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Fractal analysis of a discotic texture

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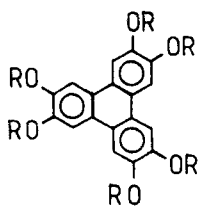
The dendritic-type texture displayed by low molar mass discotic charge transfer systems possessing a columnar hexagonal ordered phase has been subjected to a fractal analysis. The diffusion limited aggregation approach was used to simulate the growth of the texture. The results are that the texture displays a fractal geometry and that the prominent features of the discotic texture are correctly reflected by the simulated clusters, including the fractal dimension. The conclusion is that the texture is conditioned by the lattice structure of the discotic phase and the kinetic processes, the sticking rules in the terms of diffusion limited aggregation model, responsible for the growth of the texture.

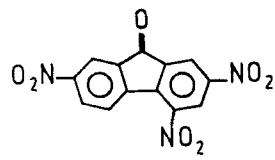
Liquid-crystalline textures as observed by polarizing light microscopy have been successfully analysed to obtain information on the nature of the liquid-crystalline phase, i.e. on its molecular structure [1, 2]. This can be achieved despite the large difference in scale (μm versus nm) since the point symmetry of the liquid-crystalline phase manifests itself in the curvature elastic properties of the phases which, in turn, control the formation of specific textures [1, 2]. Examples in case are the nematic schlieren texture and the smectic focal conic texture. The textures which develop in the course of a liquid-crystalline phase transition are frequently not as distinct as in these two cases. One reason, which is particularly valid for liquid-crystalline polymers is that the kinetics of the phase transition control the growth of a particular texture which may subsequently relax towards an equilibrium texture corresponding to a director field distribution having the lowest elastic energy. This relaxation of the transient texture can be expected to be rapid for lower viscosity and slow for higher viscosity systems. Such transient textures often show very irregular geometries. They, nevertheless, should reflect features characteristic of the growth process and the underlying molecular structure. This is the topic of this preliminary communication. It is concerned with the evaluation of such textures in discotic systems using fractal analysis.

The discotic systems considered in this communication are hexa-substituted triphenylene derivatives, doped with trinitrofluorenone (see figure 1). Thermodynamic and structural properties of such doped charge transfer systems have been reported previously [3]. Figure 2 shows the structure of such systems as obtained from the X-ray analysis; a hexagonal ordered columnar phase (D_{ho}) is formed where the trinitrofluorenone molecules are incorporated within the columns. The phase is thus characterized by a sixfold symmetry as far as the two dimensional lattice built up by the columns is concerned.

The dendritic-type textures observed for such systems are shown in figures 3 (*a*) and (*b*) for two different doped systems. The textures are obviously conditioned by a



H3T : R = C_3H_7
H5T : R = C_5H_{11}



TNF

Figure 1. Chemical structures of hexaalkyloxytriphenylenes (H3T/H5T) and trinitrofluorenone (TNF).

