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MONTE CARLO STUDIES OF DOMAIN GROWTH IN TWO DIMENSIONS*

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ABSTRACT

Monte Carlo simulations have been carried out to study the effect of temperature on the kinetics of domain growth. The concept of "spatial entropy" is introduced. Is is shown that "spatial entropy" of the domain can be used to give a measure of the roughening of the domain. Most of the roughening is achieved during the initial time ($t \lesssim 10$ Monte Carlo cycles), the rate of roughening being greater for higher temperatures. For later times the roughening of the domain for different temperatures proceeds at essentially the same rate.

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INTRODUCTION

Various phenomenological theories[1-4] have been proposed to explain the growth of domains or grains in the ordering of a three dimensional alloy with two equivalent sublattices quenched from high to low temperature. All these theories predict the size or area of the domains to shrink linearly with time as $A(t) = A_0 - \alpha t$, where A_0 and $A(t)$ are the initial and instantaneous areas of the domain respectively. The temperature dependence of the growth law is however not clearly understood, especially at temperatures approaching the critical temperature T_c. For temperature $T \ll T_c$, both the phenomenological theories of Lifshitz[1], and Allan and Cahn[2] predict an exponential temperature dependence arising from the Arrhenius behaviour of the attempt frequency, in agreement with the experimental results[2]. For temperatures close to T_c, the theory of Lifshitz[1] predicts a temperature dependence of the surface free energy which is not borne out by experimental results. The experimental verification of the theory of Allan and Cahn involves a measurement of a geometrical factor and a kinetic factor, both of which have still to be measured.

Recently Sahni et al.[5] have carried out Monte Carlo simulations to study the effect of thermal or roughening fluctuations on the growth of domains. Their calculations carried out on circular domains in two dimensions show that the slope α remains constant for $T < 0.6\ T_c$ as expected from phenomenological theories. However for $T \geq 0.6\ T_c$, α decreases linearly with increasing temperature. This deviation is explained as a result of roughening fluctuations.

The importance of roughening fluctuations in the kinetics of domain growth has prompted us to study this phenomenon in more detail. A quantity which can be used to measure the roughening of the domain wall is the "spatial entropy" of the domain. In their study of the "measurement of shapes" Rogers and Trofanenko[6] find it convenient to introduce the concept of "spatial entropy", which affords a good measure of the complexity of the shape. As applied to our study of the domain growth, this spatial entropy can be defined as

$$S = - \sum_i p_i \ln p_i$$

where p_i is the fraction of atoms having i nearest neighbours of the same type. The spatial entropy will increase as the domain roughens up (complexity increases), and will tend to a maximum value of ln4 when the domain is completely disordered ie: when all p_i are equally probable.

MODEL

The model we have used to study the kinetics of domain growth is essentially the one used by Sahni et al.[5] We monitor the time evolution of a circular domain of one sublattice surrounded by a sea of another degenerate sublattice on an NxN square lattice. We use the standard procedure of transformation of a lattice gas to an antiferromagnetic Ising model. This system is described by the Hamiltonian

$$H = - J \sum_{<ij>} S_i S_j$$

where $S_i = \pm 1$ and the notation $< >$ signifies that the summation is only over nearest neighbours. J is the exchange interaction, for our antiferromagnetic case J<0. The critical point of this system known from the Onsager solution is $\frac{T_c}{J} = 2.27$.

The initial radius of the domain is taken to be 20 lattice constants in length. This is quite small compared to the size of the lattice which is a 100 x 100 square matrix. Periodic boundary conditions are used and the spins are flipped using the Glauber dynamics[7]. In this dynamics a spin is chosen at random and flipped, and the change in energy ΔE calculated. If this energy change is negative the new direction is retained. In case it is positive, we calculate the transition probability given by

$$W = \frac{1}{\tau} e^{- \Delta E/k_T}$$

where k is the Boltzman constant, T is the temperature and τ is a constant that sets the time scale. We take $\tau = 1$[5]. The transition probability W is compared with a random number r ($0 \leqslant r \leqslant 1$). If $W \geqslant r$ the flip is allowed otherwise the old direction is retained.

