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Computer simulations of discommensuration patterns

Yoshihisa Enomoto and Kiyoaki Araki
Department of Physics, Faculty of Science, Nagoya University, Nagoya 464-01, Japan

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Abstract. We study the dynamical behaviour of discommensuration patterns that have been observed in commensurate–incommensurate phase transitions. Using a method based on a phenomenological dynamics model proposed by Enomoto and Kato, two-dimensional simulations are performed to discuss the time evolution of the model system towards equilibrium states from the initial disordered state.

The dynamics of discommensurations (DC) plays an important role in commensurate–incommensurate (C–IC) phase transitions (for a review, see [1]). Discommensurations are interfaces that separate commensurate domains. The DC patterns have been observed in electron microscopic studies of charge-density waves in 2H-$TaSe_2$ [2], superconducting Bi–Ca–Sr–Cu–O [3] and long-period superlattices of A_3B-type alloys with $L1_2$ structure like Ag–Mg and Au–Zn [4]. In these systems the spatial patterns of the structure have been found to exhibit fascinating time-dependent behaviour and also to affect various thermal and dielectric properties.

Interesting developments in the study of the C–IC transitions are their theoretical interpretations in terms of 'stripples' and the soliton picture of incommensurate phases [1, 5]. No dynamical theory of these fascinating phenomena appears to exist, except for an interfacial approach to the motion of DC [6] and the molecular dynamics simulations [7]. However, the time-dependent behaviour of the system discussed below has not yet been investigated.

Recently we have proposed the dynamical model equation [8] for the C–IC transition using the phenomenological free energy [9], and performed two-dimensional simulations of the model system. This model has been found to yield experimentally the observed typical evolution patterns, although we consider the case in which only one type of DC is involved and also ignore interlayer couplings as is required for real materials. Moreover, we have found that, starting from the initially disordered state, the system gradually reaches an equilibrium state, which is characterized by the number of DC, via the intersections and recombinations of the DC and stripples. However, these simulations were inadequate to study long-time behaviour, such as the growth law for the average ordered domain size. Thus, the purpose of the present work is to perform a long-time simulation with a large system size. In particular, simulating the model system from the initially disordered state, we study the time evolution of the system towards equilibrium states by changing the magnitude of the misfit, defined below.

Let us consider the spatial modulation described by a complex scalar field

$$g(\boldsymbol{r},t) \equiv F(\boldsymbol{r},t)\exp[\mathrm{i}S(\boldsymbol{r},t)]$$

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at position r and time t. Here F ($\geqslant 0$) and S are the amplitude and phase variables, respectively. The coarse-grained free energy functional $G[g]$ of the system considered here is taken to be [9]

$$G[g] \equiv \int \mathrm{d}r \, \{|(\nabla - \mathrm{i}\delta)g|^2 + w[g]\} \tag{1}$$

with

$$w[g] \equiv -|g|^2 + \tfrac{1}{2}|g|^4 - \tfrac{1}{2}v(g^p + g^{*p}) \tag{2}$$

$$= -F^2 + \tfrac{1}{2}F^4 - vF^p \cos(pS) \tag{3}$$

where p is a positive integer, which denotes the number of different commensurate domains (for example, $p = 3$ for the charge-density wave (CDW) states in 2H-$TaSe_2$), δ is a misfit vector, and g^* denotes the complex conjugate of g. Here the p ordered commensurate phases are characterized by spatially uniform states $(F(r,t), S(r,t)) = (F_e, S_j)$ for $j = 0, 1, \ldots, p-1$ with [10, 11]

$$\delta \cdot \delta - 1 + F_e^2 - \tfrac{1}{2}vpF_e^{p-2} = 0 \tag{4}$$

$$S_j = (2\pi/p)j. \tag{5}$$

Moreover, we have assumed that the dynamics can be described by the following equation for $g(r,t)$ as [8]

$$(\partial/\partial t)g(r,t) \equiv -L \, \partial G/\partial g^* \tag{6}$$

which gives

$$(\partial/\partial t)g(r,t) = L[\nabla^2 g - 2\mathrm{i}\delta \cdot \nabla g + g(1 - |g|^2 - \delta \cdot \delta) + \tfrac{1}{2}vpg^{*p-1}] \tag{7}$$

where L is a positive constant. This model is the continuum version of the kinetic p-state vector Potts model involving the misfit vector δ. Note that in the present phenomenological model changing the magnitude of the misfit might correspond to changing the temperature. However, at the present stage, we do not discuss the relationship between them any more. Notice also that within the present model nucleation cannot be dealt with, since we have neglected the thermal noise.

