Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713926090

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Online publication date: 29 June 2010

To cite this Article Mikulin, D. J. , Coley, D. A. and Sambles, J. R.(1997) 'Fitting reflectivity data from liquid crystal cells using genetic algorithms', Liquid Crystals, 22: 3, 301 — 307
To link to this Article: DOI: 10.1080/026782997209360
URL: http://dx.doi.org/10.1080/026782997209360

LIQUID CRYSTALS, 1997, VOL. 22, NO. 3, 301–307

Fitting reflectivity data from liquid crystal cells using genetic algorithms

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(*Received 29 June 1996; in final form 14 October 1996; accepted 20 October 1996*)

The half-leaky guided mode technique for quantifying thin optical layers is here combined with a data fitting routine based on a genetic algorithm to provide an immensely powerful procedure for detailing the director profile in liquid crystal cells. This approach not only provides a full description of the optical parameters of the cell, but also gives quantitative uncertainties in these parameters. It is tested here, first by fitting to theoretically produced data and then applied to real experimental data.

1. Introduction

The principal optical tool for the study of liquid crystals is that of polarizing optical microscopy. Because this technique integrates the optical response through the entire thickness of the cell, only a weighted average of the director orientation through the cell is obtained and thus little detailed information can be gleaned about the structure within it, without the use of many assumptions. Thus microscopy could not establish the presence of a chevron structure in the smectic C* phase of a surface stabilized ferroelectric liquid crystal cell as discovered by Reiker, Clark *et al.* [1] in 1987 using X-rays. X-rays, however, only provide information about the layering within the cell. Thus X-rays and optical microscopy combined still can only lead to limited information on the spatial variation of the director through the cell. A better knowledge of the director profile could be used to test model theories of the elastic response of cells and would also provide the potential for better cell design. What is needed is a probe that can give details of the way in which the director varies through the cell. The development of the Half-Leaky Guided Mode (HLGM) technique [2, 3] has provided just such a probe, being used to unravel the various complicated structures adopted by, for example, surface stabilized ferroelectric liquid crystals.

Since its inception, the main problem with the use of the HLGM technique with LC cells has been that of finding the parameter values characterizing the LC cell by fitting theoretically modelled data to that obtained experimentally. Whilst there may be merely half a dozen unknown parameters in an experimental test cell consisting of only two glass plates and a nematic liquid crystal, in typical commercial cells, which are much more complex, with numerous surface layer coatings, and especially when the liquid crystal is in a more highly structured phase such as smectic C*, the number of unknown parameters to be fitted can rise to over sixty.

Steepest-gradient based automatic minimization routines fail to navigate through the complex multi-dimensional function minimization hyperspace to the global minimum. It is thus an extremely difficult and time consuming process to find the correct solution to the data, with the need simultaneously to find values for such a large number of parameters. Moreover, even when the answer is found it is difficult to estimate the error associated with each parameter and even harder to quantify any degeneracy of solution.

Here we show the development of an automated genetic algorithm (GA) fitting procedure which allows rapid fitting of the HLGM data to a multi-variable model of an LC cell, leading to a true global minimum, together with error estimation and limitations of degeneracy.

2. HLGM technique

A variety of methods for optically probing materials has been investigated over the past decade based on the excitation of resonance modes in the liquid crystal cell by measuring the angle dependent reflectivities which characterize these resonances. These include the use of surface plasmon-polaritons [4, 5], and a range of guided structures from fully guiding [6–8] to fully leaky [9, 10]. The fully guiding, or attenuated total reflection geometry is very powerful, but the need for metallic layers prevents

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their resembling real devices. By contrast the fully-leaky geometry, with no metal layers and only high index glass plates, replacing the low index plates found in real devices, gives much less detailed information since the optical modes which are excited are much broader in angle (i.e. a lower Q cavity). This makes it more difficult to extract the desired optical tensor profile from the reflectivity data.

