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Numerical Three Dimensional Relaxation of Liquid Crystal Director Fields

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We have written a FORTRAN program which minimizes the elastic free energy of a liquid crystal director field in three dimensions using the ordinary Oseen–Frank equations plus an additional (divergence) term. The novel features of this program are: (1) it allows for disclinations and (2) because of disclinations, directors are not connected globally but locally. This program was used to find minimum energy configurations for various models of the cholesteric blue phase.

INTRODUCTION

Finding a minimum energy configuration of a liquid crystal director field is a problem well suited for the computer. However, this kind of work has been limited mostly to problems in one dimension.[1-2] When the director varies with all three space variables, the problem becomes much more complex to solve. The main difficulty in three dimensional simulations is the limited amount of computer memory and slowness of computation. With access to a CRAY-1 computer,[3] these simulations now become more feasible to do in terms of time and money.

The recent interest in the cholesteric blue phases[4-10] has encouraged us to write a FORTRAN program which relaxes a given director field in three dimensions and calculates the elastic free energy density. This program was used to investigate the stability of three models of the blue phase. From these calculations the temperature range over which the models predict that the blue phase will exist has been determined. There is good agreement with other theoretical predictions.[11] However,

these results are not reported here since this paper is a qualitative discussion of the numerical method used.

The ordinary Oseen–Frank equations are used, including the divergence (K_{24}) term to obtain the minimum energy configuration. The Oseen–Frank expression for the free energy per unit volume is given by

$$F_1 = \frac{K_{11}}{2}(\nabla\cdot\mathbf{n})^2 + \frac{K_{22}}{2}(\mathbf{n}\cdot\nabla\times\mathbf{n} + q_0)^2 + \frac{K_{33}}{2}(\mathbf{n}\times\nabla\times\mathbf{n})^2 \quad (1)$$

where $\mathbf{n}$ is a unit vector representing the average orientation at a given point in space, q_0 is 2π over the pitch length and K_{11}, K_{22} and K_{33} are elastic constants corresponding to splay, twist and bend deformations respectively. The additional term[12] which is included is given by

$$F_2 = \frac{(K_{22} + K_{24})}{2}\nabla\cdot[(\mathbf{n}\cdot\nabla)\mathbf{n} - \mathbf{n}(\nabla\cdot\mathbf{n})]. \quad (2)$$

F_2 is a term which is usually discarded since it has the form of a divergence. From Gauss' theorem the volume integral of a divergence term can be transformed into a surface integral. For large samples the surface term can be neglected. However, if there are singularities in the sample volume, they must be excluded when doing the surface integral. The surface of each excluded volume contributes to the surface integral. Therefore for a given density of disclinations, the amount which is discarded is proportional to the volume. This additional term can make an important contribution to the free energy. The cholesteric blue phase is such a system which has a lattice of disclinations.

The program calculates the free energy density for a given initial director field and then relaxes the field by minimizing

$$\int dV(F_1 + F_2). \quad (3)$$

The exact algorithm of how this is done will be described later.

FREE ENERGY

An initial director field must be given to the program. This is analogous to a trial solution for a differential equation. A three dimensional array is used for storing the directors. This array corresponds to a unit cell with discrete mesh points. Directors are generated at the mesh points. The appendix describes in more detail what was done to generate the directors. To keep the problem simple the unit cell is divided into equal parts along the x, y and z axes. As the number of divisions is

increased, the number of storage locations goes up as the third power. One can easily see that limited memory capacity can become a handicap when choosing a fine mesh grid. Periodic boundary conditions are imposed on the faces of the unit cell by extending the mesh beyond the unit cell one step. This is done so that derivatives at the boundaries may be calculated. It should be pointed out that there is no fixed director configuration at the unit cell boundaries. The directors on the walls of the unit cell are allowed to relax freely to their equilibrium positions.

