Metastability in Monte Carlo simulation of 2D Ising films and in Fe monolayer strips

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Abstract: Effective Curie-temperatures measured in Fe monolayer strips agree reasonably with computer simulations of two-dimensional Ising model strips. The simulations confirm the domain structure seen already by Albano et al.

Iron is a ferromagnetic metal, while the Ising model uses only localized spins. Thus in principle one should not expect good agreement if the Ising model is compared with experiments on iron. Nevertheless, experiments on Fe films and Fe strips [1-3] could be discussed in terms of 2D Ising model simulations. In particular, experiments on Fe(110) monolayer strips prepared on W(110) [1] could be reasonably well interpreted through Ising model simulations [4]. However, quantitative comparison was not possible both because of incomplete information on the Fe monolayer width and because of limited extent of the simulations. Thus we improve the simulations of ref.4 (using a 512 processor Cray-T3E instead of a 136 processor Intel Paragon), generalize them to non-zero magnetic fields, and compare them with the old critical temperatures of arbitrarily oriented, widely spaced Fe strips of incompletely defined width [1] as well as with new ones of well oriented, more closely spaced Fe strips with better defined width, which were prepared by step flow growth on miscut W(110) substrates [5].

The Monte Carlo simulations, at temperatures below the bulk Curie temperature $T_c$ of the two-dimensional Ising model (square lattice with nearest-neighbour interactions between spin 1/2 atoms), were made with standard Glauber kinetics and free boundary conditions along the long sides of the $L \times W$ films, $L \to \infty$, $W < 10^2$. In our multi-spin coding method, spins are denoted as zero or two instead of the usual zero or one, in order that the vacuum outside the films can be characterized by one. One Cray-T3E processor tried to update nearly 14 sites per microsecond.

In principle, the above $\infty \times W$ geometry of the Ising model does not have a sharp phase transition, as is well known: If we wait long enough, the magnetization decays to zero even if (as in our simulations) initially all spins are parallel. In this sense the strips behave as one-dimensional chains and have a critical temperature of zero. However, similar to investigations of glasses, experiments are made with a finite observation time $1 \ldots 10^3 \text{s}$ and thus may correspond to $10^{12} \ldots 10^{15}$ microscopic time units (Monte Carlo steps per spin). We thus ask for the temperature $T_c(W)$ at which the relaxation time $\tau$ for the magnetization in the Ising strip reaches $10^{12}$ or $10^{15}$. This temperature is only an effective critical temperature; its determination requires extrapolations via an Arrhenius law, since our simulations are restricted to one million time steps.
Figure 1 shows an example how the magnetization, averaged over many samples, decays towards zero as \( \exp(-t/\tau) \), and how this \( \tau \) increases for decreasing temperature:

\[
\tau = B(W) \exp(A(W)T_c(\infty)/T)
\]

due to an energy barrier \( AT_c \) linear in the strip width \( W \) which needs to be overcome. Figure 2 gives this roughly linear variation of the energy barrier \( A(W) \) with increasing strip width \( W \). We estimate

\[
\tau = 658 \exp([aT_c(\infty)/T - b]W - 3.31T_c(\infty)/T)
\]

with \( a = 3.13 \pm 0.05, \ b = 3.03 \pm 0.06 \). Equating this time with \( 10^{12} \) and \( 10^{15} \) we find the upper and lower curve in figure 3, while the data correspond to ref.1 (larger error bars) and ref.5 (smaller error bars). We find surprisingly good agreement. (The calibration of the \( W \)-axis, which could been done in ref. 1 by a rough estimate only, was rescaled by a factor 1.5, compatible with the data of ref. 1, to better fit both the new experiments and the simulations. The influence of magnetostatic coupling on \( T_c \) in the closely spaced new films will be discussed in [5].) However, hysteresis experiments [5] for closely spaced films disagree with simulations in a magnetic field, suggesting that the elementary magnetic dipoles are then larger than single spins.

Figure 4 shows the magnetization \( M(x)/2 \) for \( 0 < x < L = 10^4 \) defined as the number of up spins across the narrow strip of width 20. We add suitable constants to \( M \) to make the whole length \( L = 10,000 \) visible in ten strips of length 1000 each; these constants give the horizontal lines in figure 4 corresponding to 16 up spins and 16 down spins. We see that as in [6], large domains separated by relatively sharp domain walls are formed, similar to the time dependence in the “tunneling” of the magnetization [7]. However, the size of the domains varies appreciably, mostly between \( 10^2 \) and \( 10^3 \).

These domains now could be regarded as our basic magnetic units but it would be wrong to identify them with our Ising spins. Instead they form a one-dimensional chain, with dipole-dipole interactions within one chain and, for closely spaced iron films [5], also dipolar interactions from one chain to the neighbouring chains. Because of the long range of dipolar forces, such a system might be described well by a mean field approximation, and such a theory [5] will be presented together with the new experiments. It may give even a sharp phase transition for infinitely long waiting times, due to the coupling between different chains.

In summary, we found a surprisingly good qualitative agreement between widely spaced iron strips [1] and two-dimensional Ising models, while for closely spaced iron films [5] the Ising model without magnetic dipolar interactions is too simple.

We thank H.J. Elmers for pointing out an error in a draft of the manuscript, PS and DS thank SFB 341 for support, UG the Max-Planck-Institut für Mikrostrukturphysik Halle for hospitality.
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Figure captions:
Fig. 1: Part a shows the decay of the magnetization with time, part b the resulting relaxation time as a function of temperature (Arrhenius law).
Fig. 2: Dependence of Arrhenius parameter $A$, eq.(1), on strip width $W$.
Fig. 3: Effective transition temperature (curves) where $\tau$ from eq.(2) reaches $10^{12}$ and $10^{15}$. The bars indicate the width of the transition, not an error of measurement. Wide transitions from widely spaced strips [1] have large “error” bars, and narrow transitions from closely spaced strips [5] have small ones.
Fig. 4: Snapshot of equilibrium domain distribution at $T/T_c(\infty) = 0.90, 10000 \times 20, t = 10^6$. 
Fig1a, magnetization vs. time, $W = 32$, $T/T_c = 0.94$, fit: $\exp(-t/22954)$
Fig 1b, relaxation times, $W = 32$
Fig. 3, Effective critical temperature $T_c(W)/T_c$ for $t = 10^{12}$ and $10^{15}$
Fig. 4, 10,000 * 32 Ising model at $T/T_c = 0.92$, $t = 2$ million, $-16 < M < 16$