Subsequently the HLGM geometry [2, 3] was developed to enable real cells to be studied with the one proviso that the glass plates had to be of different refractive indices. It has much of the sensitivity of the guided mode geometry, without the metal layers. Ideally the high index glass plate should have a refractive index greater than the highest index of the liquid crystal and, similarly, the low index glass plate should have a lower refractive index than the lowest of the liquid crystal. With such a geometry there is a window of angles over which the optical field is evanescent in the substrate, yet propagates in the liquid crystal producing quite sharp half-leaky resonances within it. Monitoring the angle-dependent reflectivities over the range of angles which encompass the half-leaky window then gives data which when compared with model theory yield the director profile through the cell.

The incident laser beam is arranged to be either p- or s-polarized (TM or TE, respectively) and either the p- or s-polarized reflected light measured. This gives rise to four possible output data sets, two of which are the straightforward reflected signals (R_{pp} and R_{ss}) and the other two are polarization conversion or ps mixing signals (R_{ps} and R_{sp}), where R_{ps}, for example, signifies p-polarized light incident on the cell and s-polarized light reflected. The output data thus consist of various plots of reflectivity (R_{pp}, R_{ps}, R_{sp}, R_{ss}) versus angle. A typical data set is shown in figure 1.

All the optical parameters of every layer within the cell are in some way 'encoded' into such reflectivity data. It is this information that needs to be de-crypted to give the director profile and other parameters. The method employed is to match theoretically modelled data to the experimental set. Theoretical data are created by a computer program based on Fresnel's equations, together with a model of the cell as a series of discrete optical layers corresponding either to real layers such as the ITO or polyimide, or sub-layers of the liquid crystal chosen such that any individual layer is optically thin. That is to say, each layer has a thickness that is less than the wavelength of the incident laser beam divided by the refractive index of that layer. In this way the stack of layers representing the cell appears optically continuous. For a nematic LC it has been found that the LC layer can be assumed to be a single layer with a linear twist and tilt profile. For the complicated mesophases like S_C^*, this approach is taken using multiple thin layers because the available continuum theories are not readily tractable to simple modelling.

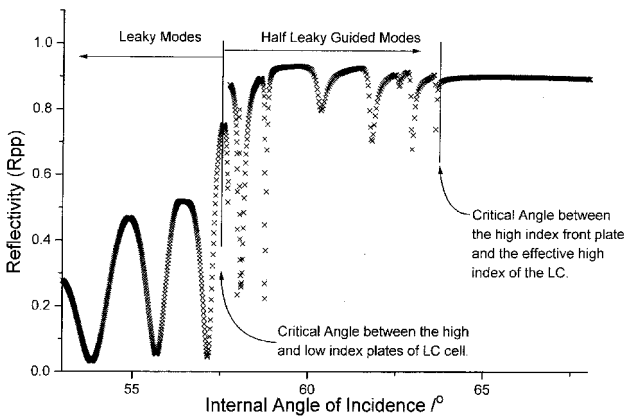

Figure 1. Example of a typical HLGM experimental reflectivity trace.

Prior to this study, the fitting process involved iteration, by hand, successively changing one or more of the parameters and then running the modelling program to see how the output is changed as a result. This is repeated until the theoretically generated curve virtually overlays the experimentally recorded data. At this point the steepest-gradient minimization routine could find the true minimum. The optical parameters for each layer, which typically include real and imaginary optical permittivities, thicknesses and twist and tilt Euler angles for the liquid crystal, can then be obtained.

3. Problems in using the HLGM technique

As indicated above, until now, for anything other than the most simple liquid crystal structures the fitting process has been carried out largely by hand, eventually switching when the solution is close enough, to an automatic fitting routine based on the *quasi*-Newton method, a rigorous direct calculus-based routine for minimization of functions. Such routines are used to minimize the sum of squares error (SOS) between the theoretically modelled and experimentally recorded reflectivity traces. These routines work by following the steepest local gradient to reach the function minimum. Unfortunately, when used to fit HLGM theory to data, it is found that these routines often have great difficulty converging to any solution within the set bounds. The reasons for these problems centre on the complex multi-dimensional function-minimization hyperspace [11]. This is the multi-dimensional landscape that represents every point in the solution space. The solution is found when the function is minimized for all parameters represented by the lowest point in the landscape.

