that the magnetic behavior in thin ferro-magnetic films is Ising-like.

In this study, a more complete picture of the magnetic phase transition in thin-films in all cubic structures especially at the critical point under the framework of the mean-field analysis was aimed for as the main objective. The study was firstly done by investigating how the magnetic properties, including their layer resolution, depend on temperature and thickness. Secondly, the shift of the critical temperatures T_C from a 2D to the bulk limit was investigated. After that, using an empirical fit, the shift exponents of the critical temperatures and their convergence from 2D- to the 3D-values were calculated. Finally, the results were quantitatively compared with the previous theoretical prediction.

Background and Methodology

In the mean-field analysis of magnetic properties, the magnetic spins are assumed to align in an average field created by all surrounding spins. In this study, it is assumed that the average field is the same for all spins in the same layer but different for different layers. Then, within this single site approximation, in each layer (plane), there are two different probabilities of a site being occupied by an up-spin or a down-spin denoted by $P_{i,\sigma}$, where i = 1,...,l is the layer index and $\sigma = \uparrow,\downarrow$ are the spin indexes referring to up-spin and down-spin respectively. The magnetization (the average spin) for all atomic sites in the i^{th} layer can be defined as

$$m_i = P_{i,\uparrow} - P_{i,\downarrow}, \qquad i = 1,...,l. \tag{1}$$

Then, the Ising Hamiltonian was considered; that is

$$H = -\sum_{<jk>} J_{jk}\sigma_j\sigma_k - h\sum_j \sigma_j, \tag{2}$$

where $\sigma_j = \pm 1$ is a spin at site j, J_{jk} is the exchange interaction, and h is the external field. The sum $<jk>$ takes only on the first neighboring. Hence, the interaction energy on the i^{th} layer (E_i) of the films is given by

$$E_i = -N_{//}\left\{\frac{Z_0}{2}J_{i,i}m_i^2 + Z_1 J_{i,i+1}m_i m_{i+1}\left(1-\delta_{i,l}\right) + Z_1 J_{i,i-1}m_i m_{i-1}\left(1-\delta_{i,l}\right) + hm_i\right\}, \tag{3}$$

where m_i is the average of all spins in layer i, Z_0 is the number of nearest neighbors to a lattice (atomic) point in the same layer and Z_1 is the number of nearest neighbors in one of its adjacent layers. The values of Z_0 and Z_1 for each cubic structure are given in Table 1. In each layer (plane), there consists of $N_{//}$ spins (atomic sites). The terms 1-$\delta_{i,1}$ and 1-$\delta_{i,1}$ in the equation refer to the use of free surfaces below the bottommost and above the topmost layer. Next, the entropy for an Ising system can be written as

$$S_i = -k_B N_{//}\left[P_{i,\uparrow}\ln P_{i,\uparrow} + P_{i,\downarrow}\ln P_{i,\downarrow}\right] = -k_B N_{//}\left[\frac{1+m_i}{2}\ln\frac{1+m_i}{2} + \frac{1-m_i}{2}\ln\frac{1-m_i}{2}\right]. \tag{4}$$

Thus, by minimizing the free energy $F_i = U_i - TS_i$ with respect to m_i; that is

$$\frac{\partial F_i}{\partial m_i} = 0, \qquad i = 1,...,l. \tag{5}$$

(where the internal energy $U_i = E_i$ is the sum of the interaction energy from all spins in the considered layer i), the equilibrium magnetization in layer i was obtained by solving the following l-coupled equations for l-layered films (Hong, 1990),

$$-J\left(Z_0 m_i + Z_1 m_{i+1}\left(1-\delta_{i,l}\right) + Z_1 m_{i-1}\left(1-\delta_{i,l}\right)\right) - h + \frac{k_B T}{2}\ln\left[\frac{1+m_i}{1-m_i}\right] = 0; \qquad i = 1,...,l. \tag{6}$$

Here, for simplicity, the homogeneity was assumed and $J_{i,i} = J_{i,i-1} = J_{i,i+1} = J$ was set (See Appendix A for details). However, to solve these coupled equations analytically is very complicated especially when the films are thick. As a result, a numerical method (root finding) was used to solve. Unfortunately, for h = 0, $\{m_i\}$ = 0 is also a solution. However, this zero-magnetization solution is a stable solution only in the para-magnetic phase. Then, to find a

Table 1. Number of nearest neighbors to a lattice point in the same layer (Z_0) and number of nearest neighbors in one of the adjacent layers (Z_1) for cubic lattices.

