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Structure, odd lines and topological entropy of disorder of amorphous silicon

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A continuous random network model of amorphous silicon, subject to periodic boundary conditions, is partitioned into cells bounded by irreducible rings. An algorithm has been developed to find the cells and the rings that bound them. A thread can be imagined to pass through odd rings (rings containing an odd number of atoms) without passing through even rings. Such a thread is an algorithmic realization of an odd line, which is the only topological defect in glass or amorphous condensed matter. The topological entropy of disorder associated with these odd lines is found to be approximately 80% of the value for an ideal tetrahedrally bonded random network of atoms for which the rings that bound the cells are statistically independent.

1. Introduction

Amorphous silicon is well described as a continuous random network of Si atoms. Each Si atom is covalently bonded to four nearest neighbors at a distance that varies by only a few percent from the nearest-neighbor distance of 3.5 Å that is found in the diamond cubic structure of crystalline Si, and the angular deviation from perfect tetrahedral bonding of 109.47° is of the order of 10°.

A crystalline structure has characteristic topological defects that determine its physical behavior. Besides point defects such as vacancies and interstitials, or walls like a grain boundary, there exist extended line defects, dislocations and disclinations (at least in nematic liquid crystals), resulting from breaking translational or rotational symmetry, respectively. In amorphous materials, such as glass or amorphous Si, only one line defect survives the breaking of translational and rotational symmetries: the wedge disclination line (Rivier, 1979), which is commonly known simply as an odd line. Odd lines are the only topological defects in a fully tetrahedrally coordinated continuous random network of Si since there are no dangling bonds *etc.*

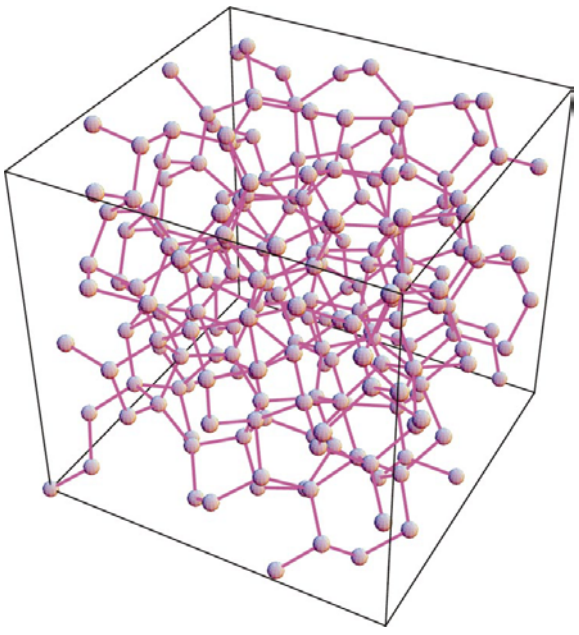

Figure 1
A 216-atom model of amorphous silicon.

Fig. 1 pictures a 216-atom random network model of amorphous Si subject to periodic boundary conditions. It is one of many computer-generated models obtained by using the method of simulated annealing. This one was chosen because it was the first (Wooten *et al.*, 1985) and the smallest, the small size making it a simpler case to deal with in a first effort at solving the 'odd-line problem'. The model was constructed by randomizing and annealing a supercell of Si that was initially in the diamond cubic structure. (Wooten *et al.*, 1985, Wooten & Weaire, 1987, 1995). In the crystal, there are rings of covalently bonded atoms. Each *irreducible* ring (roughly speaking, each shortest ring) consists of exactly six atoms. (A precise definition of irreducible rings will be given in §2.1.) The process of randomization introduces fivefold and sevenfold rings into the structure. Eventually, even larger rings are introduced. The model is subsequently relaxed by simulated annealing. The result is a model in remarkably good agreement with experiment as determined by the two-body correlation function found from X-ray scattering and, compared to other models, it gives the best agreement with three-body correlations (Filipponi *et al.*, 1989) found from X-ray absorption. It is fully randomized as indicated by ring statistics but the structure factor $|S(q)|^2$ associated with those reciprocal-lattice vectors labeled (111) for the diamond cubic structure is outside the standard deviation for a 'thoroughly'

randomized model (Wooten & Weaire, 1986). Nonetheless, because of its agreement with experimentally measured properties, its frequent use in calculations of the properties of amorphous silicon (see references in Wooten & Weaire, 1995) and, especially for the reasons of size cited above, it was chosen as a test case for developing an algorithm for finding odd lines.