Once the directors have been generated throughout the unit cell the program starts by calculating the elastic energy in a particular mesh cube. This cube is illustrated in Figure 1. To compute the free energy density associated with this small cube a director is calculated at the center on each of the six faces of the cube. The simplest way to do this is to average the four directors on the corners of the particular face. However, before the averaging is done, it must be determined whether all the directors in the cube can be connected topologically. This problem occurs because the computer assigns a head to the director whereas in physical reality the liquid crystal itself does not care about heads and tails. The problem is illustrated in Figure 2. The two orientations (a) and (b) are energetically the same as far as the liquid crystal is concerned but very different when calculated on the computer. Therefore,

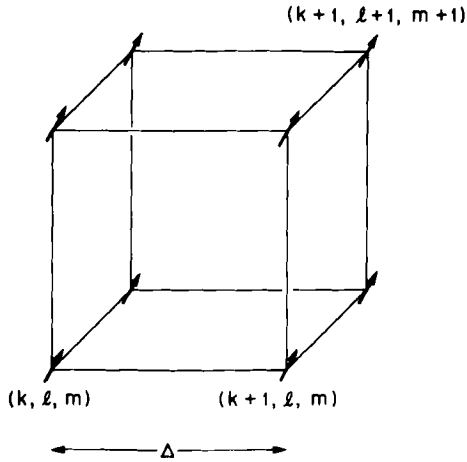

FIGURE 1 A mesh cube in the unit cell showing directors at corners. A director is generated at the center of each of the six faces by averaging the four directors adjacent to the particular face. The directors at the center of the faces are used in calculating energies and relaxation. The cube has sides of length Δ, where Δ is the unit cell size divided by the number of divisions. The program iterates the indices (k, l, m) from their minimum to maximum values, thus covering all the mesh cubes in the unit cell.

(a) (b)

FIGURE 2 Two representations for director configurations having the same energy. The arrows denote the heads which the computer assigns to the directors. The liquid crystal only cares what relative angle the molecules have between one another whereas the computer assigns an absolute angle. The program checks the dot product between the directors. If the result is negative, one director is flipped. If this were not done, higher estimates for the free energy would result.

to make sure that the directors in the cube can be connected in a head-to-head tail-to-tail fashion, the director which has the lowest x, y, z-indices is taken as the reference. The dot product of it with the seven other directors is computed. If the dot product is negative, the director at that particular corner is flipped. That is to say, the components of the director change sign. Once this is done, the program uses the flipped directors in the expression for the free energy described below.

To illustrate how the energy density is calculated for the cube the splay term is used as an example. The splay term is given by

$$\frac{K_{11}}{2}(\nabla\cdot\mathbf{n})^2. \tag{4}$$

To write this differential expression as a difference expression, a notation is introduced that indexes the directors relative to the lowest indexed director in the mesh cube. If the energy of a cube whose lowest indexed director is given by (k, l, m) is being calculated, Eq. (4) can be written

$$E_{k,l,m}(\text{splay}) = \frac{K_{11}}{2\Delta^2}\left[\sum_{b,c=0}^{1}(X_{1,b,c} - X_{0,b,c}) + \sum_{a,c=0}^{1}(Y_{a,1,c} - Y_{a,0,c}) + \sum_{a,b=0}^{1}(Z_{a,b,1} - Z_{a,b,0})\right]^2 \tag{5}$$

where $X_{a,b,c}$, $Y_{a,b,c}$ and $Z_{a,b,c}$ are the x, y, z-components of the director at $(k + a, l + b, m + c)$ and Δ is the distance over which the derivative is calculated. Since the program divides the lengths of the unit cell up into equal mesh points, this allows the Δ^2 to be factored outside the brackets. If the expression inside the summation sign is written out one can see this is just the average director on one face minus the average director on the opposite face. This quantity is the change in orientation of the director over the distance Δ. The two faces are planes perpen-

dicular to the direction along which the derivative is being calculated. Energy expressions for twist, bend and the K_{24} term are computed in a similar fashion. The indices (k, l, m) are then iterated from their minimum to maximum values and the corresponding energies at each cube are stored and summed.

DISCLINATIONS

One of the difficulties with three dimensional problems is how to handle disclinations. Disclinations are discontinuities in the director field and are analagous to dislocations in crystals. As one approaches the center of a disclination things tend to blow up. What has been done essentially is to construct a region around the disclinations in our unit cell and take this region containing the disclination as an isotropic material. This volume is excluded in calculating energies and relaxing the directors throughout the unit cell, that is to say, the core exerts no orienting torque on the outside material.

