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Percolation and transport in an assembly of anisotropic conductors

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Abstract. The percolation surface was calculated for a cubic lattice where each active site is occupied by a cube that only conducts along planes normal to one of the three cartesian directions. The transport properties of the assembly of cubes, found using a resistor network approximation, are more adversely affected by the presence of vacant sites than by the anisotropy of the different cubes. Studies of the correlation length and conductivity exponents indicate that the behaviour of the material is in general three dimensional, though systems comprised of voids and cells oriented in one direction have critical exponents corresponding to two-dimensional systems. An effective medium treatment gave simple analytical results for the percolation surface and effective conductivity that were quite accurate in some limits.

1. Introduction

Redner and Stanley (1979) introduced anisotropic percolation by occupying bonds in different directions with different probabilities. Since then, this problem has been extensively studied in two dimensions (Torrie *et al* 1982, Zhang 1984, da Silva *et al* 1985). In the present three-dimensional work anisotropy is introduced in a different, physically motivated, manner by occupying sites with elements that cannot bond to all nearest neighbours.

The system studied consists of a cubic lattice with sites located at the lattice points. Each active site may be thought of as a cube composed of layers of planes normal to one of the three cartesian axes. Cubes cannot bond (conduct) in the two directions normal to the planes and thus connect with at most four neighbours. Sites may also be left unoccupied. An equivalent perspective is to regard each site as occupied by individual two-dimensional square planes, with no transport normal to the square. Thus in the rest of the paper 'square' may be substituted for 'cube'.

The motivation for the study was to investigate the effect of anisotropy in the transport properties of single crystals on the behaviour of polycrystalline materials. Planar conductors such as the beta-aluminas are of considerable industrial importance (Farrington and Briant 1979). Furthermore, the newly discovered high-temperature superconductors also appear to show planar anisotropy (Tozer *et al* 1987). The cubic array discussed in this paper may be considered to be an elementary model for such materials, where the cubes correspond to individual grains, and the unoccupied sites correspond to impurities and defects in the crystal structure. Testing the possibility

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that the materials will conduct is analogous to investigating the connectedness of the array.

The physical requirement that some sites be left unoccupied means that the percolation problem may be classified as an anisotropic bond-site study. Bond-site percolation (Frisch and Hammersley 1963, Hammersley and Welch 1980) allows both bonds and sites to be occupied independently. This idea was first combined with the concept of anisotropic percolation by Guttmann and Whittington (1982). They considered a square lattice with a diagonal bond in each square (distorted triangular lattice) where separate occupation probabilities were defined for sites and for bonds in each of two different directions. Site and bond percolation on square and triangular lattices are special cases of this general system, as indeed is one-dimensional percolation.

In the present system sites are occupied with one probability, but different orientations of the cubes occur with different frequencies corresponding to the probabilities of forming bonds in different directions. This model includes two-dimensional site percolation as a limiting case, and consequently is analogous to the two-dimensional work of Guttmann and Whittington (1982) which encompassed a one-dimensional problem.

The focus of Guttmann and Whittington's work was to show that the critical exponents for site, bond and bond-site percolation are all the same, except for the choice of parameters corresponding to the one-dimensional limit. This conclusion is consistent with the results of Nakanishi *et al* (1981) who showed that anisotropic percolation on the two-dimensional square lattice was in the same universality class as isotropic percolation. The problem considered here was similarly found to be in the same class as three-dimensional bond and site percolation.

We note parenthetically that systems of one-dimensional conductors in a two-dimensional environment show a markedly different behaviour from that of two-dimensional conductors in a three-dimensional system as studied here. The percolation threshold for one-dimensional conductors is trivial, with all conduction paths eventually trapped in spirals (Johnson 1987). For the present problem, however, there is a well defined percolation surface.

The onset of percolation as a function of the percentage of cubes with each orientation defines the percolation surface, and this surface is discussed § 2. The correlation length exponent was calculated for one of the curves that serves to define the surface. As discussed in § 3, the exponent agrees with the three-dimensional bond or site percolation exponent except at a singular point. The conductivity exponent for the same limiting curve is found in § 4 and the behaviour at the singular point is analysed in more detail. An effective-medium theory analysis of the system is given in § 5, while § 6 is devoted to the conclusions from the work.

2. The percolation surface

Percolation was sought in the z direction as a function of the fraction of occupied sites and the probability that an active site would be occupied by a cube that could bond in the yz, xz or xy planes (referred to by their normals as x, y and z cubes respectively). Note that because the individual cells are anisotropic, the direction in which percolation is being sought must be specified. The percolation surface is calculated using Stauffer's (1985) algorithm. Durand (1989) discusses the algorithm in the context of the current problem.

2.1. Calculation of the percolation surface

The fraction of voids at incipient percolation in the z direction was found for a given ratio of the three types of cubes (i.e. a given $x:y:z$ ratio). However, if the fraction of z cubes is too large, there may be no percolation even in the absence of voids. A somewhat different percolation problem arises in this case, namely to find the critical fraction of z cubes for a given $x:y$ ratio. The methodology for the two problems is very similar.