One can pass a thread through the odd rings of a network such that each odd ring is threaded once and only once and such that the thread returns to the starting point to complete a loop, or ends at a surface in a finite system, or repeats itself in a lattice subject to periodic boundary conditions without passing through any even rings. This process can be continued until *every* odd ring has been threaded once and only once. These threads are an algorithmic realization of the odd lines of the topologist or the theoretical condensed-matter physicsist. Fig. 2 shows an example of odd lines threading the odd rings for the model of Fig. 1. Finding them and relating them to the topological entropy of disorder in a model of amorphous silicon is the subject of this paper.

2. Cells, corners, odd lines and rings

A cell can be defined for a periodic lattice as either the traditional unit cell of a Bravais lattice or as the Wigner–Seitz (Voronoi) polyhedron constructed about each atom. The notion of a cell is unambiguous even for a liquid of like atoms or for an amorphous solid such as *a*-Si, where the construction of Voronoi polyhedra is unique.

Although the Voronoi cell is the traditional choice for amorphous materials, there is another choice for defining cells in a covalent random network, where one can think in terms of a ball-and-stick model. It is to choose as cells those regions of space bounded by irreducible rings of atoms as illustrated in Fig. 3. This is the choice that will be used here. It will have to be developed in greater detail to deal with the complexity introduced by rings that overlap and which are not planar. It is this complexity that complicates the process of defining and finding cells, but the simpler description suffices for now.

The cell in Fig. 3 is a topological 'tent', with a six-ring base (atoms 167, 169, 170, 171, 166, 152), and four odd rings meeting three by three at an apex, one at each end of the edge 173–190. The point *P* in Fig. 3 is the centroid of the cell. Four lines connect *P* to the centroids (*A*, *B*, *C* and *D*) of each of the four odd rings. These four odd rings together with the sixfold ring on the bottom of the cell are the boundaries that define the cell. All cells are necessarily bounded by an even number of odd rings (four in this case), which is the basis for the theorem (Rivier, 1979): *uninterrupted lines closing as loops or terminating at the surface of the material or repeating themselves in a periodic lattice can be threaded through all odd faces avoiding even faces*. These odd lines are the topological defects in a liquid, glass or amorphous solid.

2.1. Irreducible rings

Our common-sense definition of a ring is a set of atoms (or vertices) such that, starting on any one of the atoms one can progress along a bond (edge) to an adjacent atom and from there to another atom and so forth until after *n* steps one returns to the starting atom. That defines an *n*-fold ring. There is no limit to the size of a ring defined that way. What we want are rings analogous to *smallest* rings, which we shall call *irreducible rings*. For this we need to refine our understanding of an irreducible ring with a precise definition.

Definition. A ring is irreducible if there is no shorter path between any two vertices on the ring than a path on the ring itself.

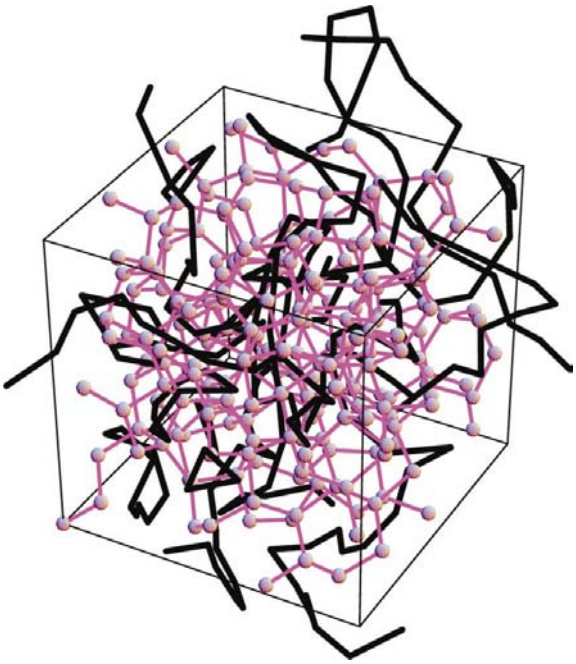

Figure 2
Odd lines in the amorphous silicon model of Fig. 1.