Thin-films structures	Z_0	Z_1
Simple cubic	4	1
Body centered cubic	0	4
Face centered cubic	4	4

non-zero solution, i.e. in the ferro-magnetic phase, from the root finding, the starting (guess) answer is required to be close to 1. The optimal choice is 1.0-10^{-15} as to avoid the rounding error in the double precision variables. For the magnetic susceptibility in a zero field, it can be calculated from $\chi_i = \left.\frac{\partial m_i}{\partial h}\right|_{h=0}$; that is

$$-J\left(Z_0\chi_i + Z_1\chi_{i+1}\left(1-\delta_{i,l}\right) + Z_1\chi_{i-1}\left(1-\delta_{i,l}\right)\right) + \frac{k_B T\chi_i}{1-m_i^2} = 1. \quad (7)$$

Apart from the magnetization and the susceptibility, the critical temperatures (T_C's) were also extracted from Equation 6. When the temperature T is very close to T_C, the magnetization $\{m_i\}$ becomes very small which leads to $\ln\frac{1+m_i}{1-m_i} \approx 2m_i$. In this way, the critical temperatures of thin-films in the zero magnetic field ($h = 0$) can be extracted by solving a set of equations

$$\mathbf{AM} = \mathbf{0}, \quad (8)$$

where **A** is an $l \times l$ matrix with elements

$$A_{ij} = (k_B T - Z_0 J)\delta_{i,j} - Z_1 J[(1-\delta_{i,l})\delta_{i,j+1} + (1-\delta_{i,1})\delta_{i,j-1}], \quad (9)$$

and **m** is an $l \times 1$ column matrix, $\{m_1,..., m_l\}$. Next, by solving det **A** = 0, the largest eigenvalue T can be associated as the critical temperature T_C of the thin-films because m is very small so this T should be insignificantly different from T_C.

Results and Discussion

From the calculations, the unit J/k_B is used for temperatures. The magnetization m and the susceptibility χ were extracted by solving Equations 6 and 7, and the results were found to present the crossover of their behavior from 2D-like for the monolayer (bilayer in bcc since the first nearest neighbor does not exist in the monolayer bcc) to 3D-like at around 20 layers e.g. see Table 2 and Figure 1. That the phase transition point moves from 2D- to 3D-value with increasing film thickness is in a good agreement with previous Monte Carlo studies (Binder, 1974; Laosiritaworn *et al*., 2004). Furthermore, from the layer-dependence of magnetic properties, the magnitudes of m and χ are found to increase from the lowest values at the surface layers to the largest values in the

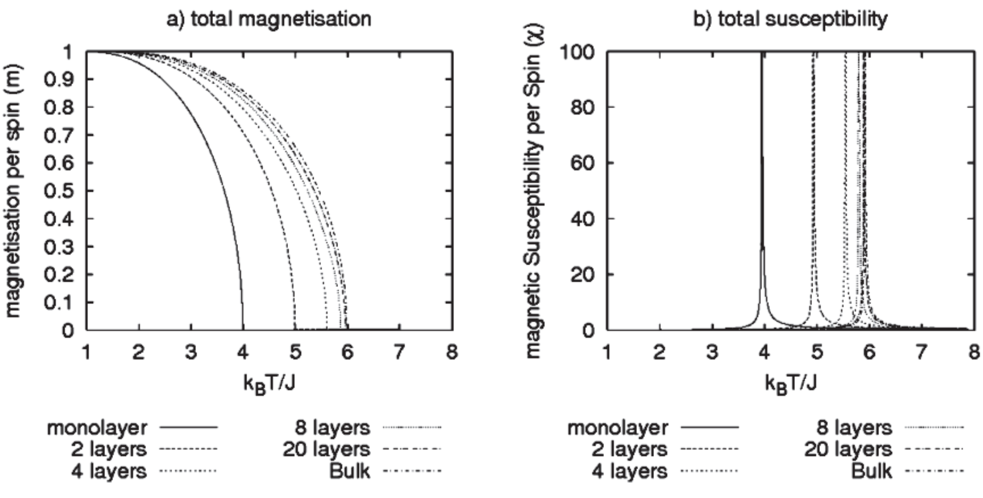

Figure 1. Examples of magnetic properties of Ising sc thin-films from mean-field calculations. As in the figure, (a) and (b) show a crossover of the magnetization m and the magnetic susceptibility χ from the 2D ($\frac{k_B T_C}{J} = 4$) to the bulk limit ($\frac{k_B T_C}{J} = 6$).

Table 2. Examples of magnetic properties of Ising sc thin-films from mean-field calculations from monolayer to bulk limit. As a summary, the temperature-dependent data are presented with a step of T = 0.2 J/k_B, and the precision digits are truncated at the fifth. A crossover of from the 2D to the bulk limit is found.