For a typical model set of data, a set of enumerative

searches has been performed around the solution vector (global minimum) in order to obtain a picture of the landscape to find why the calculus based routines fail. It is found that the hyperspace is not a simple, smooth parabolic-like surface, but a highly featured space containing many local minima. The routine may thus follow the steepest local gradient and drop to the bottom of any number of these local minima, tending to become trapped and unable to reach the global minimum. Another problem is that due to the high degree of covariance between many of the parameters, the optimum value of a given parameter depends on values for the others. Thus any routine that tries to optimize them in series is likely to have very limited success; the parameters should be optimized in parallel to find the correct solution.

A further problem concerns that of degeneracy of solution, the root cause of which is that there are only a small number of sharp features in the angle-dependent reflectivity data for a real cell. This can result in the possibility of there being many combinations of parameters that can lead to similar theory traces. Degeneracy has been reduced in the past by two methods. Firstly, the cell is fabricated in a series of stages, one surface layer at a time, and at each stage the new layer (e.g. ITO) is characterized to find its optical parameters. Secondly, when the final cell is constructed, data are taken at combinations of polarizations and over a range of leaky as well as the entire half-leaky window of angles. This increases the amount of data and the number of features to which to fit, and thus greatly reduces the levels of degeneracy; at the same time of course, it inevitably lengthens the fitting process.

4. The genetic algorithm

To automate the laborious fitting process, a fitting routine is needed that has the ability to navigate through a highly featured landscape of local minima, plateaux and other features to reach the global minimum. Calculus based routines tend to be rigorous and efficient, but not robust and are thus best suited to the rapid solution of relatively simple functions. Enumerative searches by comparison are rigorous and robust, but very inefficient since the entire search space is covered, which takes considerable processor time. A third category [11] is that of random searches, which have been found to be surprisingly effective and highly robust, but which are once again inefficient. There are, however, a sub-set of random searches that use a random feature in a directed search making them both robust and efficient, the required combination for fitting HLGM reflectivity data.

Genetic algorithms [12–20] are one of a set of routines based on either artificial intelligence or mimicking of the processes found in nature. GAs are based on the processes of natural selection [21] and genetics, a set of parameters representing one point (or solution) in the multi-dimensional space being one 'individual'. While calculus based routines need to be supplied with a previously created, guessed set of parameters from, for example, the best obtained hand-fit, genetic algorithms, by contrast, use coded sets of the parameters, search from many points simultaneously (an individual is one coded set and a population is the set of all the individuals). They require only a very loosely specified initial guess working within a very wide set of bounds for each parameter, and progress to the solution using only the fitness (e.g. SOS) of each 'individual' as the criterion for future iterations.

The simple GA consists of four basic steps: initialisation, reproduction and crossover, mutation, and selection.

Initialisation: Initially a set of parameters is chosen at random from within the assigned bounds for that parameter. Many of these random individuals are created, forming a population. Each parameter value within each individual is converted into binary strings. The strings of each individual are then concatenated to form a single binary string representing that individual in the bounded hyperspace.

Reproduction and crossover: Pairs of individuals are typically selected at random and are both cut at the same, random position anywhere along their lengths. The end portions of both strings are then swapped and joined on the front part of the other of the pair.

Mutation: There is a small probability of spontaneous reversal of any binary digit in any of the offspring.

Selection: At this point the population consists of the first generation and a second generation of offspring. All individuals are tested for fitness and a rule [22] is imposed for survival to the next generation; for example, the population size can be kept constant, in which case the least-fit half of the population might be discarded.

The average fitness of each successive generation is, on average, better than that of the preceding one (i.e. lower SOS). Thus, as this process iterates through reproduction and crossover, mutation and selection, the optimum solution is approached.

Though simple in essence, for a GA to work in practice on any particular problem, it must be customized by appropriate selection of system variables such as population size, number of generations, mutation rate, binary word lengths, size of bounded hyperspace and the rules for the selection and mating processes [23–26].