The user must tell the program where the disclinations occur in the unit cell. This problem was solved by setting up a three dimensional logical array. Each logical element has a corresponding small cube in the unit cell. If the disclination line goes through the volume occupied by a small cube, a "false" value is generated in the logical array at the point corresponding to the small cube. When the energy is calculated the program first checks the cube's truth value to see whether any of its eight corners lie on a disclination. If a false value is found, the program returns zero free energy for that particular cube. This method essentially corresponds to making an isotropic volume around the disclination with a radius roughly $r_d \approx D/N$ where D is the length of the unit cell and N is the number of divisions on each axis. As the number of mesh points is increased, the radius of this excluded volume decreases for a given unit cell size.

It should be pointed out that one must start out with the right topology of the director field. For example, following the director on a closed path around a $(-\frac{1}{2})$ disclination, the director is found pointing in the opposite direction upon returning to the starting point. The starting field of the computation must satisfy all the topological properties of the model. The relaxation process does not change the topology; i.e. disclinations stay where they are originally located and do not disappear. The program is not smart enough to find other structures.

RELAXATION

Once the free energy for a small cube has been calculated, the program then relaxes the director at (k, l, m). This is done by computing the change in energy as a function of change in the director components. The derivatives are then used in the following expressions:

$$\Delta X = \frac{f}{K_{\text{avg}}}\left\{-\frac{\partial E}{\partial X} + \left[X\left(X\frac{\partial E}{\partial X} + Y\frac{\partial E}{\partial Y} + Z\frac{\partial E}{\partial Z}\right)\right]\right\}$$

$$\Delta Y = \frac{f}{K_{\text{avg}}}\left\{-\frac{\partial E}{\partial Y} + \left[Y\left(X\frac{\partial E}{\partial X} + Y\frac{\partial E}{\partial Y} + Z\frac{\partial E}{\partial Z}\right)\right]\right\}$$

$$\Delta Z = \frac{f}{K_{\text{avg}}}\left\{-\frac{\partial E}{\partial Z} + \left[Z\left(X\frac{\partial E}{\partial X} + Y\frac{\partial E}{\partial Y} + Z\frac{\partial E}{\partial Z}\right)\right]\right\} \quad (6)$$

where f is a parameter which controls the rate of relaxation and K_{avg} is an average value for the elastic constants. The result $(\Delta X, \Delta Y, \Delta Z)$ tells the program how much and in which direction to move the director to reduce the free energy. The quantity inside the square brackets in the above expressions is the result of introducing Lagrange multipliers. It can be shown that the vector $(\Delta X, \Delta Y, \Delta Z)$ is orthogonal to (X, Y, Z), i.e. the director being relaxed. This keeps the magnitude of the director unity to first order. The relaxed directors are always renormalized after each relaxation to keep higher order variations in the magnitude from accumulating.

In Figure 3 the method for calculating the energy derivatives used in Eqs. (6) is illustrated. The splay term will be used again as an example. A volume of eight small cubes is taken around the director at (k, l, m). In each of the eight cubes energy derivatives are calculated with respect to the director components at (k, l, m). In cube A this corresponds to the derivative with respect to the components which have the lowest indices. Using notation as in Eq. (5), this can be written as

$$\frac{\partial E_{k,l,m}(\text{splay})}{\partial X_{000}} = -\frac{K_{11}}{\Delta^2}\left[\sum_{b,c=0}^{1}(X_{1,b,c} - X_{0,b,c}) + \sum_{a,c=0}^{1}(Y_{a,1,c} - Y_{a,0,c}) + \sum_{a,b=0}^{1}(Z_{a,b,1} - Z_{a,b,0})\right]. \quad (7)$$

One notices that in this case the derivatives with respect to Y_{000} and Z_{000} are the same expression as Eq. (7).

After the derivatives with respect to all the components have been

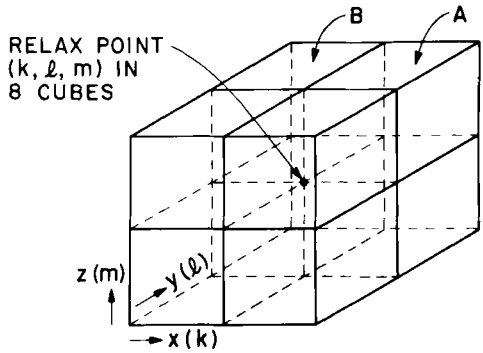

FIGURE 3 Illustration showing the eight cubes used to relax the director at (k, l, m). Cube A would be the cube used for calculating the energy only. As with the energy, directors are generated on the faces of the eight cubes. This results in 36 directors being generated.