T	Magnetization per spin (*m*)						Magnetic susceptibility per spin (χ)					
	1 layer	2 layers	4 layer	8 layers	20 layer	Bulk	1 layer	2 layers	4 layer	8 layers	20 layer	Bulk
1.0	0.99933	0.99991	0.99995	0.99997	0.99998	0.99999	0.00136	0.00018	0.00010	0.00006	0.00004	0.00002
1.2	0.99741	0.99952	0.99971	0.99981	0.99987	0.99991	0.00438	0.00081	0.00048	0.00032	0.00022	0.00015
1.4	0.99316	0.99840	0.99901	0.99932	0.99950	0.99962	0.01013	0.00231	0.00142	0.00098	0.00072	0.00054
1.6	0.98562	0.99605	0.99747	0.99818	0.99860	0.99889	0.01921	0.00505	0.00321	0.00231	0.00177	0.00140
1.8	0.97398	0.99195	0.99470	0.99606	0.99687	0.99741	0.03222	0.00933	0.00608	0.00450	0.00355	0.00292
2.0	0.95750	0.98562	0.99031	0.99260	0.99398	0.99490	0.04989	0.01537	0.01021	0.00773	0.00624	0.00525
2.2	0.93553	0.97667	0.98397	0.98751	0.98964	0.99106	0.07336	0.02342	0.01574	0.01212	0.00995	0.00850
2.4	0.90733	0.96472	0.97537	0.98050	0.98357	0.98562	0.10440	0.03376	0.02285	0.01783	0.01482	0.01281
2.6	0.87207	0.94941	0.96426	0.97131	0.97554	0.97836	0.14586	0.04680	0.03174	0.02501	0.02096	0.01827
2.8	0.82863	0.93041	0.95038	0.95972	0.96532	0.96905	0.20262	0.06312	0.04268	0.03385	0.02856	0.02503
3.0	0.77552	0.90733	0.93348	0.94549	0.95270	0.95750	0.28353	0.08352	0.05602	0.04464	0.03781	0.03326
3.2	0.71041	0.87973	0.91331	0.92841	0.93747	0.94351	0.40640	0.10923	0.07224	0.05771	0.04901	0.04320
3.4	0.62950	0.84707	0.88959	0.90823	0.91941	0.92686	0.61284	0.14211	0.09203	0.07357	0.06253	0.05517
3.6	0.52543	0.80866	0.86200	0.88468	0.89827	0.90733	1.02778	0.18510	0.11631	0.09289	0.07892	0.06960
3.8	0.37949	0.76355	0.83017	0.85745	0.87378	0.88467	2.27589	0.24314	0.14644	0.11662	0.09890	0.08709
4.0	0.00622	0.71041	0.79364	0.82616	0.84560	0.85856	9.3×10^{2}	0.32512	0.18438	0.14611	0.12355	0.10850
4.2	0.00000	0.64722	0.75183	0.79037	0.81333	0.82863	5.00000	0.44890	0.23315	0.18336	0.15439	0.13508
4.4	0.00000	0.57059	0.70399	0.74949	0.77645	0.79442	2.50000	0.65611	0.29760	0.23138	0.19377	0.16871
4.6	0.00000	0.47400	0.64911	0.70279	0.73429	0.75529	1.66698	1.07170	0.38616	0.29496	0.24539	0.21234
4.8	0.00000	0.34083	0.58569	0.64929	0.68596	0.71041	1.25000	2.32033	0.51503	0.38218	0.31542	0.27094
5.0	0.00000	0.00622	0.51130	0.58761	0.63019	0.65857	1.00000	8.3×10^{2}	0.72071	0.50775	0.41508	0.35341
5.2	0.00000	0.00000	0.42134	0.51568	0.56505	0.59793	0.83333	5.00000	1.10866	0.70212	0.56701	0.47760
5.4	0.00000	0.00000	0.30414	0.42999	0.48735	0.52543	0.71429	2.50002	2.17111	1.04213	0.82516	0.68520
5.6	0.00000	0.00000	0.08722	0.32311	0.39093	0.43515	0.62508	1.66667	2.6×10^{1}	1.80818	1.35681	1.10111
5.8	0.00000	0.00000	0.00000	0.16740	0.25994	0.31199	0.55558	1.25011	5.22761	5.97931	3.04956	2.35000
6.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00622	0.50001	1.00000	2.50046	7.50000	3.8×10^{1}	7.7×10^{2}
6.2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.45455	0.83333	1.64634	2.86472	4.10458	5.00008
6.4	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.41667	0.71429	1.22881	1.78369	2.21055	2.50026
6.6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.38462	0.62500	0.98107	1.29942	1.51926	1.66667
6.8	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.35714	0.55556	0.81684	1.02383	1.15941	1.25000
7.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.33333	0.50000	0.70000	0.84560	0.93820	1.00005
7.2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.31250	0.45457	0.61258	0.72070	0.78827	0.83334
7.4	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.29412	0.41667	0.54469	0.62823	0.67986	0.71429
7.6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.27778	0.38462	0.49043	0.55697	0.59779	0.62500
7.8	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.26316	0.35714	0.44606	0.50035	0.53347	0.55556
8.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.25003	0.33333	0.40913	0.45425	0.48171	0.49525

interior of the films e.g. see 10-layered Ising sc films in Table 3 and Figure 2. This layer-variation of magnetic properties is expected because the exchange ferro-magnetic energy associated with each spin is greater in the bulk than at the surfaces owing to the increase in numbers of nearest neighbors.

For the critical temperature T_C, it was calculated by solving (see Equations 8 and 9), and the largest eigenvalue T was associated as the critical temperature T_C. The results are presented in Table 4. A change from 2D to bulk values as the thickness l is increased was found. As increasing the thickness, the critical temperature moves

Table 3. Examples of the layer dependence of the magnetization (m_k) and the magnetic susceptibility (χ_k), where k is the layer index, for 10-layered sc films. Due to the interaction symmetry, the properties in the layer *k* and layer 10-*k* are the same. As a summary, the temperature-dependent data are presented with a step of $T = 0.2\ J/k_B$, and the precision digits are truncated at the fifth.