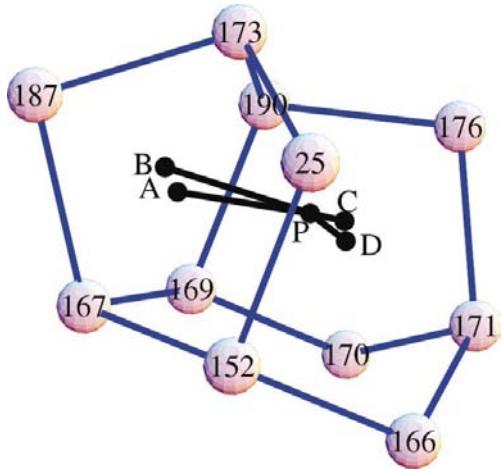

Figure 3
A cell belonging to the model of Fig. 1 with four odd rings: *A*, *B*, *C*, *D*.

Ring *A* in Fig. 3 consists of atoms 25, 152, 167, 187 and 173. (The atom numbers correspond to the numbering in the original crystalline supercell before randomization and annealing.) Ring *B* consists of atoms 190, 169, 167, 187 and 173. Is the sixfold ring consisting of atoms 25, 152, 167, 169, 190 and 173 irreducible, thereby constituting, together with rings *A* and *B*, a smaller cell bounded by two fivefold rings and a sixfold ring? No. Fig. 4 shows the topological arrangement of these rings projected onto two dimensions, where it is clear that the (outer) sixfold ring is *reducible* because the path from atom 173 to atom 167 *via* atom 187 is topologically shorter (two edges) than either path (three edges) between these two atoms that lies on the sixfold ring itself.

Henceforth, any reference to a ring means an *irreducible* ring unless otherwise stated and cells are bounded by irreducible rings.

Given a model for which the atomic coordinates and neighbors are known, one needs to first find all the irreducible rings.

The present model has 95 irreducible fivefold rings, 166 sixfold rings, 118 sevenfold rings, 32 eightfold rings and 4 ninefold rings. (All irreducible rings have been counted, even if they overlap. See discussion of Fig. 7 in §2.3.)

2.2. Corners

Cells are built from corners. A *corner* is defined by three rings that share a common atom (vertex) and such that each *pair* of rings shares a common bond (edge). Finding and identifying cells, and their bounding rings, by their *corners* is the central idea of this paper. It is the basis for finding the odd lines needed to determine the combinatorial topological entropy.

Fig. 5 shows one corner (shaded) that belongs to the example cell of Fig. 3. The vertex of the corner is atom 173.

The triangle (187, 173, 25) belongs to ring *A*. The triangle (187, 173, 190), which is hidden, belongs to ring *B*. These two rings share a bond (173–187). The triangle (25, 173, 190) belongs to the sevenfold ring *C* (atoms 25, 173, 190, 176, 171, 166, 152). It shares a bond (25–173) with ring *A* and a bond (173–190) with ring *B*. Thus, rings *A*, *B* and *C* form a corner as defined above.

Fig. 6 shows a second corner belonging to the example cell of Fig. 3. This corner is formed from rings *B*, *C* and *D*.

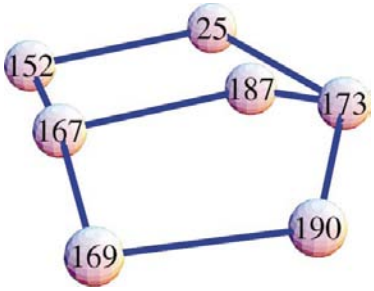

Figure 4
An (outer) sixfold ring from Fig. 3 is reducible to two fivefold rings.

Two corners that share two rings in common belong to the same cell. (Consider two adjacent corners of a cube for easy visualization. But keep in mind that cubic cells bounded by planar polygons are much simpler than the cells of a random lattice.)

The two corners emphasized in Figs. 5 and 6 have two rings in common (*B* and *C*) and thus belong to the same cell. Thus the second step in finding cells is to find all pairs of corners with two rings in common and join them to form a dihedral wedge. Next, join all pairs of dihedral wedges with two rings in common, and continue this process until finally a complete cell has been found.