For the calculation of the "spatial entropy" an average over several runs is performed. An average over 40 runs is taken for T = 0.9 and 0.7 T_c while an average over 20 runs is taken for T = 0.6 and 0.4 T_c.

RESULTS AND DISCUSSION

In Fig. 1 we plot $A(t)/A_0$ as a function of t/A_0 . It is seen that the slope $\alpha(T)$ decreases almost linearly with time. This is in agreement with the results of Sahni et al.[5]. In Fig. 2a we show the time evolution of the change in "spatial entropy" during the initial period of evolution (t<20 Monte Carlo cycles) and in Fig. 2b we reproduce the same for later times. The following points are to be noted:

(i) The rate of change of "spatial entropy" is different for different temperatures during the initial period of evolution ($t \lesssim 10$ M.C. cycles). The change being greater for the higher temperatures.

(ii) For times greater than about 10 M.C. cycles the rate of change of "spatial entropy" is almost the same for the four temperatures chosen.

We conclude that most of the roughening is achieved during the initial period (t <10 M.C. cycles). The roughening being greater for higher temperatures. This is in agreement with Sahnis' snapshot displays, which show that for $T \leqslant 0.5$ T_c the circular domains remain essentially circular throughout the evolution, whereas for $T \gtrsim 0.8$ T_c thermal fluctuations are so strong that the domain becomes extremely wavy in less than 10 Monte Carlo cycles.

For $t > 10$ Monte Carlo cycles we can express the "spatial entropy" at time t by the relation

$$S(t) = S_0 + Bt \qquad \text{for } t > 10 \text{ M.C. cycles} .$$

Here B is a constant independent of temperature. This suggests that the roughening of the domain proceeds at essentially the same rate for all temperatures and for $t > 10$ Monte Carlo cycles. The entropy will achieve the maximum value when the entire domain is completely disordered. The higher the temperature the earlier will be the approach to saturation. This is in sharp contrast to the fact that the rate of change of area is different for temperatures $T \geq 0.5\ T_c$.

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FIGURE CAPTIONS

Fig. 1. The normalized area $A(t)/A_0$ vs. t/A_0 for different temperatures.

Fig. 2a. The change in "spatial entropy" vs. time for the initial period.

Fig. 2b. The change in "spatial entropy" vs. time for later times.