Before carrying out computer simulations, we comment on the ground state of the present model as a function of δ with $\delta = (\delta, 0)$. By the analogy of [1], the ground state of incommensurate phases exhibited by this sytem is described in terms of the DC line lattices, where the flat DC lines are regularly arranged along the x direction with average spacing z. The free energy density of such a DC lattice system, $f(z,\delta)$, is given by [9, 11, 12]

$$f(z,\delta) = (\bar{\sigma}/z) + 4(\sigma/z)\exp(-z/\xi) \tag{8}$$

with

$$\sigma \equiv 2v_e^{1/2}F_e^2/p \tag{9}$$

$$\bar{\sigma} \equiv \sigma - (2\pi/p)F_e^2\delta \equiv (2\pi/p)F_e^2(\delta_c - \delta) \tag{10}$$

$$\delta_c \equiv (p/2\pi)\sigma/F_e^2 \tag{11}$$

$$v_e \equiv \tfrac{1}{2}vF_e^{p-2} \tag{12}$$

where σ is the isolated DC energy per unit length in the absence of misfit, $\xi \equiv (pv_e)^{-1/2}$ is the width of a DC line, and δ_c is the value of δ at the transition to the commensurate phase. In obtaining the above expression for $f(z,\delta)$, we have assumed that all the parameters in the system, except for the misfit δ, are taken to be fixed and also have omitted unimportant parts like the DC wandering [11]. Then, the ground state of the present model is determined by minimizing equation (8) with respect to z. Therefore, we have approximately the equilibrium value of z, denoted as z_e, for $\delta > \delta_c$,

$$z_e/\xi \simeq -\ln[(\pi/4v_e^{1/2})(\delta - \delta_c)] \tag{13}$$

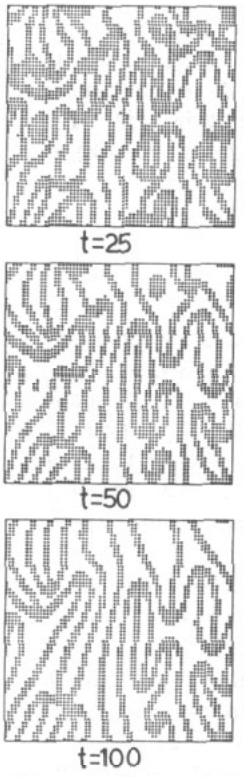
which is similar to the well known mean-field result [1]. This is understood as follows. In general, the late-stage dynamics of the dissipative systems described by complex order parameters, like in the present model, is known to be dominated by slow variations of the phase variable of the order parameter [11]. Thus, the essence of the present model in the late stage becomes similar to that of the model discussed in [1]. On the other hand, for $\delta < \delta_c$ regularly arranged DC lattices cannot exist stably. Thus an equilibrium state in this case is a spatially homogeneous state with $(F(r,t), S(r,t)) = (F_e, S_j)$ where the value of j is fixed to a certain constant for the whole space, which depends on the initial conditions. In fact, from recent computer simulations [13] we have found that the system for $\delta < \delta_c$ gradually approaches such an equilibrium state via the annihilation of vertices.

Now we carry out two-dimensional computer simulations of the above equation on an $N_x \times N_y$ square lattice with periodic boundary conditions by changing the magnitude of the misfit. In the following, we set $p = 3$ and $\delta = (\delta, 0)$. To obtain a single positive solution of equation (4), we must restrict ourselves to the case with $0 \leqslant \delta < 1$. In this case we have

$$F_e = \tfrac{3}{4}v + \left(\tfrac{9}{16}v^2 + 1 - \delta^2\right)^{1/2}.$$

Moreover, in the present simulations we use the simple Euler method with the time step $\Delta t = 0.05$, lattice spacing $\Delta x = \Delta y = 1$, $L = 1$ and $v = 0.2/3$. Note that to solve equation (7) numerically, it is convenient to use two real fields, A and B, defined by $g(r,t) \equiv A(r,t) + iB(r,t)$, rather than the amplitude and phase variables of $g(r,t)$. Initially at each lattice site both real fields, A and B, are chosen to be a Gaussian random number with average 0 and variance 0.01, which represents the disordered state with random noise. Note also that we have examined the other parameter values, and the results below do not change qualitatively.