T	Magnetization per spin (m)					Magnetic susceptibility per spin (χ)				
	Layer 1,10	Layer 2,9	Layer 3,8	Layer 4,7	Layer 5,6	Layer 1,10	Layer 2,9	Layer 3,8	Layer 4,7	Layer 5,6
1.0	0.99991	0.99999	0.99999	0.99999	0.99999	0.00018	0.00002	0.00002	0.00002	0.00002
1.2	0.99952	0.99991	0.99991	0.99991	0.99991	0.00081	0.00015	0.00015	0.00015	0.00015
1.4	0.99840	0.99962	0.99962	0.99962	0.99962	0.00230	0.00055	0.00054	0.00054	0.00054
1.6	0.99606	0.99888	0.99889	0.99889	0.99889	0.00501	0.00141	0.00140	0.00140	0.00140
1.8	0.99200	0.99740	0.99741	0.99741	0.99741	0.00921	0.00296	0.00292	0.00292	0.00292
2.0	0.98576	0.99485	0.99490	0.99490	0.99490	0.01506	0.00535	0.00525	0.00525	0.00525
2.2	0.97699	0.99094	0.99106	0.99106	0.99106	0.02273	0.00874	0.00851	0.00850	0.00850
2.4	0.96538	0.98537	0.98562	0.98562	0.98562	0.03240	0.01329	0.01282	0.01281	0.01281
2.6	0.95067	0.97787	0.97835	0.97836	0.97836	0.04428	0.01918	0.01829	0.01827	0.01827
2.8	0.93261	0.96817	0.96903	0.96905	0.96905	0.05867	0.02663	0.02509	0.02503	0.02503
3.0	0.91099	0.95602	0.95746	0.95750	0.95750	0.07596	0.03593	0.03339	0.03327	0.03326
3.2	0.88559	0.94115	0.94341	0.94350	0.94351	0.09669	0.04748	0.04346	0.04322	0.04320
3.4	0.85616	0.92324	0.92668	0.92685	0.92686	0.12157	0.06186	0.05566	0.05520	0.05517
3.6	0.82247	0.90195	0.90700	0.90731	0.90733	0.15152	0.07985	0.07053	0.06967	0.06960
3.8	0.78423	0.87687	0.88408	0.88462	0.88466	0.18782	0.10260	0.08880	0.08726	0.08711
4.0	0.74115	0.84749	0.85756	0.85847	0.85855	0.23216	0.13179	0.11159	0.10887	0.10855
4.2	0.69290	0.81317	0.82696	0.82845	0.82861	0.28684	0.16997	0.14063	0.13587	0.13520
4.4	0.63917	0.77311	0.79166	0.79406	0.79437	0.35504	0.22108	0.17867	0.17039	0.16901
4.6	0.57963	0.72625	0.75081	0.75460	0.75517	0.44116	0.29150	0.23038	0.21598	0.21315
4.8	0.51403	0.67119	0.70316	0.70908	0.71013	0.55150	0.39187	0.30409	0.27895	0.27310
5.0	0.44222	0.60606	0.64688	0.65600	0.65790	0.69556	0.54104	0.41600	0.37166	0.35948
5.2	0.36429	0.52832	0.57906	0.59287	0.59629	0.88933	0.77486	0.60068	0.52171	0.49581
5.4	0.28055	0.43450	0.49479	0.51520	0.52123	1.16606	1.17047	0.94370	0.80279	0.74668
5.6	0.19136	0.31955	0.38486	0.41322	0.42339	1.62170	1.93997	1.71792	1.48155	1.36109
5.8	0.09503	0.17271	0.22600	0.25712	0.27104	2.87583	4.32857	4.68792	4.57384	4.42361
6.0	0.00000	0.00000	0.00000	0.00000	0.00000	5.00052	9.00104	12.00153	14.00193	15.00216
6.2	0.00000	0.00000	0.00000	0.00000	0.00000	1.75671	2.86476	3.54577	3.93593	4.11327
6.4	0.00000	0.00000	0.00000	0.00000	0.00000	1.15479	1.77151	2.09682	2.26084	2.32919
6.6	0.00000	0.00000	0.00000	0.00000	0.00000	0.88376	1.29779	1.49048	1.57746	1.61091
6.8	0.00000	0.00000	0.00000	0.00000	0.00000	0.72457	1.02879	1.15605	1.20814	1.22674
7.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.61798	0.85394	0.94384	0.97756	0.98880
7.2	0.00000	0.00000	0.00000	0.00000	0.00000	0.54081	0.73060	0.79711	0.82014	0.82734
7.4	0.00000	0.00000	0.00000	0.00000	0.00000	0.48197	0.63871	0.68962	0.70602	0.71084
7.6	0.00000	0.00000	0.00000	0.00000	0.00000	0.43541	0.56748	0.60751	0.61956	0.62291
7.8	0.00000	0.00000	0.00000	0.00000	0.00000	0.39753	0.51060	0.54275	0.55183	0.55423
8.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.36617	0.46431	0.49060	0.49762	0.49937