The estimate of the critical fraction for each configuration was found to an accuracy of ± 0.015. In all cases, the system size was at least 50 (i.e. 125 000 cubes and voids were used) and periodic boundary conditions were imposed in all three directions to mitigate finite-size effects. Averaging results for many (typically 100) configurations gave the critical fractions to an accuracy of ± 0.003 at 95%. The error limits are based on the assumption that there are no systematic errors such as finite-size effects.

2.2. The features of the percolation surface

The percolation surface (figure 1) was established by considering four limiting cases, namely systems with no z cubes, equal amounts of x and y cubes, no y cubes, and no voids (i.e. all sites are active). Interpolating between the four curves, labelled as A, B, C and D on figure 1, gives the percolation surface. Curves A, B and C are shown separately as figures 2(a), 2(b) and 2(c) respectively. The overall surface is in essence a phase diagram, and shows the critical void fraction on the vertical axis as a function of the fractions of x, y and z cubes. Phase diagrams with three components are discussed in general terms below before the features of each of the four curves are

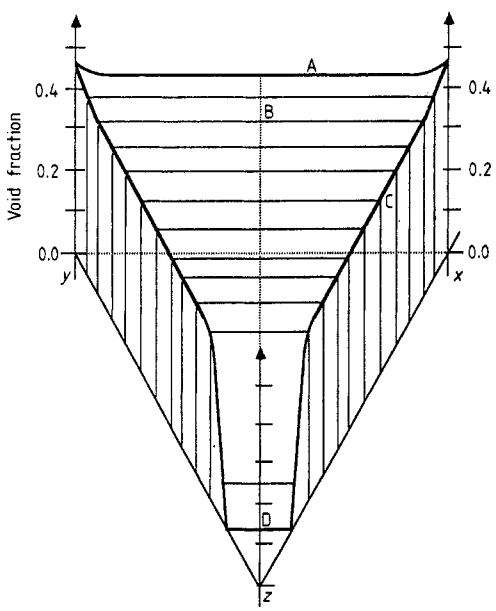

Figure 1. Schematic of the percolation surface for the system of planar conductors. The vertex labelled x corresponds to all conducting cubes having normal in the x direction. The vertical axis gives the void fraction at incipient percolation.