5. Use of GA to fit to theoretically produced data

The GA was first tested by fitting to theoretically created data, so that the answer was known and the

success of the GA could be analysed. The data were created to simulate a typical low surface tilt, parallel polyimide aligned, nematic liquid crystal whose director has a slight linear twist and tilt (splayed) variation from the top to the bottom surfaces in a cell made of ITO coated glass plates. Four data sets were created representing the acquisition of data at two polarizations, at two azimuthal angles.

By the end of the initial development process the GA, starting with wide bounds which were typically the entire possible range of values that any of the materials could assume over a large temperature range, could find the solution to all 27 fitting parameters within a day on a fast desktop PC. Because of the randomness of the GA search it is easy to estimate the error associated with each parameter from the final spread of parameter values in the last population of individuals.

The accuracy and degeneracy in the solution for any particular cell will depend both on the configuration of the cell itself and on the 'quality' of the reflectivity data. 'Quality' here is defined as data of high experimental quality that contain enough features that are as a whole sufficiently sensitive to each parameter which is to be found. Put very simply, if any particular parameter has no effect on any feature of any of the sets of experimentally measured reflectivity data, its value will not be able to be ascertained.

Figure 2 shows an example of the quality of fit obtained with the GA. The figure shows the two polarization data sets at one of the two azimuthal angles used, together with their fitted reflectivity traces. The quality of fit for the other azimuthal angle data sets is similar. Table 1 shows the accuracy to which the parameters were found. Many are accurate to well within the required accuracy limit of an experiment. Note the parameters that have relatively large deviation from the true values: ITO and polyimide ε_i values, and the values for the grading of the low index plate. The reflectivity data were seen to be less sensitive to these parameters in the enumerative searches showing that they do not have a large enough effect on the reflectivity to allow the search routine to lock onto their true values. It is also seen that whilst the LC twist angles can be found to $\pm 0{\cdot}05°$, the tilt angles can only be found to $\pm 0{\cdot}4°$. The tilts in this cell are very small and have only a relatively small effect on the reflectivity trace.

As a further test of the fitting routine, some theoretical data were independently produced by a colleague, once again for a nematic cell. Fitting proceeded with the author having no knowledge of the actual parameters used. This was to avoid any influence of prejudice by the author in setting the initial bounds for the GA. This resulted in the fit shown in figure 3. The accuracies of the most important parameters are listed in table 2. From these results, the GA is clearly performing very well and the power of the HLGM technique is illustrated. The next step was to fit to some real nematic cell data.

6. Use of GA to fit experimental data

Data were taken on a cell consisting of ITO coated glass plates, coated in turn with parallel-rubbed polyimide and filled with Merck SCE13 ferroelectric liquid crystal raised in temperature to its nematic phase. These data were fitted by hand with limited success; it seemed that a large number of different combinations of parameters led to ostensibly similar quality fits. An added difficulty was that the data had been taken at only two polarization combinations at a single azimuthal angle.

The final GA fit was over an order of magnitude poorer in the SOS error than those obtained using

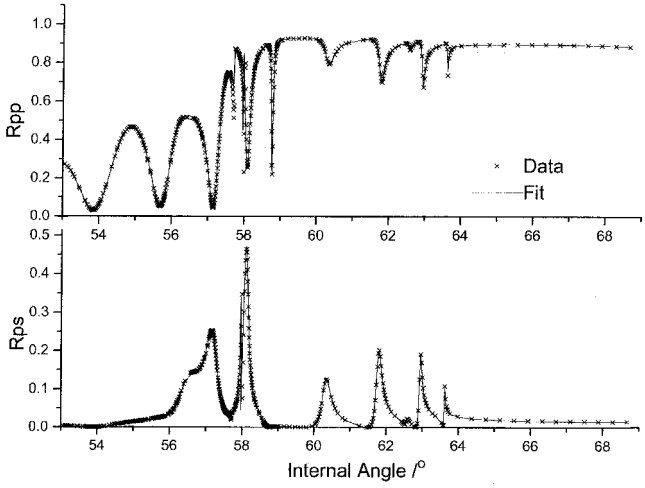

Figure 2. GA fit to theoretically produced nematic liquid crystal cell reflectivity data.

