Notes

Annealing Method for Modeling Liquid Crystal Textures

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Introduction

The texture of liquid crystalline polymer samples, observed, for example, by optical microscopy between crossed polars, gives information on the characteristic spatial distribution of the local directors in these self-orienting materials. The interpretation of these textures may be aided by models that simulate texture formation.[1,2]

Recently, Bedford *et al.*[2,3] proposed a simple lattice model for textures in liquid crystals, where the lattice site simply indicates a region of uniform director orientation that may include many chains. In their method, they minimized the total energy of the system by repeatedly selecting lattice sites at random and minimizing the energy of the sites. The minimization process for a multivariable function sometimes has difficulty in finding the global minimum because the process becomes trapped in one of numerous local minima. An "uphill" mechanism, such as is employed in Monte Carlo methods, might be useful for getting out of a local minimum, but it would require lengthy computation. In this paper, we introduce a rapid method of minimization in which selection of lattice sites is not random but instead proceeds from the fixed boundary toward the inside of the system. The method can bring the system to a lower energy state with shorter computational time. The idea employed in this method is useful for both polymeric and low molecular weight liquid crystal systems if an appropriate interaction energy is chosen.[2]

Bedford *et al.*[3] applied their method to two- and three-dimensional (2D and 3D) systems. They described their algorithm for the 2D system in some detail but not that for the 3D system. Although the extension to 3D seems straightforward, some modification is required. In this paper, we describe briefly the 3D algorithm. The algorithm presented here is basically that of Bedford *et al.*,[3] but the details may be different.

Algorithm for a Three-Dimensional System

We use a cubic lattice model in which the director vector $\mathbf{n}_k$ with unit length at lattice site k interacts with six adjacent director vectors to give the interaction energy

$$E_k = \sum_{k'} \sin^2 \Psi_{kk'} \tag{1}$$

where k' runs over six adjacent cells and $\Psi_{kk'}$ indicates the angle formed by $\mathbf{n}_k$ and $\mathbf{n}_{k'}$. Equation 1 is rewritten as

$$E_k = \sum_{k'} |\mathbf{n}_k - \mathbf{n}_{k'}|^2 \tag{2}$$

with the truncation of the quadratic term in $|\mathbf{n}_k - \mathbf{n}_{k'}|$. This approximation may be acceptable, as it was for the 2D algorithm,[3] as long as the difference between the adjacent director vectors is not too great. If we express the director vector in terms of local Cartesian coordinates embedded in each lattice site, eq 2 becomes

$$E_k = \sum_{k'} \{(x_k - x_{k'})^2 + (y_k - y_{k'})^2 + (z_k - z_{k'})^2\} \tag{3}$$

Using Lagrange's method of undetermined multipliers, the minimum of eq 3, under the restriction $|\mathbf{n}_k| = 1$, is given as

$$E_k^{\min} = 2(m - R) \tag{4}$$

by substituting the following values into eq 3

$$x_k = \sum_{k'} x_{k'}/R, \quad y_k = \sum_{k'} y_{k'}/R, \quad z_k = \sum_{k'} z_{k'}/R$$

with

$$R = [(\sum_{k'} x_{k'})^2 + (\sum_{k'} y_{k'})^2 + (\sum_{k'} z_{k'})^2]^{1/2} \tag{5}$$

Here, m is the number of adjacent lattice sites. Due to the π redundancy of the director vector ($\mathbf{n}$ is equivalent to $-\mathbf{n}$), the length of R may take 2^{m-1} different values. Therefore, the true minimum is attained by choosing that combination of redundant orientations that makes R a maximum. This 3D algorithm is readily applied to 2D systems. It should be noted that the minimizing operation given by eq 5 will not change the value (x_k, y_k, z_k) for every k when the system is in a minimum.

Annealing Method

The repetition of a random hit of a lattice site k and the minimization of the energy E_k of the site is regarded as the minimization of the total energy E ($=\sum_k E_k/2$) because $\partial E/\partial \mathbf{n}_k = \partial E_k/\partial \mathbf{n}_k$. However, minimizing this multivariable function is difficult because of a number of local minima. Even for a small 2D system with $n=2$ under the $s=1/2$ type boundary condition, where s stands for the strength of disclination, we find five configurations which are in local minima. Among these, the $s=1/2$ disclination pattern gives the lowest energy. For small systems such as the one above, it might be possible to list all the local minima and determine the global minimum. For larger systems, however, this is actually impossible because of the vast number of local minima.