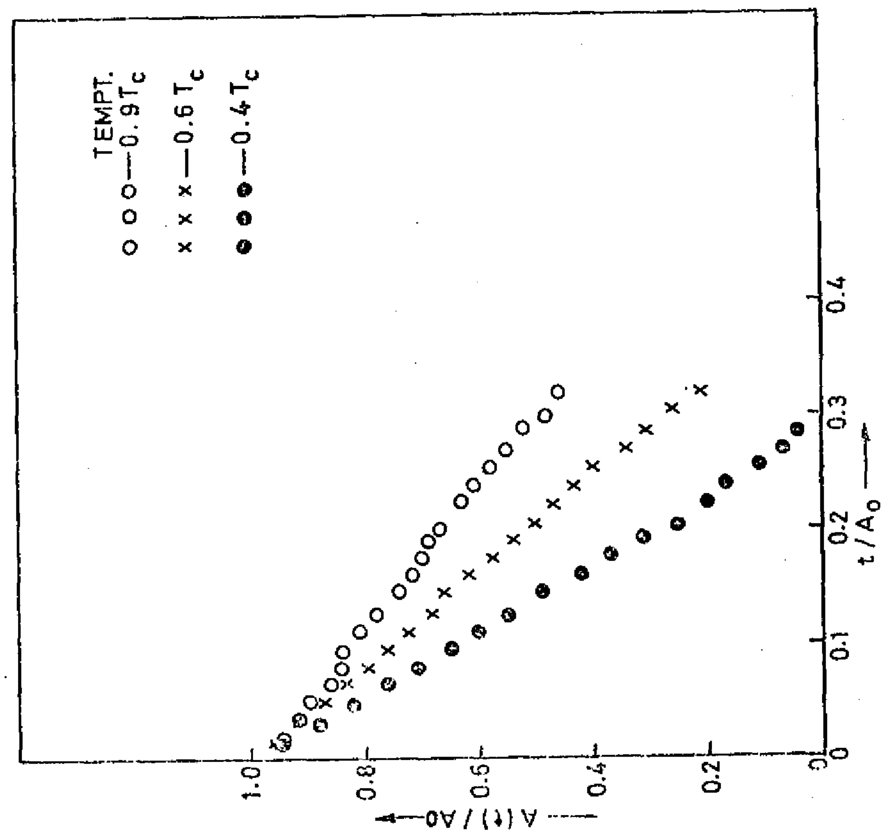

Fig. 1.

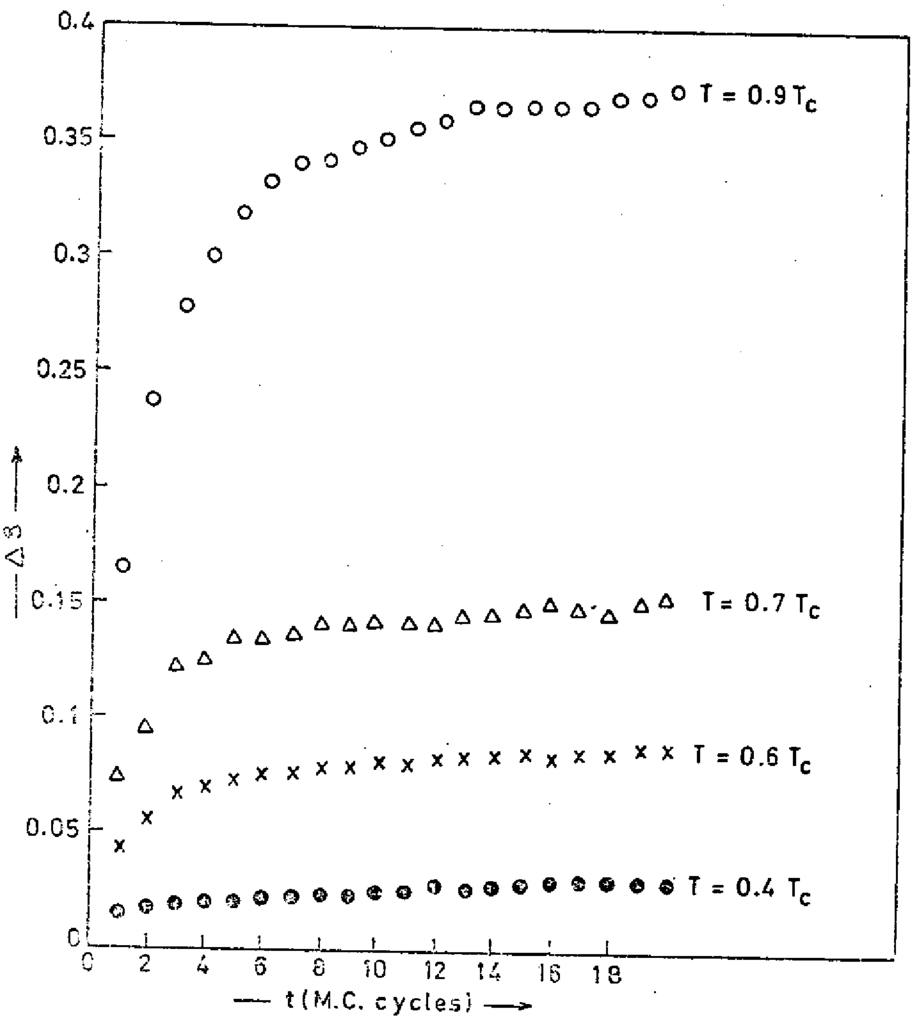
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
Δ 9
0 2 4 6 8 10 12 14 16 18
t (M.C. cycles)
T = 0.9 T_c
T = 0.7 T_c
T = 0.6 T_c
T = 0.4 T_c

Fig. 2a.