We have ignored this: At least two rings belong to each triangle. For example, consider the triangle (187, 173, 25) belonging to ring *A*. Atom 187 is bonded to two other atoms, not shown in Fig. 3. Call one of them 187′. Similarly, atom 25 is bonded to another atom 25′. If the ring (. . . 187′, 187, 173, 25, 25′, . . .) is irreducible, the triangle (187, 173, 25) belongs to at least one ring other than ring *A* and the *corner* belongs to at

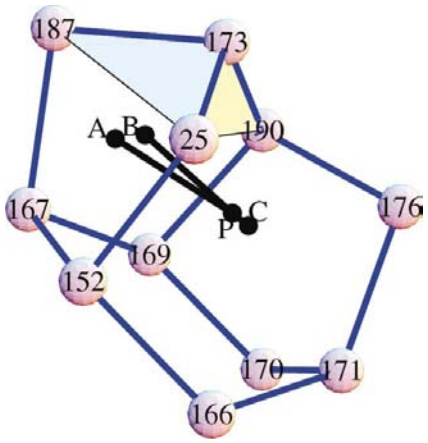

Figure 5
A corner (shown shaded) of the cell of Fig. 3. See Fig. 3 for a better perspective of the line segments from point *P*.

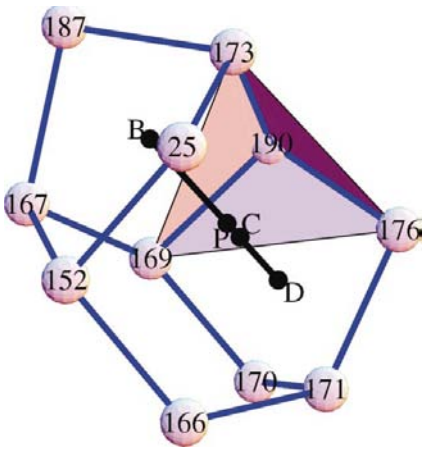

Figure 6
A second corner (shown shaded) of the cell of Fig. 3. See Fig. 3 for a better perspective of the line segments from point *P*.

least eight different combinations of rings. How do we choose the correct combination?

An approximation to the centroid of the corner is found by taking the vector sum of the three bonds belonging to the corner, using the vertex atom as the origin. Then, those three rings having centroids closest to the centroid of the corner are selected. (Taking account of periodic boundary conditions in this process requires close attention to detail.) As a check on these choices, it is required that the pairs of rings have at least one atom in common in addition to those belonging to the corner.

2.3. Pseudo-rings

The procedure to this point is conceptually simple because we have ignored the complexities and ambiguities introduced by overlapping rings. To resolve these ambiguities, it is convenient to introduce the concept of pseudo-rings.

Fig. 7 shows two overlapping sevenfold rings and a sixfold ring. These three rings are irreducible but cause problems in defining a cell because of the overlap. The difficulties can be removed by defining a pseudo-bond (dashed line in Fig. 8), which creates a fivefold *pseudo-ring* as the overlap region of the two sevenfold rings. The fivefold pseudo-ring is shown in Fig. 8 as the shaded region. In the process, two fourfold pseudo-rings are created by dividing the sixfold ring.

The cluster of rings from Fig. 8 is shown again embedded in the structure of Fig. 9.

There appear to be two cells in Fig. 9, one bounded above by the pseudo fivefold ring and the other bounded below by the pseudo fivefold ring. The role of the pseudo-rings is twofold: First, they clarify the boundaries more clearly. But, what is more important and subtle, is that they prevent the merging of cells. Note that if pseudo-rings were not used the cell below would be bounded partially by both of the two overlapping sevenfold rings, as would the cell above, so that one should merge the cells since they would seem to have two rings in common. This ambiguity is removed by defining the single fivefold pseudo-ring to replace the two sevenfold rings. However, the two cells would then still have two rings in common (the pseudo fivefold and the sixfold) and the cells would still merge. Thus it is also necessary to replace the sixfold ring by two pseudo fourfold rings.

This use of pseudo-rings is fraught with opportunities to miss when considering possible overlaps. Sevenfold rings can overlap with four atoms in common, which requires introducing a pseudo fourfold ring and two pseudo fivefold rings. Introducing pseudo-rings must be extended to overlapping eightfold and ninefold rings in this model. In larger models (4096 atoms), even tenfold and elevenfold rings exist. There are numerous combinations of overlapping rings to be dealt with.