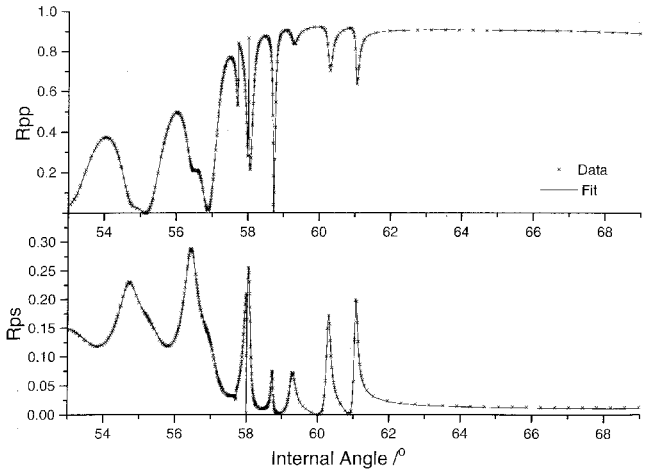

Figure 3. GA fit to unseen theoretically produced nematic liquid crystal cell reflectivity data.

Table 1. Comparison of real and fitted values for theoretically produced nematic data.

Layer	Parameter	Real value	Fitted value
Matching fluid (thickness in metres)	ε_r	2·995	2·9949
	ε_i	3·000E-6	2·905E-6
	thickness, d	7·0E-4	6·9E-4
ITO	ε_r	3·85	3·85
	ε_i	1·0E-2	1·1E-2
	thickness, d	6·800E-8	6·815E-8
Polyimide alignment	ε_{r1}	3·00	3·00
	ε_{i1}	0·0060	0·006
	ε_{r3}	3·05	2·98
	ε_{i3}	0·009	0·008
	thickness, d	3·30E-8	3·52E-8
Nematic LC	ε_{r1}	2·2000	2·2000
	ε_{i1}	3·0E-4	3·0E-4
	ε_{r3}	2·6000	2·5997
	ε_{i3}	3·5E-4	3·8E-4
	thickness, d	3·200E-6	3·196E-6
Nematic LC director profile Euler angles/°	upper surface twist	41·50	41·49
	lower surface twist	40·00	39·96
	upper surface tilt	89·00	88·63
	lower surface tilt	91·00	90·76
Index grading on the low index glass plate	ε_r	2·17	2·17
	d	2·50E-7	2·26E-7
	ε_r	2·16	2·16
	d	3·00E-6	2·99E-6
	ε_r	2·144	2·144
	d	5·0E-7	6·0E-7
Bulk low index plate	ε_r	2·1403	2·1403

Table 2. Comparison of real and fitted values for unseen theoretically produced nematic data.

Layer	Parameter	Real value	Fitted value	± Estimated error
Polyimide alignment	ε_{r1}	2·69	2·64	1·0E-2
	ε_{i1}	7·99E-3	8·50E-3	8·5E-3
	ε_{r3}	2·752	2·6	2·0E-1
	ε_{i3}	8·25E-4	6·9E-3	6·9E-3
	thickness, d	2·30E-8	2·9E-8	5·0E-9
Nematic LC	ε_{r1}	2·1980	2·1980	5·0E-5
	ε_{i1}	7·7E-4	7·5E-4	3·0E-5
	ε_{r3}	2·5910	2·591	2·0E-3
	ε_{i3}	6·8E-4	6·6E-4	1·5E-4
	thickness, d	3·17E-6	3·16E-6	1·0E-8
Nematic LC director profile Euler angles/°	upper surface twist	33·10	33·2	2·0E-1
	lower surface twist	42·50	42·4	2·0E-1
	upper surface tilt	88·70	88·8	2·0E-1
	lower surface tilt	93·10	93·2	2·5E-1

theoretical data. This reduction in accuracy is not surprising, due to the data having random noise and experimental errors, however the accuracy was still very high. The fit is shown in figure 4 with the parameters listed in table 3.

It seems that, for simple structures such as the one examined here, there may be sufficient information from a single azimuthal angle to produce accurate, non-degenerate fits to the experimental data. Again it is seen that the liquid crystal tilt at the bottom surface cannot

Table 3. Fitted parameter values for a real nematic liquid crystal cell.