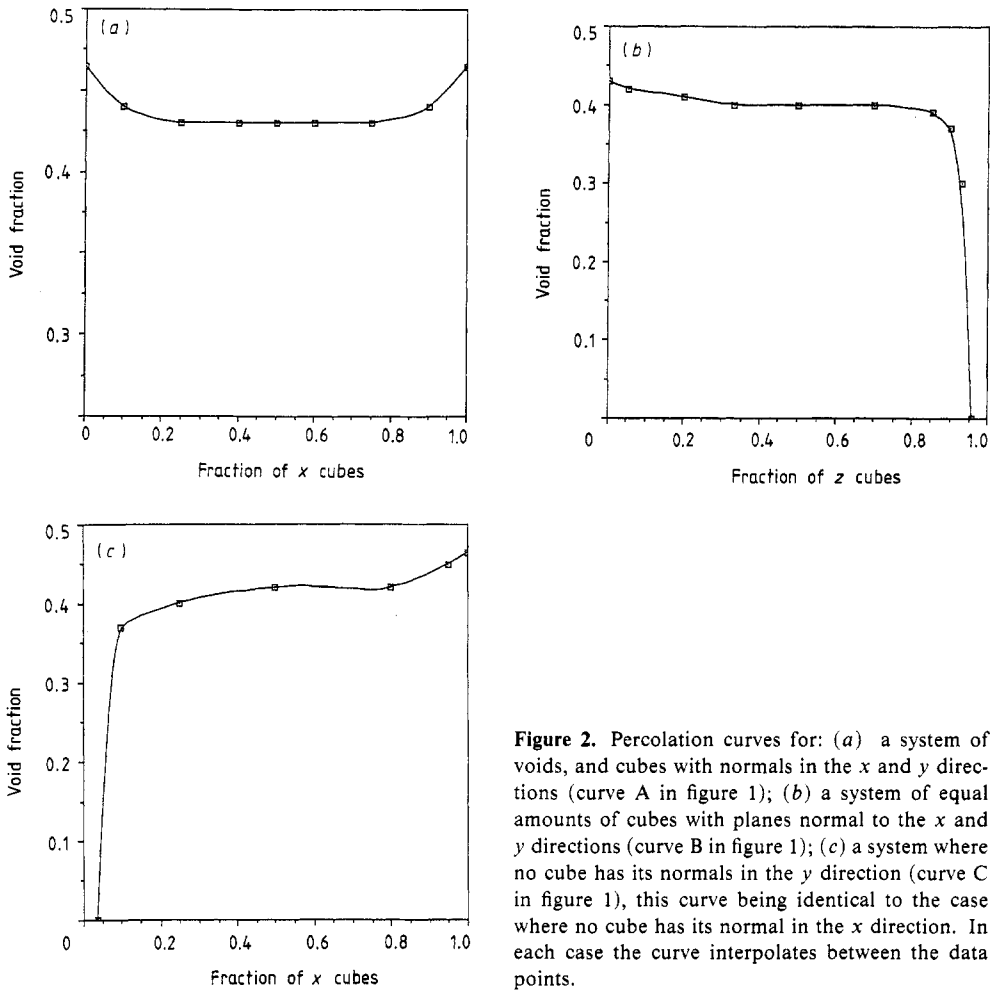

Figure 2. Percolation curves for: (*a*) a system of voids, and cubes with normals in the x and y directions (curve A in figure 1); (*b*) a system of equal amounts of cubes with planes normal to the x and y directions (curve B in figure 1); (*c*) a system where no cube has its normals in the y direction (curve C in figure 1), this curve being identical to the case where no cube has its normal in the x direction. In each case the curve interpolates between the data points.

examined in detail. Those readers conversant with the nature of such diagrams may prefer to skip to the description of curve A in § 2.2.1.

Phase diagrams with three components are typically shown as equilateral triangles, with any ratio of the three components corresponding to a unique point in the triangle. The three vertices correspond to systems containing only one of the components. The fraction of, for example, z cubes corresponding to any point on the triangular diagram is found by drawing a line from the z vertex through the point to the opposite side of the triangle. The required fraction is the portion of the line from the point to the side of the triangle. The sum of the fractions of x, y, and z cubes adds to unity.

The vertical axis in figure 1 denotes the critical void fraction; points under the surface correspond to systems that will conduct. For any point in the diagram, the fraction of the total number of cubes that have normals in a given direction is found by multiplying the fraction of cubes with normals in that direction (as read from the phase diagram) by $(1 - v_f)$, where v_f is the void fraction.

2.2.1. No cubes having planes normal to the z direction (figure 2(a)). Both x and y cubes conduct in the z direction and so, from a transport perspective, the two types

of cube are in essence equivalent when present in approximately equal amounts. Consequently, the percolation line approaches the axis of equal amounts of x and y cubes with zero slope. When the fraction of either type of cube is greater than about 0.75, two-dimensional effects start to manifest themselves. The case of purely x or purely y cubes (and voids) is a strictly two-dimensional problem.

Consider, for example, the case where all active sites are occupied by cubes with normals in the x direction. Bonds within the assembly are confined to yz planes. A system of size $L \times L \times L$ is effectively L independent two-dimensional systems of size $L \times L$. Thus, in this limit, the problem of the behaviour of an assembly of planar conductors reduces to the two-dimensional site percolation problem.

Middlemiss *et al* (1980) found the critical void fraction of the site percolation problem to be 0.406 ± 0.003 by extrapolating data from systems of up to 200×200 to infinite system size. More recently, Ziff and Sapoval (1986) reported a value of $0.407\,255 \pm 0.000\,002$. The figure found in this work in the three-dimensional simulations of $50 \times 50 \times 50$ planar conductors with all occupied cubes having normal in the x direction is considerably larger than this, namely 0.465. When the true two-dimensional problem was studied using a modified version of the three-dimensional code and a system size of 50×50, the threshold was found to be $0{\cdot}406 \pm 0{\cdot}003$, which is consistent with literature values.

The two-dimensional and three-dimensional results of the present work are not inconsistent. The disparity arises because, as noted above, in the limit of only one type of cube, the $50 \times 50 \times 50$ three-dimensional system is really 50 two-dimensional systems of size 50×50. Once any of the 50 systems percolates, the three-dimensional system is considered to percolate and consequently the void fraction that is reported as critical is actually the maximum void fraction of 50 two-dimensional systems averaged over many clusters of 50 systems. In the appendix, the mean of the maximum threshold for L systems of size $L \times L$ is compared with simulation results for systems of size $L \times L \times L$, and the two are found to be in reasonable agreement. Implicitly, different definitions of percolation are being used for the two-dimensional and three-dimensional work; this point is explored further in § 3.4.

2.2.2. Equal fractions of x and y cubes (figure 2(b)). In contrast to curve A, some sites for curve B are occupied by cubes with normals in the z direction, and these tend to inhibit conduction. Indeed, as the fraction of z cubes becomes very large (as the z vertex is approached in figure 1), conduction becomes increasingly difficult. The permitted void fraction falls to zero when 96% of the grains have normals in the z direction.

It is surprising that conduction in the z direction is possible when as little as 4% of the cells can conduct along this axis. However, transport in the xy plane is facilitated by all three types of cubes and thus in the limit of no voids, connections in each xy plane are guaranteed. Conduction in the z direction is thus seen to be dependent on having only sufficient x and y cubes to ensure alignment of grains that conduct in the z direction in different layers, and consequently the fraction of such cubes at the threshold can be very small.