calculated, the program then proceeds to the next cube out of the eight. To illustrate what happens, the cube marked B in Figure 3 will be used. In this case the meanings of the indices of the director components change. If cube B is taken as our reference, to relax the director at (k, l, m), the derivatives with respect to X_{100}, Y_{100} and Z_{100} must be calculated. This is because of the convention for calculating energies. Cube B represents the energy at $(k-1, l, m)$. Therefore we have

$$\frac{\partial E_{k-1,l,m}(\text{splay})}{\partial X_{100}} = \frac{K_{11}}{\Delta^2}\left[\ \right] \tag{8}$$

where the expression inside the brackets is the same as in Eq. (7). The program then iterates over the remaining cubes in the group of eight. As with the energy routine, each of the eight cubes is checked to see if they lie on a disclination line. If a disclination is found, the contribution from that cube in relaxing the director at (k, l, m) is set to zero.

After the derivatives from the eight cubes are calculated, they are summed and stored. Using Eqs. (6), the director at (k, l, m) is relaxed partially to its equilibrium position using a trial value of f, usually 0.1. The reason for relaxing the director partially is that if the relaxation is too rapid instabilities would develop. The appearance of instabilities results in an increase in the calculated energy. When this happens, the value of f is halved and the relaxation continues with the new value. It should also be noted that the relaxed directors are stored in a separate array. This is because if one is relaxing a mix of relaxed and unrelaxed directors instabilities could also develop. When all the directors in the

unit cell have been relaxed the new values for the directors are substituted into the original array. Energy calculations and relaxation then begin on the new values.

Execution halts in either one of two ways. The first condition resulting in termination is if the program relaxes all the directors *nmax* times (where *nmax* is the maximum number of relaxation iterations specified). It has been found empirically that on the average, the optimum value for *nmax* is 20. The second condition is a given number of reductions of the parameter *f*. This indicates that the program has found an unstable solution.

RESULTS

Figure 4 shows the output of a typical run on a CRAY-1 computer. This data is for a model of the blue phase having O^8 symmetry, a cell size of 1.5×10^{-5} cm, a pitch of -2.5×10^{-5} cm and mesh number of 24. The sign of the pitch depends upon whether one has left-handed or right-handed twist. The elastic constants K_{11}, K_{22} and K_{33} are read in to the program. K_{24} is calculated using the following expression[12]

$$K_{24} = \frac{(K_{11} - K_{22})}{2}.$$

The total energy which is the sum of the splay, twist, bend and K_{24} en-

cell size= 0.150000E-04cm, ndiv= 24
k11= .10000E-06 k22= .50000E-07 k33= .10000E-06 k24= .25000E-07

	tot. energy	splay	twist	bend	k24 term	f
0	0.10980E+03	0.11698E+04	0.78777E+03	0.11420E+04	-0.29898E+04	0.100000
1	0.64839E+02	0.11300E+04	0.79328E+03	0.11461E+04	-0.30045E+04	0.100000
2	0.47113E+02	0.11109E+04	0.79800E+03	0.11527E+04	-0.30144E+04	0.100000
3	0.36415E+02	0.10969E+04	0.80220E+03	0.11590E+04	-0.30217E+04	0.100000
4	0.28908E+02	0.10859E+04	0.80603E+03	0.11644E+04	-0.30274E+04	0.100000
5	0.23178E+02	0.10767E+04	0.80954E+03	0.11690E+04	-0.30320E+04	0.100000
6	0.18563E+02	0.10687E+04	0.81278E+03	0.11729E+04	-0.30358E+04	0.100000
7	0.14712E+02	0.10616E+04	0.81581E+03	0.11763E+04	-0.30390E+04	0.100000
8	0.11413E+02	0.10551E+04	0.81865E+03	0.11794E+04	-0.30418E+04	0.100000
9	0.85344E+01	0.10492E+04	0.82133E+03	0.11821E+04	-0.30441E+04	0.100000
10	0.59853E+01	0.10437E+04	0.82387E+03	0.11846E+04	-0.30461E+04	0.100000
11	0.37022E+01	0.10385E+04	0.82627E+03	0.11868E+04	-0.30478E+04	0.100000
12	0.16387E+01	0.10337E+04	0.82856E+03	0.11888E+04	-0.30494E+04	0.100000
13	-0.24034E+00	0.10291E+04	0.83072E+03	0.11906E+04	-0.30507E+04	0.100000
14	-0.19619E+01	0.10249E+04	0.83277E+03	0.11923E+04	-0.30518E+04	0.100000
15	-0.35471E+01	0.10208E+04	0.83472E+03	0.11938E+04	-0.30529E+04	0.100000
16	-0.50129E+01	0.10170E+04	0.83656E+03	0.11952E+04	-0.30537E+04	0.100000
17	-0.63730E+01	0.10134E+04	0.83831E+03	0.11964E+04	-0.30545E+04	0.100000
18	-0.76388E+01	0.10100E+04	0.83996E+03	0.11976E+04	-0.30552E+04	0.100000
19	-0.88195E+01	0.10068E+04	0.84153E+03	0.11986E+04	-0.30558E+04	0.100000
20	-0.99231E+01	0.10038E+04	0.84300E+03	0.11996E+04	-0.30563E+04	0.100000