Layer	Parameter	Fitted value	± Estimated error
Matching fluid (thickness in metres)	ε_r	2·9949	4·0E-5
	ε_i	3·07E-6	0·015E-6
	thickness, d	4·94E-4	0·07E-4
ITO	ε_r	4·36	0·01
	ε_i	3·7E-3	0·5E-3
	thickness, d	5·92E-8	0·05E-8
Polyimide alignment	ε_{r1}	2·65	0·04
	ε_{i1}	2·7E-3	1·3E-3
	ε_{r3}	2·86	0·005
	ε_{i3}	6·4E-3	0·5E-3
	thickness, d	2·36E-8	0·05E-8
Nematic LC	ε_{r1}	2·2047	0·0001
	ε_{i1}	2·96E-5	0·05E-5
	ε_{r3}	2·6094	0·0004
	ε_{i3}	3·23E-3	0·05E-3
	thickness, d	3·004E-6	0·001E-6
Nematic LC director profile Euler angles/°	upper surface twist	60·44	0·04
	lower surface twist	61·30	0·08
	upper surface tilt	88·60	0·01
	lower surface tilt	92·15	0·15
Index grading on the low index glass plate	ε_r	2·1577	3·0E-4
	d	4·91E-7	7·0E-9
	ε_r	2·1456	1·0E-4
	d	8·3E-7	1·6E-7
	ε_r	2·1406	3·0E-4
	d	1·34E-6	8·0E-7
Bulk low index plate	ε_r	2·1396	4·0E-4

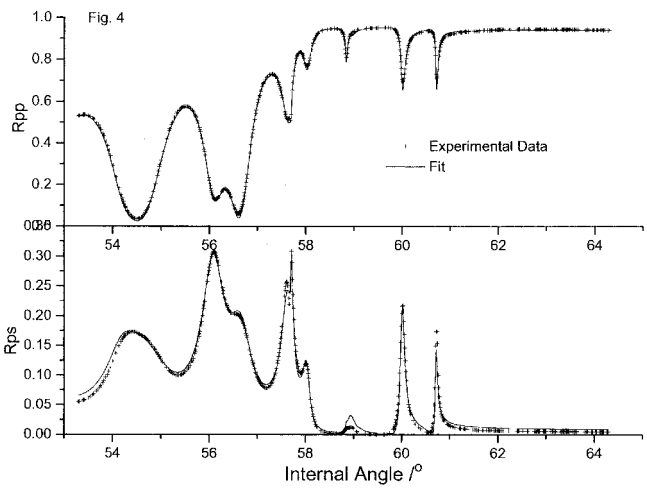

Figure 4. GA fit to real data taken from the nematic phase of a ferroelectric liquid crystal cell.

be determined to as high an accuracy as that at the top surface. This reflects the optical electric field distribution profiles which are not as concentrated at the bottom surface. The parameters that cannot be specified with great accuracy are the same ones that were very hard to find when the data were fitted by hand or when using the automatic calculus routines. These include the imaginary component of the optical permittivity of the ITO, the polyimide parameters generally and the grading on the low index plate that has always been a problem to model. Examination of the fits in figure 4 reveal that they are not perfect; this is particularly evident in the R_{ps} data due to a combination of the reflectivity axis scaling being larger than that of the R_{pp} and the lower signal levels involved. The reasons for these deviations are either errors in the data, or that the model is not accurately simulating the cell in some way. Probable causes are due to the assumption of simple linear twist and tilt variations of the nematic LC and the use of discrete three layer grading of the bottom glass plate. In reality the grading will be some continuously varying function and a three layer model may be inappropriate. One might imagine that the assumption of a linear variation of the LC director would have a far greater effect than any very thin, minor surface layer variation in the glass, but modelling has shown that this is not in fact the case and that the reflectivity is greatly affected by these surface layers.

7. Conclusions

For several years the half-leaky guided mode technique has appeared to have great potential as a tool for investigating, among other things, the structures assumed by liquid crystals in real cells. This potential has not been realised due to the nature of the labour intensive fitting process. In this study, to obviate this problem, a genetic algorithm has been developed as a minimization routine to fit model theory to HLGM data. It processes the parameters in a parallel fashion and does not easily become trapped by local minima.