Fig. 9 can be deceptive. One easily recognizes a sevenfold ring on top of the cluster. This sevenfold ring is surrounded by a pseudo fourfold ring, two fivefold rings and a sixfold ring. These rings appear to be bounded below by the (shaded) pseudo fivefold ring. Thus there may appear to be a cell bounded by four odd rings and two even rings. Actually, there are *two* cells in the top of the cluster lying above the shaded pseudo fivefold ring. The sixfold ring overlaps two sevenfold rings in a three-ring cluster topologically equivalent to the three rings of Fig. 7, but here the two sevenfold rings are sufficiently geometrically distorted as to be difficult to recognize. One must create *another* pseudo fivefold ring from the overlap region of these two sevenfold rings to separate the two cells in the top of the cluster. It is easy to find the two sevenfold rings with a computer program, but they are often difficult to recognize by visual inspection. Of course, finding eight-, nine-, ten-, eleven- and higher-fold rings is impossibly complicated without a computer program.

Finally, one must consider the case for which the ring identified as sixfold in Fig. 7 is *reducible* because of its connections to the surrounding matrix in which the cluster is

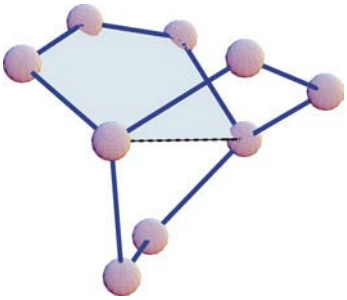

Figure 8
A pseudo fivefold ring created with a pseudo-bond.

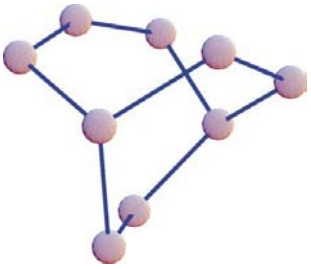

Figure 7
Two overlapping sevenfold rings and a sixfold ring.

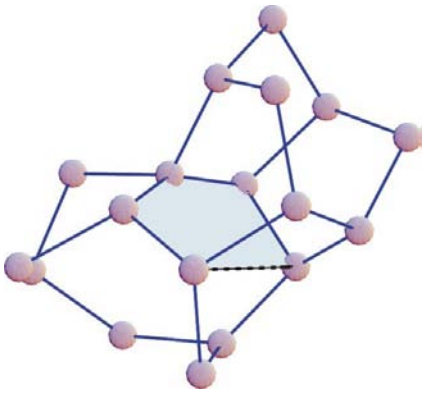

Figure 9
The rings of Fig. 8 embedded in an Si cluster.

Table 1
Odd loop statistics.

Loop length	Irreducible loops	Total loops
3-fold	3	3
4-fold	2	8
5-fold	0	7
6-fold	1	5
7-fold	2	10
8-fold	1	16
9-fold	2	35
10-fold	6	58
11-fold	3	107
12-fold	5	194
13-fold	13	331

embedded. This is a rare occurrence but, if the sixfold ring is reducible, one must not form pseudo-rings from the overlapping sevenfold rings. To do so would implicitly promote a reducible sixfold ring to the status of an irreducible ring when it is converted (improperly) into two fourfold pseudo-rings in the process of creating a fivefold pseudo-ring from the overlapping sevenfold rings.

2.4. The Rivier network

The segments of odd lines shown in Fig. 2, for example, connect to the segments of odd lines in adjoining cells, thus making up a network called the Rivier network. For the present model, it consists of 144 nodes at the centroids of cells. Of these 144 cells, 96 are bounded by two odd rings, 44 are bounded by four odd rings and six cells are bounded by six odd rings.

The Rivier network can be decomposed into loops and *irreducible loops* in the same way that the covalent network of Si atoms can be decomposed into rings and *irreducible rings*. The statistics for these loops are given in Table 1 for loops from length 3 to length 13. Of course, in addition to closed loops, there are lines that extend completely across the supercell that constitutes the model and thus correspond to odd lines that repeat themselves because of the periodicity of the model.

Of the irreducible loops, five are minimal (three threefold and two fourfold loops) in the sense that the rings through which each of these loops pass all share a common bond. Thus, if one visualizes the loop as a thread, the thread can be tightened to be of arbirarily short length looping around the common bond.