FIGURE 4 Printout of a relaxation run on a CRAY-1 computer. Energies are in ergs/cm^3. The parameter *f* (telling what fraction to relax the directors to their equilibrium position) remains the same since after each relaxation the total energy is lower than the previous value.

ergies decreases rapidly at the beginning. This corresponds to short wavelength modes being damped out. After the seventh or eighth iteration the relaxation proceeds at a slower rate. These are low frequency modes which take a long time to decay. The total energy does not contain the energy from the core regions of the disclinations. This must be calculated separately by hand.[13]

In Figure 5 results for a series of runs are plotted. This is for a blue

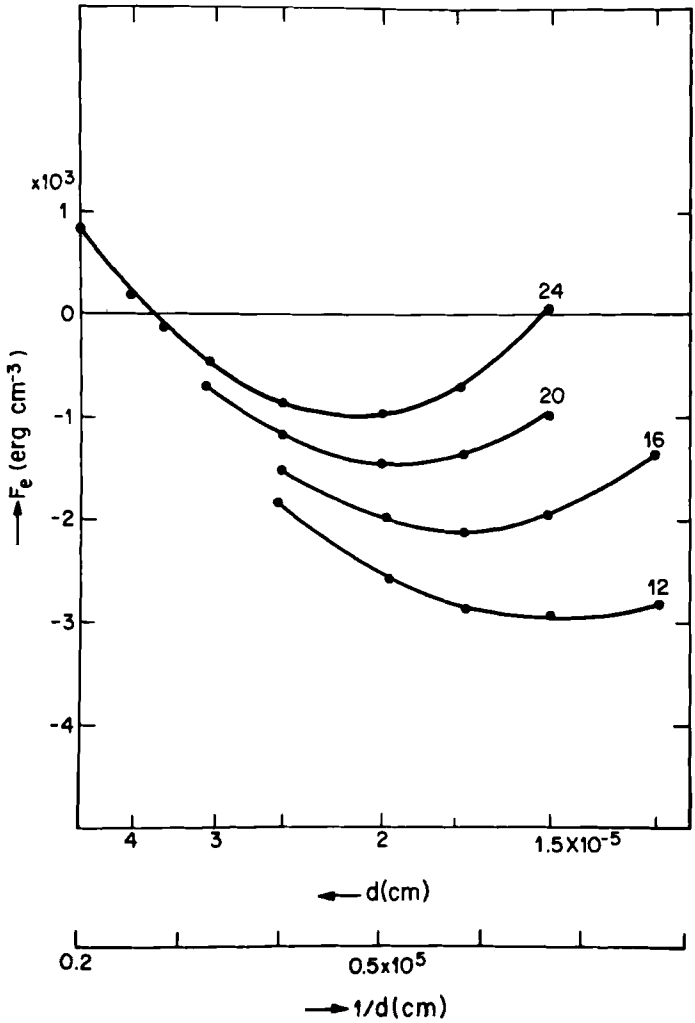

FIGURE 5 Relaxed free energy curves vs. cell size for the O^8 structure. The mesh sizes are given to the right of the curves. The parameters used are: $K_{11} = 2K_{22} = K_{33} = 3 \times 10^{-7}$ dynes; cholesteric pitch, $P_0 = 2.5 \times 10^{-3}$ cm.

phase model having O^8 symmetry. The x-axis is plotted as one over the cell size in units of cm^{-1}. The y-axis is free energy density in units of ergs/cm^3. All the energies have been multiplied by three. This scaling gives more realistic values for the elastic constants. The main features to be noted here are (1) there is a characteristic cell size which minimizes the free energy for a given mesh size and (2) the free energy increases as the mesh size becomes finer. This latter effect results because a smaller region around the disclinations is being discarded. Therefore the program calculates energies in a more highly stressed director field.