We then try to find a local minimum with as low an energy as possible, hopefully the lowest energy. The procedure of random hits applied to an initial random configuration is not efficient. It usually ends up with a multidomain structure with a higher energy; due to the orientational fluctuation present in the initial random configuration, some small regions in the system may act as seeds for the subsequent growth of local ordered structures. In this respect, this procedure might be called a *quenching method*. Instead, we introduce an *annealing method* which is simple and analogous to the physical process of annealing. Selection of lattice sites is not done randomly but starts from the fixed boundary and moves toward the inside of the system. This corresponds to a

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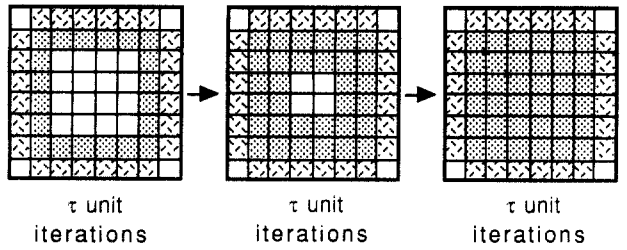

Figure 1. Diagram of the *annealing* method. The shaded area indicates cells with the fixed boundary condition, and the dotted area indicates the target region. At each stage, τ unit iterations are applied to the dotted cells.

physical process in which the phase change proceeds inward from the boundary, prompted by the controlled gradient of physical parameters such as temperature, concentration, etc. By this method, the final energy is greatly reduced.

We define a unit iteration as the number of lattice sites in the target region, the region to be subjected to random hits. During a unit iteration, each lattice site in the target region undergoes one hit on average. The following procedure can be applied to an arbitrary initial configuration or to a system in which some pairs of boundaries are subject to the periodic boundary condition. First, the outermost lattice sites attached to the fixed boundary are chosen as the target region, followed by τ unit iterations. Then, the next outermost lattice sites are added to the previous target region, and the newly enlarged target region again undergoes τ unit iterations. The same procedure is repeated all the way to the center of the system, followed by a further τ unit iteration applied to the whole system (see Figure 1). The value of τ is usually set between 5 and 15.

In order to check the efficiency of the *annealing method*, we generate 20 initial random configurations in 2D and subject them to the *annealing method* for a fixed boundary condition of $s=2$ disclination strength. For the sake of comparison, we also subject the same initial configurations to the *quenching method*. For the 20 initial random configurations, the average energy is 505.7, with a standard deviation of 16.3. The *annealing method* gives an average energy of 36.3, with a standard deviation of 7.2, and the *quenching method* gives an average energy of 54.2, with a standard deviation of 9.0. The average for the *annealing method* is significantly lower than that for the *quenching method*. In Figure 2, the final texture pattern with the lowest total energy among 20 samples is shown for each of the methods. The pattern for the *annealing method* has a fairly large region of uniform alignment, reflecting lower energy. We notice that the former pattern has a great similarity to that obtained by a matrix method.[4] This indicates that both the *annealing* and matrix methods are capable of bringing the system to a comparably low energy level, although the former method is superior for the kinetic study of texture formation.

The *annealing method* is also efficient in 3D. We start with an initial 3D 18 × 18 × 18 lattice in a random

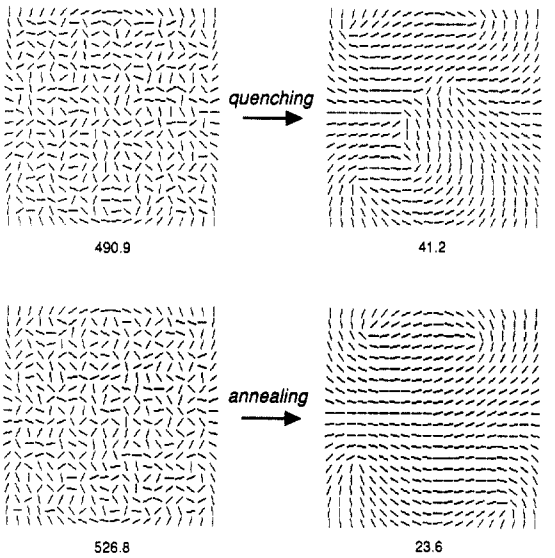

Figure 2. Comparison of the *annealing method* with the *quenching method* in 2D. The number below each pattern indicates the total energy evaluated from eq 4; the summation is performed over the whole system, including boundaries.

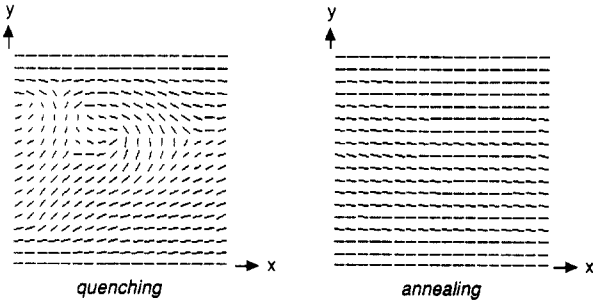

Figure 3. Comparison of the *annealing method* with the *quenching method* in 3D. Cross section at $z=10$.

configuration. Two boundaries perpendicular to the z axis are subject to fixed boundary conditions with their directors set parallel to the x direction. The other four faces of the cube are subject to the periodic boundary condition. The *annealing method* produces a uniform orientation parallel to the x direction throughout the system. The cross section at $z=10$ is shown in Figure 3, together with that for the *quenching method* for comparison.

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References and Notes

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