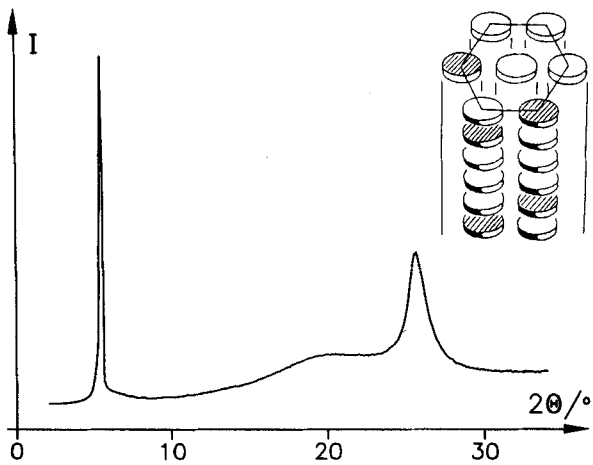
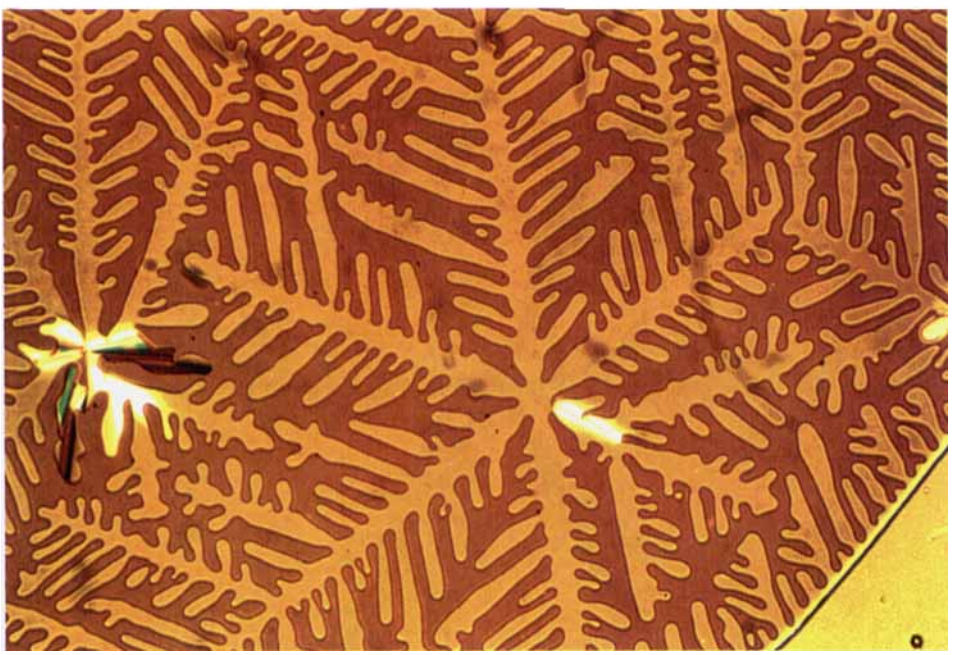


Figure 2. X-ray scattering pattern and the structural model of the D_{ho} phase for the system H5T/TNF 67/33.

sixfold symmetry, they exhibit a very irregular geometry and possess rugged boundaries and they are apparently self-similar at least for a certain range of scales. Such features are reminiscent of fractal geometries [4, 5]. It was tempting therefore to analyse such a dendritic-type of texture in terms of a fractal geometry and to simulate a fractal growth process. For this purpose the diffusion limited aggregation approach [6, 7] was selected which may be considered as a discrete version of a general dendritic growth model.

The two dimensional lattice of the discotic phase is characterized by a sixfold symmetry (see figure 2). For this reason the simulation was performed on a hexagonal lattice. We tentatively assumed, furthermore, that the texture formation takes place via a diffusion controlled aggregation of columns. The basic features of the diffusion limited aggregation model are the following. The simulation starts with a seed particle at the origin of the lattice. A second particle is added which performs random walks on the lattice. It is incorporated into the growing cluster whenever it visits an empty lattice site which neighbours an occupied cell. In addition to this simple cluster generation rule we have considered a version where the particle is incorporated into the cluster only if the lattice site has previously been visited $m - 1$ times, m being a noise reduction parameter; details are given in the literature [8]. The simulations were performed on a Silicon Graphics Iris 4D Workstation.

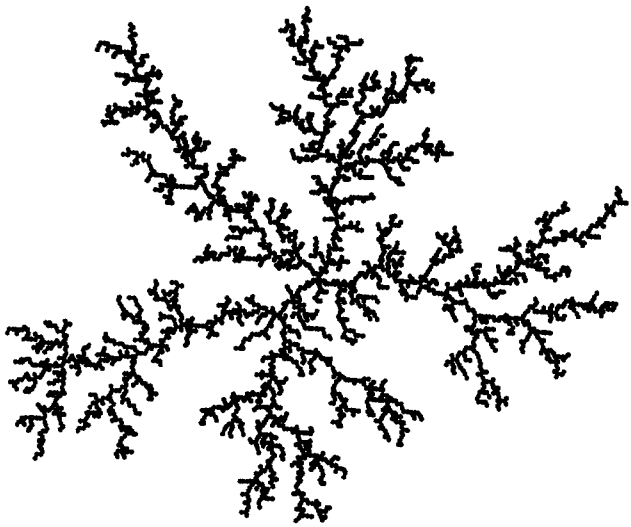
(*a*)



(*b*)

Figure 3. (*a*) Texture shown at 193°C by H3T/TNF 83/17 (Phase behaviour: C 157°C D_{ho} 210°C I). (*b*) Texture shown at 210°C by H5T/TNF 67/33 (Phase behaviour: D_{ho} 236°C I).