CONCLUSION

We have demonstrated that stable configurations of liquid crystal director fields can be found in a three dimensional simulation with locally connected directors. We have also come up with a method for treating disclinations.

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13. The energy from the disclination cores can be calculated using

$$F_{\text{core}} = \frac{a(T_c - T)\pi b}{N^2}$$

where a is the entropy of transition from the ordered phase to the isotropic, b is the length factor for the disclinations in the unit cell, N is the number of divisions and T_c is the isotropic transition temperature. For O^2 $b = 2\sqrt{3}$; for O^5 $b = 4\sqrt{3}$; for O^8 $b = 6$. See Refs. 6 and 11.
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Appendix

Generating a director field with the right topology can be easily done using an analytic function which represents the order parameter at a given point in space. Below are three tensorial expressions for order parameters which were used in blue phase relaxations.

$$\overline{\overline{Q}}_{O^4} = \begin{pmatrix} \Sigma_1 - 3\sin y\cos z & -\sin y\cos x + \sqrt{2}(\cos x\cos z + \sin x\sin y) & -\sin z\cos y + \sqrt{2}(\cos x\cos y + \sin x\sin z) \\ -\sin y\cos x + \sqrt{2}(\cos x\cos z + \sin y\sin z) & \Sigma_1 - 3\sin z\cos x & -\sin z\cos y + \sqrt{2}(\cos x\cos y + \sin x\sin z) \\ -\sin x\cos z + \sqrt{2}(\cos z\cos y + \sin x\sin y) & -\sin z\cos y + \sqrt{2}(\cos x\cos y + \sin x\sin z) & \Sigma_1 - 3\sin x\cos y \end{pmatrix}.$$

$$\overline{\overline{Q}}_{O^5} = \begin{pmatrix} 3\cos y\cos z - \Sigma_2 & \sqrt{2}(\cos x - \cos y)\sin z - \sin x\sin y & \sqrt{2}(\cos z - \cos x)\sin y - \sin x\sin z \\ \sqrt{2}(\cos x - \cos y)\sin z - \sin x\sin y & 3\cos x\cos z - \Sigma_2 & \sqrt{2}(\cos y - \cos z)\sin x - \sin y\sin z \\ \sqrt{2}(\cos z - \cos x)\sin y - \sin x\sin z & \sqrt{2}(\cos y - \cos z)\sin x - \sin y\sin z & 3\cos x\cos y - \Sigma_2 \end{pmatrix}.$$

$$\overline{\overline{Q}}_{O^2} = \begin{pmatrix} 3\cos y\cos z - \Sigma_2 & (\sqrt{2}(\cos x - \cos y)\sin z \\ -3(\cos z - \cos y) & -\sin x \sin y) + 3\sin z \\ (\sqrt{2}(\cos x - \cos y)\sin z & 3\cos z\cos x - \Sigma_2 \\ -\sin x \sin y) + 3\sin z & -3(\cos x - \cos z) \\ (\sqrt{2}(\cos z - \cos x)\sin y & (\sqrt{2}(\cos y - \cos z)\sin x \\ -\sin z \sin x) + 3\sin y & -\sin y \sin z) + 3\sin x \end{pmatrix}$$

$$\begin{matrix} (\sqrt{2}(\cos z - \cos x)\sin y \\ -\sin z \sin x) + 3\sin y \\ (\sqrt{2}(\cos y - \cos z)\sin x \\ -\sin y \sin z) + 3\sin x \\ 3\cos z\cos x - \Sigma_2 \\ -3(\cos y - \cos x) \end{matrix} \Bigg)$$

Where $\Sigma_1 = \sin x \cos y + \sin z \cos x + \sin y \cos z$ and $\Sigma_2 = \cos x \cos y + \cos x \cos z + \cos y \cos z$. The coordinates x, y, z represent the position in the unit cell and run from 0 to 2π.