towards the 3D value owing to the increase of the average exchange interaction energy. Figure 3 shows evidence of such a dimensional crossover of the critical temperatures for the Ising thin-films in all considered structures. The results are found to comply with the analytic expression for T_C being made on the basis of a mean-field T_C examination (Haubenreisser *et al.*, 1972) given as

$$T_C(l) = T_C(\infty)\frac{Z_0 + 2Z_1\cos(\pi/(l+1))}{Z_0 + 2Z_1}, \quad (10)$$

where Z_0 and Z_1 are number of nearest neighbors

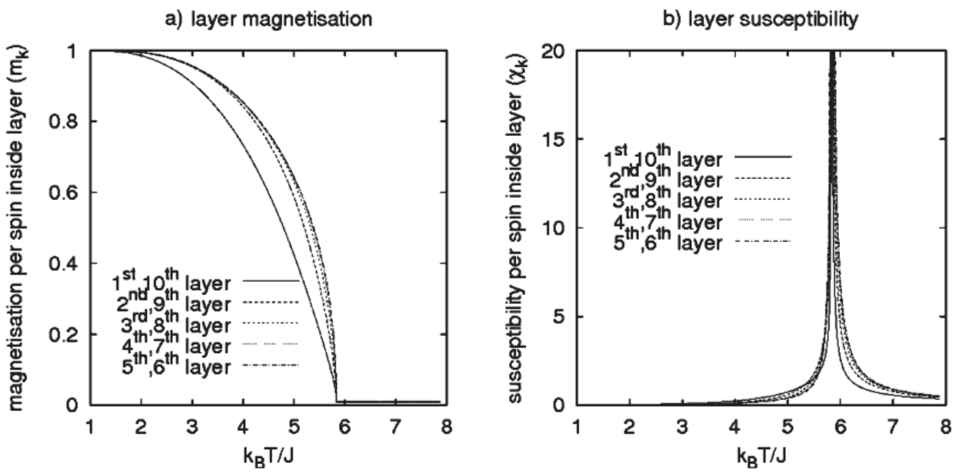

Figure 2. Examples of the layer dependence of the magnetization (m_k) and the magnetic susceptibility (χ_k), where *k* is the layer index, for 10-layered sc films. As can be seen, the magnitude of both m_k and χ_k are smallest at the surface layers (layer 1 and layer 10), but strongest at the innermost (layer 5 and layer 6).

Table 4. Critical temperatures of Ising thin-films in all 3 types of cubic lattices. The precision digits are truncated at the 15th due to the limitation of computer numerical accuracy.

Number of layers	Thin-films structures		
	Simple cubic	Body centered cubic	Face centered cubic
1	4	-	4
2	5	4	8
3	5.414213562373095	5.656854249492381	9.656854249492380
4	5.618033988749895	6.472135954999580	10.472135954999580
5	5.732050807568877	6.928203230275509	10.928203230275509
6	5.801937735804839	7.207750943219353	11.207750943219352
7	5.847759065022574	7.391036260090294	11.391036260090294
8	5.879385241571818	7.517540966287266	11.517540966287266
9	5.902113032590307	7.608452130361228	11.608452130361230
10	5.918985947228995	7.675943788915980	11.675943788915980
11	5.931851652578136	7.727406610312547	11.727406610312546
12	5.941883634852104	7.767534539408395	11.767534539408416
13	5.949855824363647	7.799423297454589	11.799423297454588
14	5.956295201467611	7.825180805870446	11.825180805870446
15	5.961570560806461	7.846282243225843	11.846282243225843
16	5.965946199367804	7.863784797470034	11.863784797471215
17	5.969615506024416	7.878462024097664	11.878462024097665
18	5.972722606805444	7.890890427219795	11.890890427221780
19	5.975376681190276	7.901506724761102	11.901506724761102
20	5.977661652450257	7.910646609801074	11.910646609801034
Bulk	6	8	12

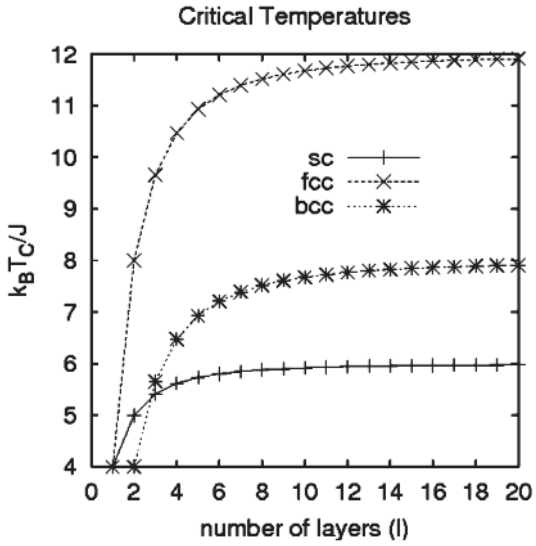

Figure 3. The critical temperatures T_C as a function of thickness l extracted from mean-field calculations. The values of $\frac{k_B T_C}{J}$ are 4 for 2D square-lattice and 6, 8 and 12 for bulk sc, bcc, and fcc respectively. Lines are added as a viewing aid.

in the same plane and one of its adjacent planes respectively (see Table 1). Also, from the T_C results, for large enough thickness i.e. $l \geq 4$, it is found that $T_C^{sc}(l) < T_C^{bcc}(l) < T_C^{fcc}(l)$. This is due to the fact that the number of neighboring sites has a strong effect on the interaction energy. Hence, the more neighboring sites the higher thermal energy is required to change from a ferro-magnetic to a para-magnetic phase which results in the higher critical temperature.