Figures 4 (*a*) and (*b*) display the results of such cluster growth simulations without ($m = 1$) and with ($m = 100$) noise reduction. It is apparent that the main features of the experimentally observed textures are represented by the cluster, particulary for the cluster generated using the noise reduction rule. The clusters display the dendritic-type texture, irregular geometries and a sixfold symmetry. It seems therefore that the



(*a*)

(*b*)

Figure 4. Results of the diffusion limited aggregation simulations of cluster formation without ((*a*) $m = 1$) and with ((*b*) $m = 100$) noise reduction.

macroscopically observed texture is conditioned by the hexagonal lattice structure of the discotic phase and by the growth process of the liquid-crystalline phase. One conclusion, therefore, is that such transient textures may provide information on structures and dynamical processes on a molecular scale.

In order to test the agreement between the experimentally observed textures and the simulated clusters on a more quantitative level the fractal dimensions both of the textures and the clusters were determined. For this purpose we have projected a net with a given mesh size on to the textures and we have counted the number of meshes covering the boundaries of the dendritic pattern as a function of the mesh size. The slope of a plot of the logarithm of the mesh size versus the logarithm of the number of covering meshes yields the fractal dimension d [4]. Figure 5 shows the results of such an analysis. It is apparent that the fractal dimensions of the textures and the clusters are close to each other, and that they are in the range of 1·57 to 1·63, i.e. close to the theoretical finding for a continuous model of 1·73. The representation of the textures in terms of fractal growth and fractal geometry is thus consistent with experiment.

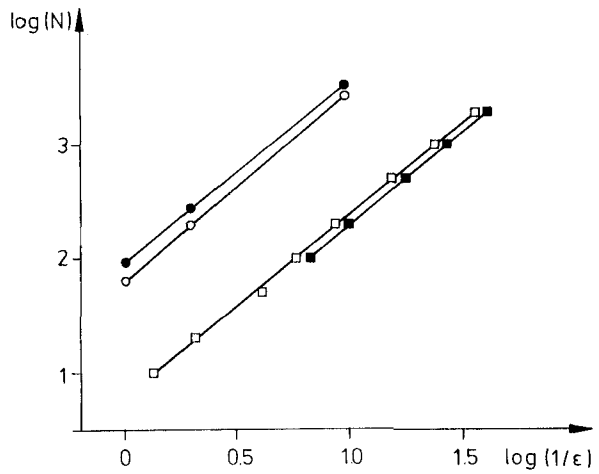


Figure 5. Analysis of the fractal dimension $d = \log(N)/\log(1/\varepsilon)$ (N, number of covering meshes; ε, mesh size) of the experimental textures (●, H3T/TNF 83/17; ○, H5T/TNF 67/33) and the simulated clusters (■, without noise reduction $m = 1$; □, with noise reduction $m = 100$).

Ideal fractal structures should display a self-similarity at all scales. This is obviously not the case for the textures given in figures 3 (*a*) and (*b*), as in most real fractal objects such as carbon black particles [5]. A cut-off value seems to exist at smaller scales below which the self-similarity ceases to exist. Our investigations show that the cut-off scale increases with increasing annealing time within the anisotropic fluid state. The reason apparently is, as for spinodal decomposition of blends [9, 10], that coarsening processes set in which are controlled by surface free energy induced flow.

The textures displayed by low molar mass discotic charge transfer systems have successfully been analysed in terms of the fractal growth of clusters. The diffusion limited aggregation model seems to be suitable as a mathematical approach to dendritic growth of discotic textures. Based on this analysis conclusions can be drawn

with respect to the symmetry of the liquid-crystalline phase and the growth mode of the textures.

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