2.2.3. No cubes having planes normal to the y direction (figure 2(c)). The discussion pertaining to curve B, where the fraction of cubes with normals in the x and y directions were constrained to be equal, is germane to the present case where there are no y cubes. However, differences between the two curves arise because the behaviour of

combinations of x and y cubes is not always equivalent to the action of an equal fraction of just x or just y cubes. Systems of cubes of different type can contribute to trapping where systems of only one type of cube cannot. Consequently, the permitted void fraction for a given $(x+y):z$ ratio for curve B, where there is a mixture of cubes, is lower than the corresponding $x:z$ ratio for curve C (see table 1). The difference in critical void fraction at zero fraction of z cubes is an artefact of the singular nature of this limit for curve D (see the earlier discussion of this point in § 2.2.1).

Table 1. Comparison of curves B and C in figure 1.

Fraction of z cubes	Void fraction	
	Curve B	Curve C
0.0	0.431	0.464
0.20	0.406	0.423
0.50	0.399	0.419

2.2.4. No voids present in the system (curve D in figure 1). The critical fraction of z cubes is reported as a function of the $x:y$ ratio. As discussed above, either x or y cubes can provide a path from one xy plane to an adjacent layer while conduction within a given xy plane is through a network of z cubes. The fraction of x or y cubes on curve D is small and so each cube may be considered to be acting independently and thus the two types of cube are equivalent. This independence contrasts sharply with curve A where, in the limit of a preponderance of y or x cubes, the presence of even small amounts of a second type of cube added a three-dimensional nature to the transport and so the different types of cells were not equivalent. One manifestation of the similarity of behaviour of x and y cubes for curve D is the invariance of the critical fraction of z cubes with respect to the $y:x$ ratio. The threshold ranges from 0.959 ± 0.003 at $y:x=1$, to 0.962 ± 0.003 at $y:x=0$, and because this variation is insignificant, no separate figure is shown for this curve.

3. The correlation length exponent

The universality hypothesis (see e.g. Fisher 1971) justifies the use of critical exponents to decribe the behaviour of percolating systems in the vicinity of the percolation threshold. Systems in the same universality class must have the same critical exponents, but the class to which a given system belongs should be independent of details such as the type of lattice used in the simulations, and whether site or bond percolation is being investigated. In the present work, the conductivity and correlation length exponents corresponding to the limit of no z cubes (curve A in figure 1) are found. The exponents are compared with those found for more conventional percolation problems.

The scaling relations used to find the critical exponents must explicitly include size dependence. The correlation length exponent, ν, was found from the relation

$$\sigma \propto L^{-1/\nu} \tag{1}$$

where σ is the standard deviation of independent estimates of the percolation threshold

(Levinshtein *et al* 1976). Thus, the exponent was calculated by finding the percolation threshold for a number of independent configurations at each of a range of system sizes. The individual thresholds were found to a precision of ±0.001 at 95% confidence. The smallest standard deviation found was 0.007, so that the calculated standard deviation was not inflated by random fluctuations in the individual thresholds. A weighted least-squares analysis was used to find the exponent. Following Bevington (1969), the weighting an individual data point received was chosen to be proportional to the reciprocal of the error associated with that point.

The uncertainty in the standard deviation, Δ_σ, was estimated to be $\sigma/\sqrt{2n}$, where n is the number of estimates of the threshold from which the standard deviation was calculated. Levinshtein *et al* (1976) showed that this simple expression for Δ_σ is a good approximation to the exact expression. In the present work, Δ_σ was kept constant for different system sizes. The error in the logarithm of the standard deviation, however, is Δ_σ/σ. Thus, counterintuitively, larger systems, which have small standard deviations, contribute more to the inaccuracy of the slopes of the least-squares lines than results for smaller systems.

The procedure for finding the critical exponents was validated by finding the exponent for the truly two-dimensional site percolation problem. The standard deviations of values of the percolation threshold corresponding to independent configurations were found for a range of different system sizes. The results are shown as the uppermost plot on figure 3. The weighted least-squares line based on the four largest

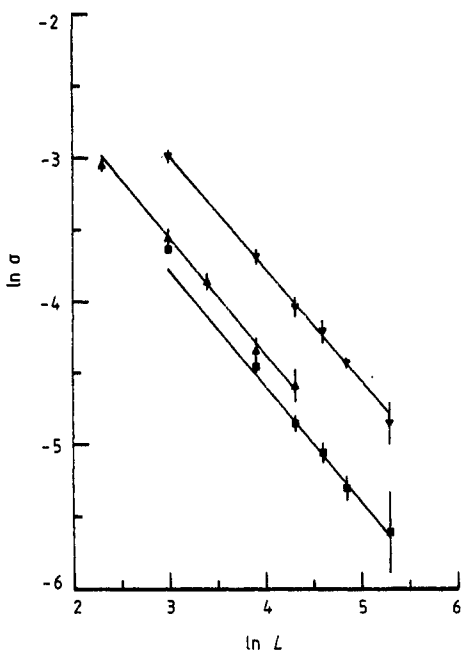

Figure 3. Scaling plots of standard deviation against system size for a system where all conducting cubes have normals in the x direction. The uppermost plot is based on two-dimensional simulations and yields $\nu = 1.3 \pm 0.16$. The middle plot is based on the data from the three-dimensional code and gives $\nu = 1.25 \pm 0.11$. The lowest plot corresponds to data for a three-dimensional system predicted from the two-dimensional data in the top curve (see appendix). The slope of this plot gives $\nu = 1.23 \pm 0.2$.

systems (75, 100, 128 and 200) gives an exponent of $\nu = 1.30 \pm 0.16$ which is consistent with the accepted result of $\frac{4}{3}$.