The evolution patterns are shown in figure 1 for $N_x = N_y = 64$ and $\delta = 0.15$. In the present and following figures we plot a dot on each disordered lattice site. Here the disordered lattice is characterized by the site with $F(r,t) < 0.975F_e$ or $|S(r,t) - S_j| > \pi/12$ with $j = 0, 1, 2$, which is thought to denote positions of DC lines and their vertices. In this figure we can see the intersections and recombination of the DC and stripples, which exhibit striking similarity to the experimentally observed DC patterns [2–4]. In figure 2 we show the DC structures at time $t = 200$ for various values of δ. The results of figures 1 and 2 are all obtained from the same initial configuration. From these figures we find that a tiny change of the misfit magnitude δ completely changes the dynamical behaviour of the system. This is understood as follows. Adopting the soliton picture of an incommensurate phase for $\delta > \delta_c$ ($\simeq$



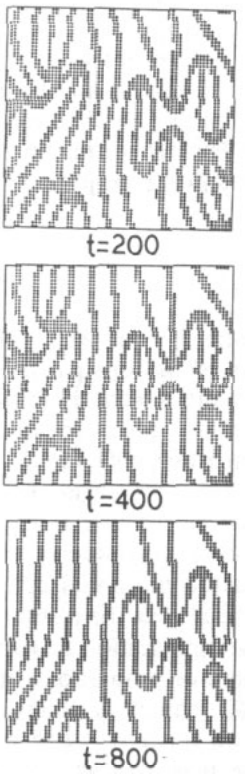


Figure 1. Time evolution of DC patterns for $\delta = 0.15$ at various times.

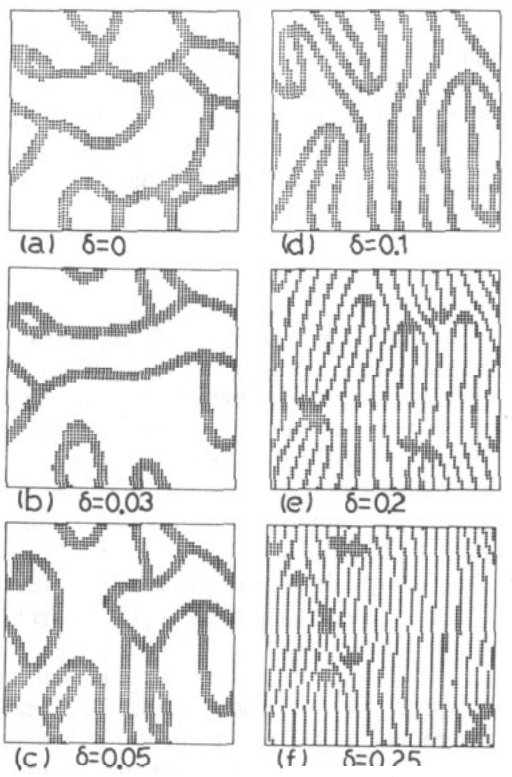


Figure 2. DC patterns at $t = 200$ for $\delta = 0$ (*a*), 0.03 (*b*), 0.05 (*c*), 0.1 (*d*), 0.2 (*e*) and 0.25 (*f*).

0.058 in this case) [1, 11], equilibrium states with different values of δ correspond to different numbers of solitons. On the other hand, for $\delta < \delta_c$ there are no flat DC lattices, which are not stable in this case.

Now we discuss the time-dependent behaviour of the system. For this purpose we simulate the model using a 256 × 256 square lattice. Moreover, the following results are obtained by averaging over 50 independent simulation runs. In figure 3 we show the time evolution of the average size of the ordered commensurate domains, $\bar{z}(t)$, for different values of δ. Here $\bar{z}(t)$ is roughly evaluated from [14]

$$\bar{z}(t) \equiv \frac{1}{N_y} \sum_{i=1}^{N_y} \frac{N_x \, \Delta x}{N(i)} \tag{14}$$

where $N(i)$ denotes the number of the DC lines in the ith row along the x axis. From this figure we find that for various values of δ the average size $\bar{z}(t)$ grows with time as

$$\bar{z}(t) = \nu \log_{10} t \qquad \text{for } t_0 < t < t_1 \tag{15}$$

but the coefficient ν in equation (15) depends on the value of δ. We have checked that $t_0 \simeq 10$, and $t_1 \simeq 1000$ for $\delta = 0.1$ and $t_1 \simeq 1000$ for $\delta = 1.0$. The