A picture of the Rivier network is not helpful. The large number of small fragments of the Rivier network that connect to neighboring supercells make for a very confusing picture. The best visualization was obtained by making a choice of loops to display. The choice for Fig. 2 was made as follows: Two of the three minimal threefold loops and the two minimal fourfold loops were chosen. (One of the threefold loops was necessarily eliminated by the choice of the first two threefold loops.) Then successively larger loops or repeating lines were chosen more or less at random. The choices become more and more restricted. If, for example, one chooses a loop containing the line segment from face A to face C in Fig. 3, the other loop extending through the cell necessarily consists of the line segments from face B to face D. The choice of Fig. 2 is one out of $\sim 5 \times 10^{25}$ choices, as we shall find in §3.

There are 15 loops or periodically repeated lines shown in Fig. 2. The number of odd rings through which each of the closed loops (or the periodic part of a line) passes are: 3, 3, 4, 4, 4, 6, 9, 9, 10, 12, 14, 17, 24, 32, 45.

In order to clearly separate the chosen loops, they are constructed such that the odd line segments in the loop go from one ring centroid to the next ring centroid without passing through the centroid of the cell. This makes a clearer picture than the Rivier network with all odd lines passing through, and connected at, the cell centroids. In the case of repeating lines, portions of the odd line that extend into neighboring cells are shown without translating them back into the supercell of Fig. 2.

3. The topological entropy of disorder

The full topological entropy of the odd-line defects has been calculated (Rivier & Duffy, 1982) under the assumption that every face (ring) can be odd or even, apart from the continuity restraint, which is satisfied by the requirement that there be an even number of odd faces per cell, for which there is a simple proof (Rivier, 1979). For the case of a monoatomic tetrahedrally bonded substance such as covalent liquid Si, the result is

$$\begin{aligned} S_t &= Nk_B \ln 2 = R \ln 2 \\ &= 5.76\ \mathrm{J\ K^{-1}\ mole^{-1}}. \end{aligned} \tag{1}$$

This is the ideal (maximum) entropy for the case in which the parity (odd or even) of the rings is statistically independent, an assumption unlikely to be valid in an actual network. Here, we are using S_t as the upper limit for amorphous silicon, which *is* a tetrahedrally coordinated covalent random network, unlike liquid Si, which is metallic with an atomic connectivity of 6 (locally, a simple cubic configuration).

The combinatorial topological entropy of the model, $S_{\rm comb}$, involving the vertices of the Rivier network, is given by

$$S_{\rm comb} = k_B \ln \Omega^{\rm OddLines}, \tag{2}$$

where $\Omega^{\rm OddLines}$ is the number of distinguishable configurations of the odd lines. The number of possible configurations for a cell is

$$\Omega^{\rm cell} = (n-1)!! = (n-1)(n-3)(n-5)\ldots(1), \tag{3}$$

where n is the number of odd rings bounding the cell. Thus, for example, a cell with four odd rings has three possible ways in which two lines can pass through the cell and one with six odd rings has $5 \times 3 = 15$ possibilities for passing three lines. The total number of possible odd-line configurations for the model with four odd cells containing six odd rings and 44 cells with four odd rings is

$$\begin{aligned}\Omega^{\text{OddLines}} &= \prod_{\text{cells}} \Omega^{\text{cell}} \\ &= (15)^4(3)^{44}(1)^{96} \\ &= 4.98 \times 10^{25} \quad \text{for 216 atoms} \\ &= 1.39 \times 10^{47} \quad \text{for one mole.}\end{aligned} \tag{4}$$

The combinatorial topological entropy arises from lifting the degeneracy of the Rivier network. Ω^{OddLines} is the number of ways in which one can lift the degeneracy. Fig. 2 shows one of these configurations.