As noted earlier, the three-dimensional system where all conducting cubes have their normal in the x direction is really a composite of many two-dimensional systems. Plotting the data for this system (middle curve in figure 3) and attributing a physical significance to the slope is of questionable validity. For completeness, the three-dimensional result is reported in table 2 below, though the more appropriate figure is perhaps $\nu = 1.30 \pm 0.16$ found for truly two-dimensional systems.

The investigation of the correlation length exponent for other three-dimensional systems was restricted to cases where there were no cubes with normal in the z direction. Systems of size 10, 20, 30 and 50 were used except for the cases where all conducting cubes had normals in the x direction, where data for a system of size 75 were also collected. The exponents reported in table 2 are based on a weighted least-squares fit through all system sizes except the smallest. The data for the case of an equal fraction of cubes having normals in the x and y directions are plotted in figure 4.

The value of the exponent ν in three dimensions was found to be 0.89 ± 0.01 by Heermann and Stauffer (1981) for random site percolation on a cubic lattice. Gaunt

Table 2. Correlation length exponents.

x fraction	0.5	0.6	0.75	0.9	1.0
y fraction	0.5	0.4	0.25	0.1	0.0
Exponent, ν	0.88 ± 0.11	0.84 ± 0.10	0.87 ± 0.08	0.89 ± 0.09	1.25 ± 0.11

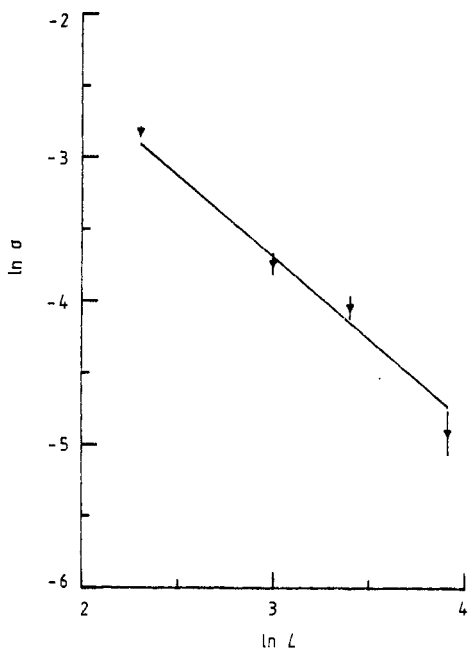

Figure 4. Scaling plot of standard deviation against system size for a system where an equal number of grains have normals in the x and y directions. The slope is based on data for the three largest systems and corresponds to an exponent $\nu = 0.88 \pm 0.11$.

et al (1981) report a value of 0.86 ± 0.06 for the same exponent. The values calculated here are consistent with both of these results, except for a fraction of x cubes greater than 0.9. Consequently, the system of planar conductors, which may be viewed as a special bond-site percolation problem, is in the same universality class as traditional three-dimensional site or bond percolation problems. This result is consistent with the two-dimensional bond-site percolation studies of Guttmann and Whittington (1982).

4. The conductivity exponent

For any system under the percolation surface of figure 1, transport is possible. Viewing the centre of the cubes as nodes and representing viable paths between adjacent active sites by links allows the assembly of cubes to be approximated by a resistor network. Application of periodic boundary conditions and solution of Kirchoff's current laws yields the conductivity of the system.

For an infinite system, the conductivity Σ follows the scaling law

$$\Sigma \propto (p_c - p)^t \tag{2}$$

where p is the probability of a site being vacant, p_c is the critical void fraction for a truly infinite system, and t is the conductivity exponent. The scaling relation for a finite-sized system is (Green 1971)

$$\Sigma = L^{-t/\nu} F((p_c - p) L^{1/\nu}) \tag{3}$$

where p_c is the critical void fraction for a truly infinite system and F is a scaling function. The scaling function is unity if the argument is zero. Consequently the exponent t/ν may be found by performing simulations for a range of system sizes where the void fraction, p, is chosen to be the critical void fraction for the infinite system. The infinite-system void fraction may be found by extrapolating the results of finite-sized systems. An alternative approach, which was adopted in the present study, is to perform simulations with the void fraction p set to the critical void fraction corresponding to the system size, $p_c(L)$. Use of the scaling relation $p_c - p_c(L) \propto L^{-1/\nu}$ indicates that with this choice of p, the term in square brackets in equation (3) is constant, and in this limit the scaling law reduces to a simple relation between L and Σ.

