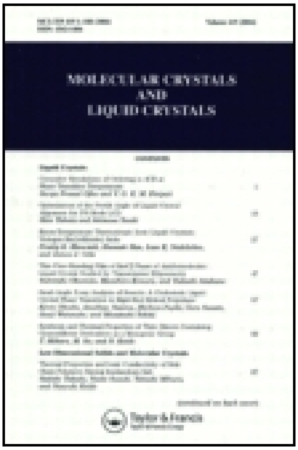

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Crystal Growth-Disorder Models and Ising Models

T. R. Welberry [a]
[a] Research School of Chemistry, Australian National University, P.O. Box 4, Canberra A.C.T., Australia
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Crystal Growth-Disorder Models and Ising Models

T. R. WELBERRY
Research School of Chemistry, Australian National University, P.O. Box 4, Canberra, A.C.T., Australia

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Crystal growth-disorder models attempt to describe the way in which disorder and short-range order are introduced into a crystal at growth in a situation where because of the shape of molecule or groups of atoms subsequent rearrangements can be ruled out. There are many examples of disordered molecular crystals some of which may reasonably be supposed to satisfy this criterion and most of which it would be difficult to imagine in complete 3-D equilibrium in the way described by the Ising model. Growth-disorder models, moreover, have the attraction that they are very easily simulated.

COMPARATIVE FORMULATION OF GROWTH-DISORDER AND GENERAL ISING MODELS

Growth-disorder

The probability that a given site is occupied by one species or another, is given in terms of previously filled sites. Using $\sigma_{ij} = \pm 1$ we write

$$P(\sigma_{ij} = 1/\text{all predecessors}) = f_n[\sigma_{i-1,\,j};\, \sigma_{i,\,j-1};\, \ldots \text{etc.}]$$

Considering only short-range interactions

$$P(\sigma_{ij} = 1/\text{all predecessors}) = P(\sigma_{ij} = 1/\text{near-neighbor predecessors})$$

The probability of a whole crystal configuration given a distant arbitrary boundary is then

$$P_c = \prod_{\text{all sites } i,\,j} P(\sigma_{ij}/\sigma_{i-1,\,j};\, \sigma_{i,\,j-1} \ldots \text{etc.}) \tag{1}$$

ISING MODEL

The probability that a lattice has configuration C is

$$P_c = \frac{\exp - [E_c/kT]}{Z} \tag{2a}$$

where Z is the partition function or normalizing factor and

$$E_c = \sum_{\text{all sites}} \sigma_{ij}(H + J_1\sigma_{i-1,j} + J_2\sigma_{i,j-1} + K\sigma_{i,j-1}\sigma_{i-1,j}\ldots) \quad (2b)$$

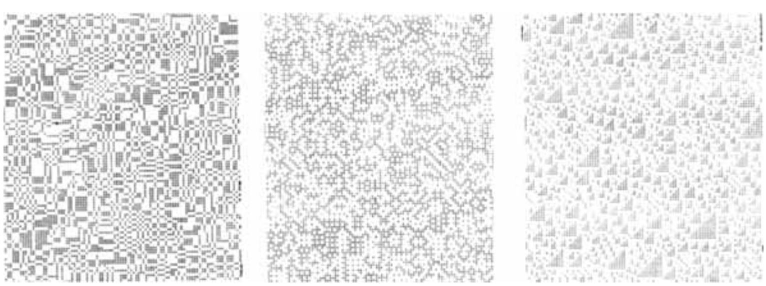
We relate the Ising model to the growth-disorder model by comparing eq. (1) and (2) after taking logarithms. The product of individual transition probabilities in (1) becomes the sum of logarithm probabilities while the form of (2) results in a sum of individual interaction energies. By equating the two for particular configurations (simple ones) the relationship between the two parameterizations may be found.

As an example in 2D we take a model based on interactions in a square. For such a model in growth-disorder terms 8 transition probabilities are available $P(+/- - -)$ $P(+/- - +)$ $P(+/- + -)$ $P(+/+ - -)$ $P(+/+ + +)$ $P(+/+ + -)$ $P(+/+ - +)$ $P(+/- + +)$, while the Ising model has 10 possible independent energy terms represented pictorially by

The Ising model has two additional degrees of freedom and so for equivalence with the growth-disorder model, is subject to 2 constraints.

However if these two constraints are satisfied the two formulations are entirely equivalent. An interesting and useful property of this fact is that the simple procedure of ensuring symmetry in the Ising model automatically forces the same symmetry on the growth-disorder model distribution despite its very non-symmetric growth.

Such symmetry imposition is possible in a number of different ways depending on whether the lattice is square or triangular but in each case the imposed symmetry enables a solution to be made for the lattice's statistical properties. One property of the models that has aroused interest is the fact that lattices having the same diffraction patterns may have very different appearances because of multiple-body interactions. All three of the realizations given below have indistinguishable diffraction patterns.

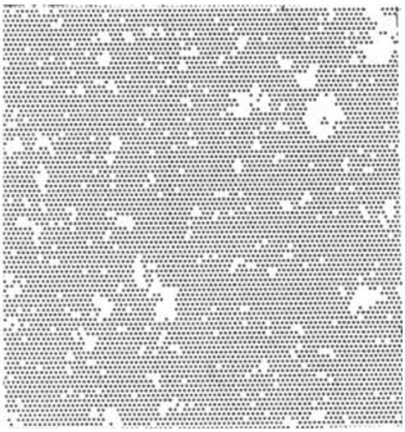


The same procedures can be carried out in 3D. A given growth-disorder model can be identified with a restricted subset of a 3D Ising model. Symmetry can be imposed in an analogous manner also and for the present purposes a simple growth-disorder model in which symmetry to reflection in the growth plane has been imposed will be discussed.

In this model we define only 2 growth-disorder probabilities. We construct the model starting from a triangular lattice boundary by adding points in the next layer above only the apex-up triangles. Further layers are added in an identical manner to generate a simple cubic lattice. We define

$$\begin{aligned} a &= P(+/+\ +\ +) \\ b &= P(+/+\ +\ -) \text{ or } P(+/-\ +\ +) \text{ or } P(+/+\ -\ +) \\ 1-b &= P(+/-\ -\ +) \text{ or } P(+/+\ -\ -) \text{ or } P(+/-\ +\ -) \\ 1-a &= P(+/-\ -\ -) \end{aligned}$$

The equivalent Ising model interactions are J along bonds in a growth plane K along bonds between planes and L a four-body interaction between three points in a plane and one in the next. Setting this last interaction to zero means the model is invariant to reflection in the growth plane. Moreover it may then be shown that the distribution of individual triangular layers is identical to that for the simple nearest-neighbor Ising model on a triangular lattice and this is well known to possess a phase transition. Equilibrium distributions on either side of the transition point are shown below, the difference between the two being a change of the value of b from 0.76 to 0.80.

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