Apart from the results for T_C, it is also interesting to examine the evolution of the thin-films critical temperatures from the monolayer to the bulk 3D-limit in terms of a power law (Privman, 1990)

$$1-\frac{T_C(l)}{T_C(\infty)} \alpha\, l^{-\lambda}. \tag{11}$$

Here, $T_C(l)$ and $T_C(\infty)$ are the thin-films and the bulk critical temperatures respectively. The shift exponent of the critical temperature λ has a value between 1.0 and 2.0 depending on the spin model used and the type of calculation. For thick-films, λ is expected to be $\lambda = 1/\nu^{3D}$ (Barber, 1983) where ν is the critical exponent to the correlation length of magnetic interaction. However, if the films' size is not thick enough, a better fit for films of a range of thicknesses l is given by (Huang *et al.*, 1994; Wu *et al.*, 1996)

$$\frac{1}{T_C(l)} = \frac{1}{T_C(\infty)}\left[1+\left(\frac{l_0}{l-l'}\right)^{\lambda'}\right], \tag{12}$$

where l_0, l' and λ' are all adjustable parameters. Similarly, λ' should tend to $1/\nu^{3D}$ as l tends to infinity (bulk limit). However, from the mean-field theory, the critical exponents are dimensional independent and obey Josephson scaling relation only at the dimension D = 4 (Binney *et al.*, 1992). This dimensional independence of the critical exponents is not true and hence the weak point of the mean-field method. So, it can be implied that the mean-field works well only at high dimensions, and it is expected that at the bulk limit (or at high dimension) the mentioned λ' should converge to $1/\nu_{\text{mean-field}} = 2$ since $\nu_{\text{mean-field}} = 1/2$. Consequently, Equation 12 was used to fit the $T_C(l)$'s arising from

Table 5. Fitting exponents of the extrapolation to bulk limit from Equations 12 and 13.

Fitting parameters	Simple cubic	Body centered cubic	Face centered cubic
l_0	$1.2342 \pm 7.2 \times 10^{-3}$	$1.6680 \pm 3.6 \times 10^{-2}$	$1.1940 \pm 1.8 \times 10^{-3}$
l'	$-0.6105 \pm 3.7 \times 10^{-3}$	$0.6290 \pm 1.5 \times 10^{-2}$	$0.2812 \pm 8.9 \times 10^{-3}$
λ'	$1.8941 \pm 3.3 \times 10^{-3}$	$1.5950 \pm 1.3 \times 10^{-2}$	$1.5810 \pm 3.7 \times 10^{-2}$
$T_C(\infty)$	$6.00204 \pm 2.2 \times 10^{-4}$	$8.03210 \pm 3.9 \times 10^{-3}$	$12.04960 \pm 5.8 \times 10^{-3}$
T_C^{bulk}	6	8	12
λ''		$1.9971 \pm 1.5 \times 10^{-3}$	

the mean-field calculations. Results of the fit are shown in Table 5. As can be seen, $T_C(\infty)$'s, which are the extrapolated thin-films critical temperatures to the bulk limit, agree well with the theoretical 3D-values, i.e. T_C^{bulk}'s, for all three structures of the films. Hence, it can be concluded that the calculated $T_C(l)$'s in this work are accurate and the fitting Equation 12 is useful.

However, as can be seen in Table 5, even up to $l = 20$, λ' is not close to the expected value i.e. 2. This may be caused by some mismatch behavior between thin-films and thick-films. Then, to clarify the evolution from 2D- to 3D-like behavior, the power law of Equation 11 was rearranged and defined (See Appendix B for details)

$$\lambda''(l) = -\log\left(\frac{T_C^{bulk} - T_C(l)}{T_C^{bulk} - T_C(l-1)}\right) \Big/ \log\left(\frac{l}{l-1}\right), \quad (13)$$

where $T_C(\infty)$ is substituted by the theoretical 3D-value T_C^{bulk} to obtain a more accurate value. After that, $\lambda''(l)$ was tabulated with l ranging from 2 to 20 layers. These $\lambda''(l)$'s should converge to 2 when l tends to infinity. A linear least square fit between $\lambda''(l)$'s and $1/l$ gives a way to obtain $\lambda''(\infty)$'s which are also given in Table 5. As can be seen, the mean-field values of $\lambda''(\infty)$'s from all structures have a same value which is very close to 2. This is satisfying since the mean-field ν is well-known to be 1/2. Furthermore, the critical exponents ($\lambda''(\infty) = 1/\nu_{\text{mean-field}}$) are structural independent and this satisfies the condition of universality.