The conductivity was calculated for the case where the fraction of cubes with normal in the z direction was zero. For each ratio of $y:x$ cubes the mean conductivity was found by calculating the conductivity for a number of independent configurations. The procedure was repeated for a range of different system sizes, with the void fraction p set to the critical void fraction corresponding to that system size, $p_c(L)$. The values of $p_c(L)$ had been found to an accuracy of ± 0.001 during the investigation of the correlation length exponent. Of course, at any given system size, not all configurations percolated. The flux through a percolating system (and hence the conductivity) was found by solving Kirchoff's laws for the system by using the ITPACK sparse matrix solver (Kincaid *et al* 1982). The conductivity for each system size was averaged until the error was less than 5% at 95% confidence, and the result was multiplied by the fraction of non-percolating configurations so that the reported conductivity was averaged over all configurations.

The slopes of the scaling plots were found using a weighted least-squares analysis for systems of size 15, 20 and 30. The results are listed in table 3. The exponent for the system with $y = 0.5$ changed by less than 2% when the system of size 10 was included, and so the regression is stable. Figures 5 and 6 are the plots for the fraction of cubes with normals in the y direction being 0.5 and 1.0 respectively.

Derrida *et al* (1983) report a value of 2.2 ± 0.1 for t/ν for a three-dimensional system of resistors and insulators while Pandey and Stauffer's (1983) result for the problem of diffusion on a three-dimensional simple cubic lattice was 2.3 ± 0.2. Thus, as for the correlation length exponent, the system behaves in a three-dimensional fashion until the fraction of cubes with normal in the x direction is greater than 0.9.

The third column in table 3 corresponds to the case where all the cubes have their normal in the x direction, but for each system the void fraction was set equal to the two-dimensional infinite-system result (0.407 25) rather than using the size-dependent

Table 3. Exponent t/ν for different systems.

Fraction of x cubes	0.5	0.9	1.0–∞
Exponent, t/ν	2.31 ± 0.10	2.11 ± 0.10	0.94 ± 0.06

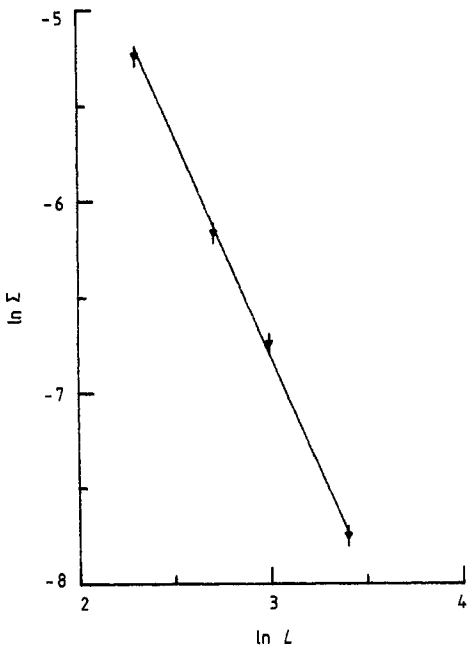

Figure 5. Conductivity as a function of system size for a system with no cubes with normals in the z direction, and equal fraction of cubes having normals in the x and y directions. The slope yields a value of $t/\nu = 2.3 \pm 0.1$.

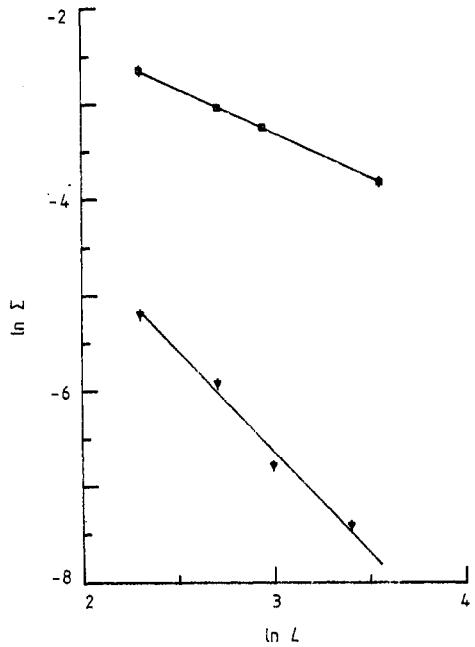

Figure 6. Plot of conductivity against system size for a system where all cubes are normal to the x direction. The void fraction was set to the system size-dependent threshold $p_c(L)$ for the lower curve and yields $t/\nu = 2.1 \pm 0.1$. It is impossible to ascribe physical significance to this result (see text). For the upper plot the void fraction was set to the two-dimensional infinite-system result (0.407 25) giving $t/\nu = 0.94 \pm 0.08$.

thresholds. As noted earlier, the case of all cubes having normals in the x direction is a two-dimensional problem and the system of size $L\times L\times L$ is really L systems of size $L\times L$. The size-dependent thresholds found from the three-dimensional simulations $p_c(L)$ do not correspond to half of the L two-dimensional systems percolating. Consequently the use of size-dependent thresholds $p_c(L)$ in equation (3) are inappropriate. This point is further discussed by Durand (1989). Setting the void fraction to the two-dimensional infinite-system result in the three-dimensional simulations yielded an exponent (t/ν) of 0.94 ± 0.06 which is consistent with the two-dimensional result of Lobb and Frank, (1984) of $0.973^{+0.005}_{-0.003}$. The change in the exponent from a three-dimensional value to a two-dimensional result in the singular limit of the fraction of cubes with normal in the x direction being 1.0 is consistent with the results presented above for the correlation length exponent, and also with the findings of Guttmann and Whittington (1982) discussed earlier.