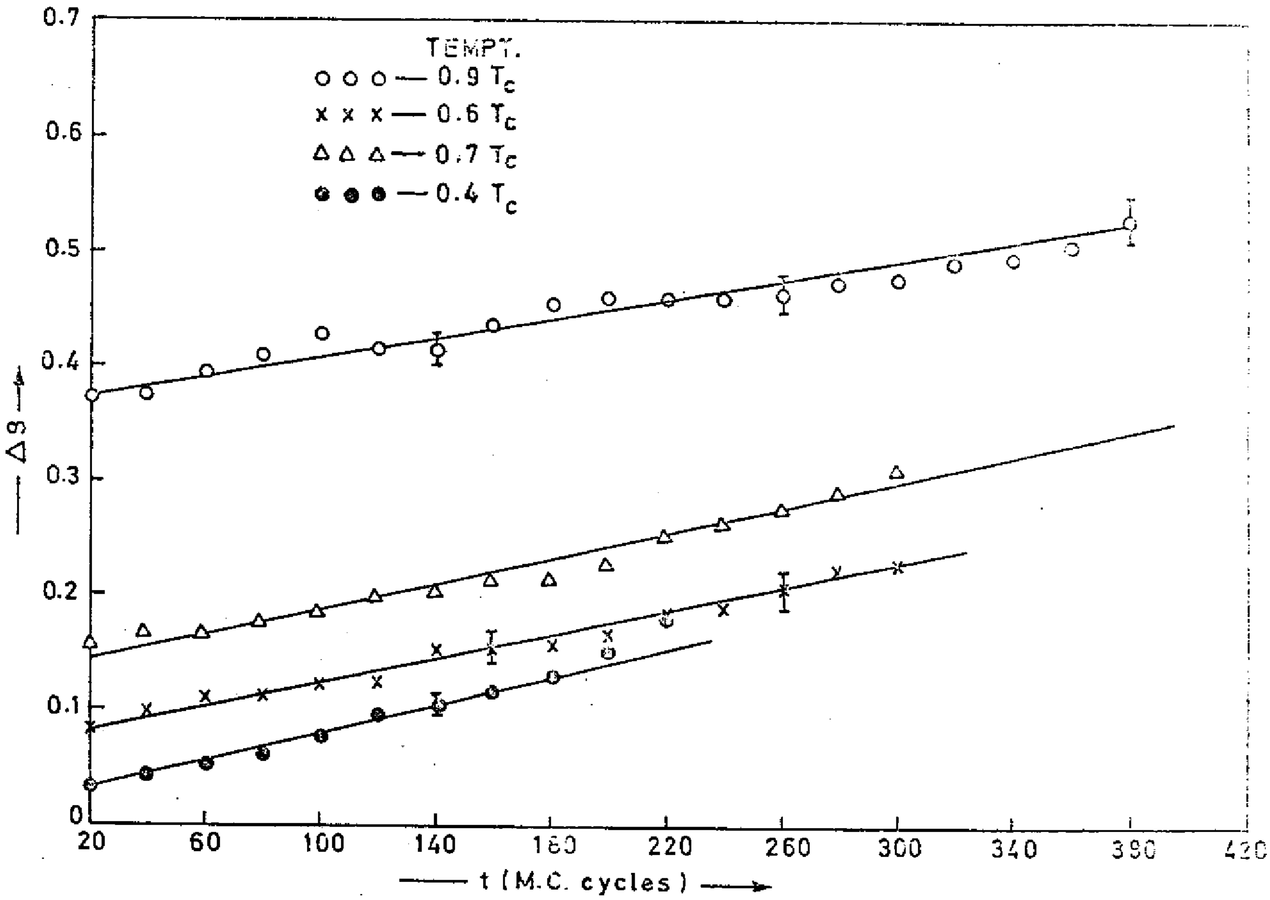
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Δ 9
20 60 100 140 180 220 260 300 340 380 420
t (M.C. cycles)
TEMPT.
— 0.9 T_c
— 0.6 T_c
— 0.7 T_c
— 0.4 T_c

Fig. 2b.

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