The combinatorial topological entropy of the model (on a molar basis) is

$$\begin{aligned}S_{\text{comb}} &= k_B \ln \Omega^{\text{OddLines}} \\ &= 2.28\,\text{J K}^{-1}\,\text{mole}^{-1}.\end{aligned} \tag{5}$$

Thus we find that

$$S_{\text{comb}} = 0.4\,S_t. \tag{6}$$

Configurational entropy, S_{config}, arises from rings that have been twisted and distorted from their configuration in the diamond cubic structure, from edges of the Rivier network which are 'wiggly' and of variable length and because the loops of the Rivier network also have a fluctuating number of topological edges. One can, in principle, measure the entropy frozen in the glass at a temperature T_1 well below the glass transition: Just cool the liquid slowly, from T_2 through the glass transition down to T_1 (at T_2, liquid silicon is metallic with six nearest neighbors but the entropy can be calculated or measured by some independent means), measure the specific heat, C_P, at each temperature and calculate the integral

$$\int_{T_1}^{T_2} (C_P/T)\,\mathrm{d}T = S(T_2) - S(T_1). \tag{7}$$

At very low temperatures, C_P is very small and the lower limit T_1 in the integral can be set to zero. Nevertheless, $S(T_1) \approx S(0)$ remains finite, although the experimental value depends on the rate of cooling. $S(0)$ measures the entropy frozen in the glass, which is the full topological entropy, $S_{\text{comb}} + S_{\text{config}}$. One can argue (Rivier, 1987, and private communication) that the two contributions are roughly equal for a 'semi-dilute' network of loops. [A semi-dilute network of loops is such that one does not know whether the nearest segment belongs to the same loop or to any other. For the Rivier network, this means that the average radius of a loop (the distance between vertices of the Rivier network) is of the same order as the wiggliness of individual loops, which appears to be the case in Fig. 2.] Thus, for a semi-dilute network of loops, the topological entropy is maximal (since there is only one length scale), with equal configurational and combinatorial contributions.

$$S_{\text{config}} \approx S_{\text{comb}}. \tag{8}$$

Since the model has been found to have $S_{\text{comb}} = 0.4S_t$, the total topological entropy for the model is

$$S_{\text{topological}} = S_{\text{comb}} + S_{\text{config}} \approx 0.8S_t, \tag{9}$$

a value that is perhaps surprisingly large in view of the very rough argument used to estimate S_{config} and of the smallness of the model. The deficit, compared to the idealized Rivier–Duffy calculation, arises from various causes, the most important being that the model is insufficiently randomized (Wooten & Weaire, 1986), the model is too small and/or the parities of the faces (rings) are not statistically independent.

If one imagines building a cubic model having free surfaces *without* periodic boundary conditions, there are no parity constraints imposed by the surface. On the other hand, if the model is to be a supercell such as that of Fig. 1, with periodic boundary conditions imposed, it is necessary that opposite sides be joined with little deviation from tetrahedral bonding or from the average Si—Si bond length. This imposes constraints on the topology and geometry of the rings in order to satisfy the boundary conditions. There is some evidence that this is indeed a constraint, for the angular deviations from perfect tetrahedral bonding in models subject to periodic boundary conditions have been found to be larger in smaller models than in larger ones. If the cell is small, the boundary constraints affect a larger fraction of the cell.

I thank D. Weaire for introducing me to the problem of odd lines and for many stimulating discussions. N. Rivier has been invaluable for his enthusiasm, encouragement, many helpful suggestions and probing questions. W. Thurston inspired me to pursue a topological approach when my attempts with purely geometrical approaches ended in failure. B. Higgins tutored me on *Mathematica* graphics. S. Holland has been a kind and helpful reviewer. J. Koch and E. Suranyi provided the irreducible ring program. I am indebted to them all.

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addenda and errata

Structure, odd lines and topological entropy of disorder of amorphous silicon. Correction

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Wooten [*Acta Cryst.* (2002), A**58**, 346–351] defines cells in amorphous Si as being bounded by irreducible rings of atoms, which can be viewed as distorted polygons. These irreducible rings are, roughly speaking, shortest rings. However, the definition used is incomplete and leads to some large rings being counted as irreducible when close examination reveals they are not. In particular, the incomplete definition counts four ninefold rings (out of a total of 1041 ninefold rings) as being irreducible. Yet a detailed examination reveals that these four rings bound a set of smaller rings, and are clearly not irreducible in any meaningful sense of the word. An extended definition has been given [Rivier & Wooten (2003). *MATCH – Commun. Math. Comput. Chem.* **48**, 145–153], and described at length, that removes the difficulties. It results in a small increase in entropy, approaching slightly closer to the ideal. The first paragraph of Wooten (2002) incorrectly states that the nearest-neighbor distance in Si is 3.5 Å, rather than the correct value of 2.35 Å. This misprint has no effect on anything else.

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