5. Effective medium theory (EMT) approximation

A simple analytical analysis of planar conductors based on a modification of effective medium theory (EMT) (for a review, see Landauer (1978)) may be used to find the percolation surface. The approximate surface is compared with the simulation (exact) results to provide insight into the particle-particle interactions that must be incorporated to represent the behaviour of the system.

EMT gives an implicit expression for the effective conductivity (k_m) of a multiphase material as a function of the volume fractions (ϕ_i) and conductivities (k_i) of each of the phases. The present system of anisotropic cells may be considered to be a material composed of four different phases, namely voids and cubes with normals in the x, y and z directions. Cubes with normals in the x and y directions conduct in the z direction, and as cells are considered to act in isolation in the effective medium theory approach, the two types of cube are equivalent. Each of these phases is assigned a conductivity k which is the product of the two-dimensional (planar) conductivity and the number of planes per unit length in a cube. The conductivity of cubes with normals in the z direction and voids is zero. Denoting the fraction of cubes with normals in the x direction by $x(1-v_f)$ where v_f is the fraction of voids, the EMT equation for the effective conductivity, k_m, is

$$x(1-v_f)\left(\frac{k-k_m}{k+2k_m}\right)+y(1-v_f)\left(\frac{k-k_m}{k+2k_m}\right)+z(1-v_f)\left(\frac{-k_m}{2k_m}\right)+v_f\left(\frac{-k_m}{2k_m}\right)=0. \tag{4}$$

The last equation may be rearranged to yield

$$\frac{k_m}{k}=\frac{1-a}{1+2a} \qquad \text{where} \qquad a=\frac{v_f+z(1-v_f)}{(x+y)(1-v_f)}. \tag{5}$$

At the threshold, the effective conductivity k_m falls to zero and so equation (5) may be used to find the critical void fraction,

$$v_{f(\text{critical})}=(1-2z)/2(1-z). \tag{6}$$

The percolation surface given by equation (6) is shown as figure 7, which should be compared with the simulation results presented in figure 1. When the fraction of cubes with normal in the z direction is zero, (curve A in figure 1), the critical void fraction is $\frac{1}{2}$, which compares well with the simulation result of approximately 0.43.

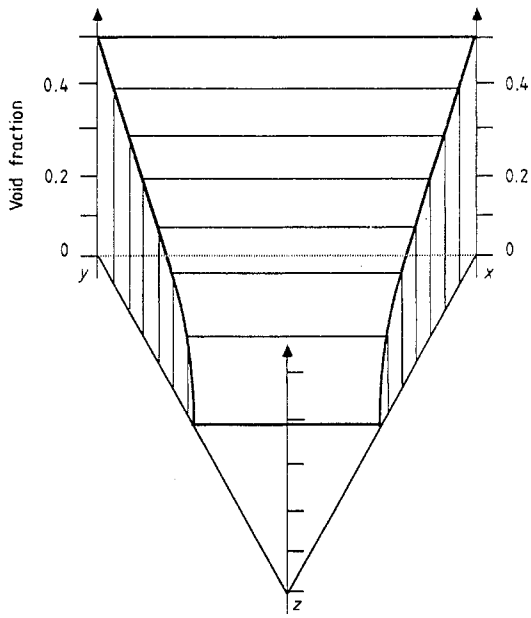

Figure 7. Schematic of the percolation surface predicted by effective medium theory.

The result for the critical fraction of cubes with normal in the z direction (curve D in figure 1) is 0.5 which is considerably less than the simulation result of 0.96. The EMT approximation for curve D in figure 1 is unsatisfactory because no distinction is drawn between cubes with normals in the z direction and voids. Cells that are void do not conduct in any direction, whereas cells that are normal to the z direction facilitate transport by providing paths in the xy plane.

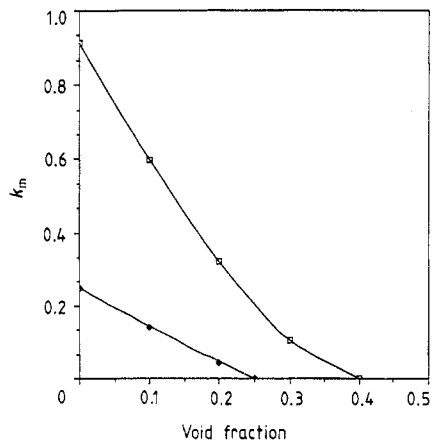

Figure 8. Comparison of effective medium theory predictions (full diamonds) and resistor network calculations (open squares) for the conductivity of a system with equal amounts of cubes with normals in the three cartesian directions. The conductivity of the assembly of cubes is normalised by the effective conductivity of one cube (see text). The lines interpolate between the data points.