Conclusion

The magnetic behavior of Ising thin films was studied in sc, bcc, and fcc structures using a mean-field analysis. The dimensional crossover of both m and χ from 2D- to 3D-like is found with increasing film thickness. The layer components of m and χ are found to have the lowest magnitudes at the surfaces while the innermost layers have the highest value due to the free boundary effect at the surfaces. That the films' T_C's evolve from 2D- to 3D-values with increasing film thickness is in good agreement with previous investigation. The empirical fit of the calculated $T_C(l)$'s for films of varying the thickness l gives the fitted T_C at the limit of infinitely thick films which agrees very well with the theoretical prediction at the bulk limit. Another empirical fit for the shift exponent also strongly suggests the usefulness of the mean-field method at a high dimension and confirms the condition of universality.

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References

Bander, M. and Mills, D.L. 1988. Ferromagnetism of ultrathin films. Phys. Rev. B, 38: 12015-12018.

Barber, M.N. 1983. Finite-Size Scaling. **In**: Domb, C. and Lebowitz, J.L. (eds) Phase Transitions and Critical Phenomena Vol. 8, Academic Press, New York.

Binder, K. 1974. Monte Carlo study of thin magnetic Ising films. Thin Solid Films, 20: 367-381.

Binder, K. and Hohenberg, P.C. 1974. Surface effects on magnetic phase transitions. Phys. Rev. B, 9: 2194-2214.

Binney, J.J., Dowrick, N.J., Fisher, A.J. and Newman, M.E.J. 1992. The Theory of Critical Phenomena: An Introduction to the Renormalization Group., Oxford University Press, New York.

Dunlavy, M.J. and Venus, D. 2004. Critical susceptibility exponent measured from Fe/W(110) bilayers. Phys. Rev. B, 69: 094411-1 - 094411-7.

Elmers, H.J., Hauschild, J., Hoche, H., Gradmann, U., Bethge, H., Heuer, D. and Kohler, U. 1994. Submonolayer Magnetism of Fe(110) on W(110): Finite Width Scaling of Stripes and Percolation between Islands. Phys. Rev. Lett., 73: 898-901.

Falicov, L.M., Pierce, D.T., Bader, S.D., Gronsky, R., Hathaway, K.B., Hopster, H.J., Lambeth, D.N., Parkin, S.S.P., Prinz, G., Salamon, M., Schuller, I.K. and Victora, R.H. 1990. Surface, interface, and thin-film magnetism. J. Mater. Res., 5: 1299-1340.

Haubenreisser, W., Brodkorb, W., Corciovei, A. and Costache, G. 1972. Status Report of Green's Function Theory in Uniaxial Ferromagnetic Unpinned Thin Films. Phys. Status Solidi B, 53: 9-40.

Hong, Q. 1990. Critical temperature of an Ising magnetic film. Phys. Rev. B, 41: 9621-9624.

Huang, F., Kief, M.T., Mankey, G.J. and Willis, R.F. 1994. Magnetism in the few-monolayers limit: A surface magneto-optic Kerr-effect study of the magnetic behavior of ultrathin films of Co, Ni, and Co-Ni alloys on Cu(100) and Cu(111). Phys. Rev. B, 49: 3962-3971.

Johnson, M.T., Bloemen, P.J.H., den Broeder, F.J.A. and de Vries, J.J. 1996. Magnetic anisotropy in metallic multilayers. Rep. Prog. Phys., 59: 1409-1458.

Laosiritaworn, Y., Poulter, J., Staunton, J.B. 2004. Magnetic properties of Ising thin films with cubic lattices. Phys. Rev. B 70: 104413-1 - 104413-9.

Li, Y. and Baberschke, K. 1992. Dimensional crossover in ultrathin Ni(111) films on W(110). Phys. Rev. Lett., 68: 1208-1211.

Newman, M.E.J. and Barkema, G.T. 1999. Monte Carlo Methods in Statistical Physics, Clarendon Press, Oxford.

Privman, V. 1990. Finite-Size Scaling Theory. **In**: Privman, V. (eds) Finite Size Scaling and Numerical Simulation of Statistical Systems, World Scientific, Singapore.

Wu, S.Z., Schumann, F.O., Mankey, G.J. and Willis, R.F. 1996. Magnetic behavior of $Fe_xNi_{(1-x)}$ and $Co_xNi_{(1-x)}$ pseudomorphic films. J. Vac. Sci. Technol. B, 14: 3189-3192.

Appendix A

Staring with the Ising Hamiltonian,

$$H = -\sum_{<jk>} J_{jk}\sigma_j\sigma_k - h\sum_j \sigma_j, \tag{2}$$

the average Hamiltonian in layer i is given by

$$\begin{aligned}\langle H_i \rangle &\equiv E_i \\ &= -N_{//}\left\{\frac{Z_0}{2}J_{1,1}m_1^2 + Z_1 J_{1,2} m_1 m_2 + hm_1\right\}, &&; \text{for } i = 1, \\ &= -N_{//}\left\{\frac{Z_0}{2}J_{i,i}m_i^2 + Z_1 J_{i,i+1} m_i m_{i+1} + Z_1 J_{i,i-1} m_i m_{i-1} + hm_i\right\}, &&; \text{for } 2 \le i \le l\text{-}1, \\ &= -N_{//}\left\{\frac{Z_0}{2}J_{l,l}m_l^2 + Z_1 J_{l,l-1} m_l m_{l-1} + hm_i\right\}, &&; \text{for } i = l,\end{aligned}$$