The fits to both theoretically generated and experimentally recorded data show the power of the HLGM technique and its ability to resolve great detail within the wave-guide structure. The GA enables the HLGM technique for the first time to be used as a powerful and useful technique within a realistic time frame.

The GA is still in the early stages of development. Once optimised it will find the solution for appropriate data sets on a fast PC within a few hours. Work is continuing to test the GA and HLGM technique fully on cells containing complex phases such as the smectic C* phase.

The authors acknowledge the support of EPSRC and Sharp Laboratories of Europe through a CASE award.

References

[1] Reiker, T. P., Clark, N. A., Smith, G. S., Parmar, D. S., Sirota, E. B., and Safinya, C. R., 1987, *Phys. Rev. Lett.*, **59,** 2658.
[2] Yang, F., and Sambles, J. R., 1993, *J. opt. Soc. Am. B*, **10,** 858.
[3] Yang, F., and Sambles, J. R., 1993, *Liq. Cryst.*, **13,** 1.
[4] Welford, K. R., Sambles, J. R., and Clark, M. G., 1987, *Liq. Cryst.*, **2,** 91.
[5] Innes, R. A., Ashworth, S. P., and Sambles, J. R., 1989, *Phys. Lett. A*, **135,** 357.
[6] Elston, S. J., and Sambles, J. R., 1989, *App. Phys. Lett.*, **55,** 1621.
[7] Elston, S. J., and Sambles, J. R., 1991, *J. mod. Opt.*, **38,** 731.
[8] Bryan-Brown, G. P., Yang, F. Z., Bradberry, G. W., and Sambles, J. R., 1993, *J. appl. Phys.*, **73,** 3603.
[9] Lavers, C. R., and Sambles, J. R., 1991, *Jpn. J. appl. Phys.*, **30,** 729.
[10] Lavers, C. R., Cann, P. S., Sambles, J. R., and Raynes, E. P., 1991, *J. mod. Opt.*, **38,** 1451.
[11] Goldberg, D. E., 1989, *Genetic Algorithms, in Search, Optimisation & Machine Learning* (Reading, Massachusetts: Addison-Wesley).
[12] Holland, J. H., 1975, *Adaptation in Natural and Artificial Systems* Ann Arbor: University of Michigan Press.
[13] Keane, A. J., 1995, *Artif. Intell. Eng.*, **9,** 75.
[14] Dandy, G. C., Simpson, A. R., and Murphy, L. J., 1996, *Wat. Resour. Res.*, **32,** 449.
[15] Turton, B. C. H., 1994, *J. Sys. Eng.*, **4,** 121.
[16] Coley, D. A., 1996, *Contemp. Phys.*, **37,** 145.
[17] Davis, L., 1987, *Genetic Algorithms and Simulated Annealing* (London: Pitman Publishing).
[18] Wanschura, T., Coley, D. A., and Migowsky, S., 1996, *Solid State Comm.*, **99,** 247.
[19] Pal, K. F., 1995, *Biol. Cybern.*, **73,** 335.
[20] Thomas, G. M., Gerth, R., Velasco, T., and Rabelo, L. C., 1995, *Comput. ind. Engng.*, **29,** 377.
[21] Darwin, C., 1859, *On the Origin of Species by Means of Natural Selection* (London: John Murray).
[22] Gulsen, M., Smith, A. E., and Tate, D. M., 1995, *Int. J. Prod. Res.*, **33,** 1911.
[23] Karafydillis, I., Thanailakis, A., 1995, *Int. J. Elec.*, **79,** 205.
[24] Greenwell, R. N., Angus, J. E., and Finck, M., 1995, *Math. Comput. Model.*, **21,** 1.
[25] Bhandari, D., and Pal, S. K., 1994, *Info. Sci.*, **79,** 251.
[26] Lin, W., Delgado-Frais, J. G., Gause, D. C., and Vasiliadis, S., 1995, *Cybern. Sys.*, **26,** 387.