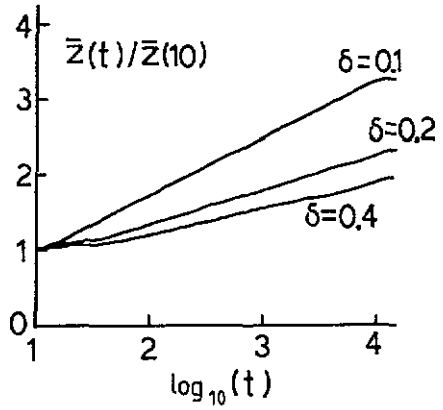


Figure 3. Time evolutions of the average ordered domain size $\bar{z}(t)/\bar{z}(10)$, against $\log_{10} t$ for different values of δ.

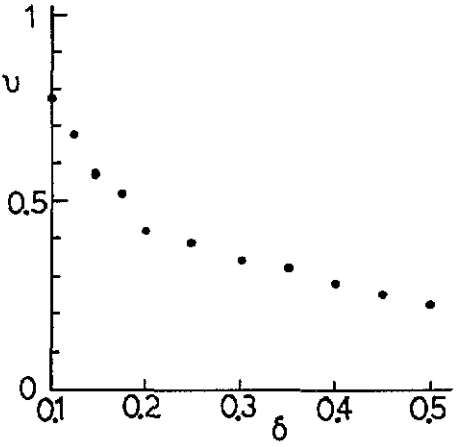


Figure 4. Variation of ν in equation (15) as a function of δ.

time region for $t < t_0$ corresponds to the initial transient regime where no DC appears, while for $t > t_1$, $\bar{z}(t)$ almost becomes constant and thus the system may be interpreted as reaching equilibrium states. We have numerically checked that for $t > t_1$, $\bar{z}(t)$ is almost consistent with z_e, defined in equation (13) as a function of δ ($> \delta_c$). In figure 4 we show the values of ν as a function of δ ($> \delta_c$). It is found that decreasing the misfit magnitude δ causes acceleration of the ordering process. This is understood as follows. The undulations of the flat DC lines have the effect of speeding up the ordering process, since these are still triggered by DC line annihilations due to attractive interactions between ordered commensurate domains with the same equilibrium phase value S_j defined by equation (5). These results are similar to those of a quasi-one-dimensional simulation for layered Ising magnets [14], where the strength of anisotropy corresponds to the misfit magnitude discussed here.

Finally we comment on the crossover of the above growth law of the average ordered domain size. Instead of the logarithmic growth law obtained here, we have obtained the $\frac{1}{2}$-power growth law for the case $\delta = 0$ [13, 15]. Thus, there must exist a crossover of the growth law at a certain value of δ. We have numerically checked that in the present simulation such a crossover occurs at $\delta \simeq 0.07$, which is comparable with the value of δ_c, defined in equation (11) ($\delta_c = 0.058$ in this case). As was discussed before, the difference between the asymptotic growth laws for these two cases is thought to be due to the difference between the equilibrium states and also the corresponding dominant dynamics in the late stage of the respective cases. In fact, for $\delta > \delta_c$ the late-stage dynamics is dominated by the intersections and recombinations of the DC and stripples, while for $\delta < \delta_c$ it is dominated by the annihilations of the vertices. To check the validity of the above results, as well as to examine the difference between the cases with $|\delta| < \delta_c$ and $|\delta| > \delta_c$ in detail, we need to calculate the scattering structure functions.

In summary, we have performed two-dimensional computer simulations of DC patterns and have studied the asymptotic growth law of the average ordered domain

size. For the case of $p = 3$, we have found that the ordering process with weak misfit (but $\delta > 0.07$) goes on faster than that with strong misfit, but for both cases the average sizes vary logarithmically in time for the late stage. On the other hand, for $\delta < 0.07$ the average sizes vary as $t^{1/2}$, which is consistent with the results of [13]. The scaling behaviour of the scattering structure function and effects of temperature, as well as the p dependence of the above results, are interesting problems and still remain to be studied.

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