The O^5 structure, which was first proposed by Saupe,[14] was taken from independent derivations by Alexander[15] and Hornreich and Shtrikman.[16] It was obtained by constructing plane wave interference patterns along the six (110) directions for a bcc configuration. The O^2 structure, proposed by Sethna,[6] was obtained by arranging cylinders of double twist along orthogonal directions and filling half the spaces between the cylinders with nematic material, and half by the director configuration of a $(-\frac{1}{2})$ disclination. The initial configuration was relaxed and afterwards Fourier analyzed.[17] The tensor was then constructed from the Fourier components. For the O^8 structure, proposed by Horneich and Shtrikman,[18] the above methods become more difficult. The resulting tensor was arrived at from group theory calculations. A more detailed explanation can be found in Ref. 11. Other possible structures were considered[19] but were ruled out as being subgroups of the aforementioned spacegroups.

To generate directors from these expressions the tensor is diagonalized to get the eigenvalues and eigenvectors. The eigenvector corresponding to the largest positive eigenvalue is chosen as the director (normalized to unity) at the point (x, y, z) in the unit cell. Figure 6 shows the positions of the disclination lines for the O^8 structure in the unit cell. The disclinations were found by looking for two positive, nearly equal eigenvalues. The third (negative) eigenvalue has been plotted in the figure. It is interesting to note that for this particular structure the disclination is really not a straight line but a spiral. This can be shown by solving for the points where the two eigenvalues are exactly equal. These points give the positions of the centers of the disclination lines. The centers lie less than one percent of the unit cell size away from the

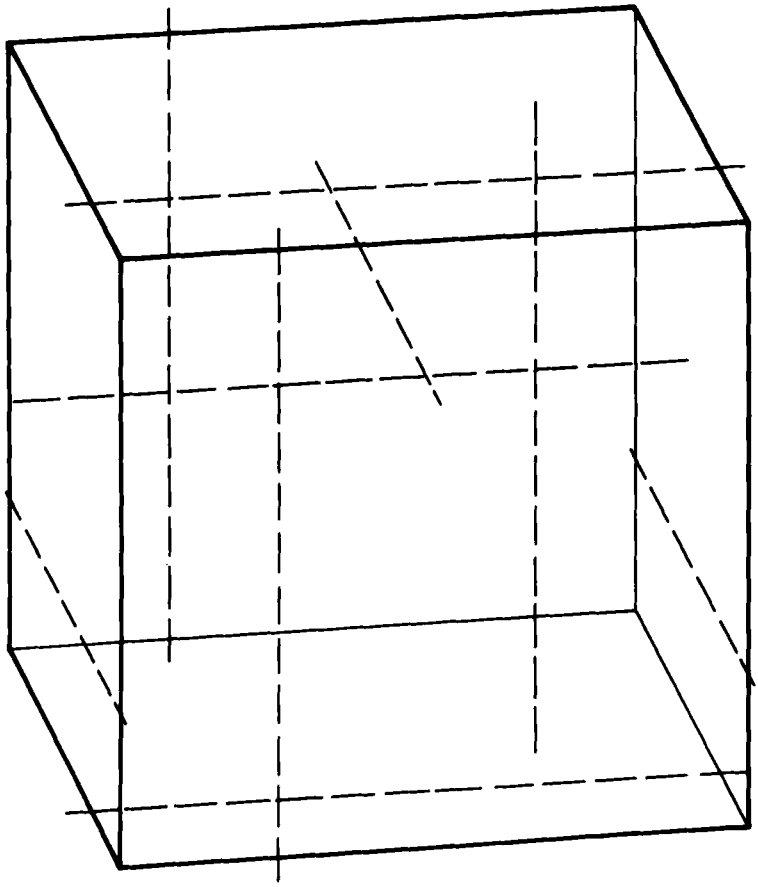

FIGURE 6 O^8 symmetry showing the disclinations in the unit cell. The program checks for two nearly equal eigenvalues. If two are found, the eigenvector corresponding to the negative eigenvalue is plotted.

lines shown in Figure 6. Therefore, these lines are only close approximations of where the disclination lines actually exist. If we had an infinitely fine grid the computer could actually trace the center of the disclination line for this particular symmetry through the unit cell.