where the average of spin in layer i ($<\sigma_i>$), under the mean-field framework, is the magnetization in that layer (m_i), and $N_{//}$ is the number of spins in one layer. In general, we can write

$$E_i = -N_{//}\left\{\frac{Z_0}{2}J_{i,i}m_i^2 + Z_1 J_{i,i+1} m_i m_{i+1}(1-\delta_{i,l}) + Z_1 J_{i,i-1} m_i m_{i-1}(1-\delta_{i,1}) + hm_i\right\}, \tag{3}$$

or $$E_i = U_i = -N_{//}J\left\{\frac{Z_0}{2}m_i^2 + Z_1 m_i m_{i+1}(1-\delta_{i,l}) + Z_1 m_i m_{i-1}(1-\delta_{i,1}) + hm_i\right\},$$

where the exchange interaction $J_{i,j}$ is assumed isotropic i.e. $J_{i,i} = J_{i,i-1} = J_{i,i+1} = J$, and U_i denotes the internal energy in layer i. Next, the entropy of all spins j in layer i can be written as $S_i = \sum_{j\in i}\left(-k_B \sum_{\text{all possible states at } j} P_j \ln P_j\right)$, where P_j is the spin-probability at site j. In the Ising Hamiltonian, in layer i, the probability can be only $P_{i,\uparrow}$ or $P_{i,\downarrow}$, where $\uparrow$ and $\downarrow$ refer to up (+1) and down (-1) spin respectively. In this study, $P_{i,\uparrow}$ or $P_{i,\downarrow}$ are allowed to vary from to layer to layer. Since $m_i = P_{i,\uparrow} - P_{i,\downarrow}$, $P_{i,\uparrow} + P_{i,\downarrow} = 1$, and there are $N_{//}$ in each layer, it is possible to write

$$S_i = -k_B N_{//}[P_{i,\uparrow}\ln P_{i,\uparrow} + P_{i,\downarrow}\ln P_{i,\downarrow}] = -k_B N_{//}[P_{i,\uparrow}\ln P_{i,\uparrow} + (1-P_{i,\uparrow})\ln(1-P_{i,\uparrow})].$$

$$S_i = -k_B N_{//}\left[\frac{1+m_i}{2}\ln\frac{1+m_i}{2} + \frac{1-m_i}{2}\ln\frac{1-m_i}{2}\right] \tag{4}$$

Next, by considering the free energy in layer i,

$$\begin{aligned}F_i = U_i - TS_i = -N_{//}J&\left\{\frac{Z_0}{2}m_i^2 + Z_1 m_i m_{i+1}(1-\delta_{i,l}) + Z_1 m_i m_{i-1}(1-\delta_{i,1}) + hm_i\right\} \\ &-k_B T N_{//}\left[\frac{1+m_i}{2}\ln\frac{1+m_i}{2} + \frac{1-m_i}{2}\ln\frac{1-m_i}{2}\right],\end{aligned}$$

it is possible to calculate the stable magnetization in layer *i* i.e. m_i from where the free energy in layer *i* has its minimum i.e. $\frac{\partial F_i}{\partial m_i} = 0.$ Then, from this derivative, it is easy to obtain

$$-J(Z_0 m_i + Z_1 m_{i+1}(1-\delta_{i,l}) + Z_1 m_{i-1}(1-\delta_{i,1})) - h + \frac{k_B T}{2}\ln\left[\frac{1+m_i}{1-m_i}\right] = 0; \quad i = 1,\ldots,l. \tag{6}$$

As a result, by performing the root-finding method to solve these *l*-coupled equations, the set $\{m_i\}$ is obtained as a function of temperature.

Appendix B

Starting with Equation 11,

$$1 - \frac{T_C(l)}{T_C(\infty)} \alpha\, l^{-\lambda}, \tag{11}$$

for *l* layered and *l*-1 layered films, we may write $1 - \frac{T_C(l)}{T_C(\infty)} \approx cl^{-\lambda''}$ and $1 - \frac{T_C(l-1)}{T_C(\infty)} \approx c(l-1)^{-\lambda''}$, where *c* is a proportional constant. As a result,

$$\frac{1 - \frac{T_C(l)}{T_C(\infty)}}{1 - \frac{T_C(l-1)}{T_C(\infty)}} = \frac{cl^{-\lambda''}}{c(l-1)^{-\lambda''}},$$

$$\frac{T_C(\infty) - T_C(l)}{T_C(\infty) - T_C(l-1)} = \left(\frac{l}{l-1}\right)^{-\lambda''},$$

and $$\lambda'' \equiv \lambda''(l) = -\log\left(\frac{T_C^{bulk} - T_C(l)}{T_C^{bulk} - T_C(l-1)}\right) \Big/ \log\left(\frac{l}{l-1}\right), \tag{13}$$

where $T_C(\infty)$ is substituted by T_C^{bulk} and $\lambda''(l)$ is *l*-dependent (see text).