The EMT and resistor network approaches can also be compared by computing effective conductivities. A sample of material containing equal amounts of the three types of cube with varying amounts of voids was studied. Such a composition might arise from a manufacturing process where a totally random mixture of the different cubes is obtained but some control over the void fraction is possible. The resistor network calculations were based on a system of 27 000 cubes. The effective conductivity for the zero voids case was found to be $0.91 \pm 4\%$ of the conductivity k of the individual cubes and the threshold void fraction was 0.401 ± 0.003. The simulation and EMT results are compared in figure 8. The failure of the approximate theory is again due to ignoring the difference between cubes with normals in the z direction and voids.

6. Conclusions

The percolation surface was found for an assembly of voids and planar conducting cubes with normals in any of the three cartesian directions. The simulation results emphasise that the extreme anisotropy of the individual conductor has little effect on transport through the system. The effective conductivity with three types of cubes present, but zero void fraction, is 90% of the value for conduction in the preferred direction, however the role of voids is pronounced. The implication of these results is that effort should be expended to develop manufacturing techniques that eliminate voids rather than seeking to align individual conductors.

Studies of the correlation length and conductivity exponents for systems of planar conductors where no cubes have normals in the conduction direction indicated that the behaviour of the material was in general three dimensional. Systems of voids and only one type of cube were found to have critical exponents corresponding to two-dimensional systems.

An effective medium treatment of the problem of planar conductors gave simple analytic results for the percolation surface and the effective conductivity. The theory does not distinguish between cubes with normals in the x or y directions or between voids and cubes with normals in the z direction. Such a simplification does not account for conduction in the xy plane by z cubes and hence gives rise to increasingly poor predictions as the ratio of cubes with normals in the conduction direction to voids increases.

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Appendix. Behaviour when all occupied cubes have normals in the y direction

The case of all active sites being occupied by cubes with normals in the y direction (or the x direction) is a truly two-dimensional problem. The data for the three-dimensional simulations of this system have been interpreted by assuming that a

three-dimensional system of size $L \times L \times L$ is really L independent systems of size $L \times L$. This was interpreted as meaning that once any of the two-dimensional systems had percolated then the three-dimensional system had also percolated. The critical void fraction that was reported for any configuration of the system of size $L \times L \times L$ was then the largest void fraction of any of the L independent systems. The validity of this explanation of the difference between the results for simulation of two-dimensional site percolation using a three-dimensional or two-dimensional code may be checked by finding the mean of the maximum threshold of L systems of size $L \times L$ and comparing with those found in the three-dimensional simulations. The individual estimates of the percolation threshold from the two-dimensional systems of size $L \times L$ were found to be distributed normally and so the mean of the maxima $\bar{m}$ may be found from the expression

$$\bar{m} = \int_{-\infty}^{\infty} dx\, xL\left[\int_{-\infty}^{x} dx \frac{1}{\sigma\sqrt{2\pi}} \exp\left(\frac{-(x-m)^2}{2\sigma^2}\right)\right]^{L-1} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(\frac{-(x-m)^2}{2\sigma^2}\right) \qquad \text{(A1)}$$

$$= E(x)$$

where m, the value for the mean of the distribution of the samples of size $L \times L$, will be taken to be the result for the mean percolation threshold from the true two-dimensional simulations. Similarly the standard deviation, σ, is the dispersion of thresholds for many independent two-dimensional configurations. The standard deviation of the maxima, σ_m, may be found from

$$\sigma_m^2 = E(x^2) - (\bar{m})^2. \qquad \text{(A2)}$$

Table 4 below compares the two-dimensional values for the mean threshold and the dispersion of the values of the critical void fraction from different configurations with three-dimensional results.

Table 4. Comparison of the two-dimensional and quasi-two-dimensional results.

System size	Two dimensions		Three dimensions			
			Predicted by (A1) and (A2)		Simulations in 3D	
L	$m \pm 0.003$	σ	$\bar{m}$	σ_m	m	σ
20	0.4048	0.050 08	0.5174	0.0233	0.5060	0.028 45
50	0.4059	0.024 89	0.4619	0.0116	0.4645	0.012 98
75	0.4064	0.017 57	0.4486	0.0078	0.4543	0.010 14

The predicted and actual three-dimensional values below agree to the second decimal place. The data for the standard deviations are plotted in figure 3, where the uppermost curve corresponds to the two-dimensional calculations, the squares denote the predicted data, and the middle curve with upward pointing triangles is the result of the three-dimensional simulations at $y = 1.0$.

The behaviour of the system with only one type of cube and voids is two dimensional, as verified by the agreement between the predictions and the data above and as given by the ratio of the correlation length and conductivity critical exponents. Consequently, the percolation threshold for the system should be the two-dimensional result.

In the limit of large system size, the three-dimensional percolation threshold might be expected to yield the two-dimensional result. However, there is no guarantee that this will be the case. Consider the scaling function for the percolation probability (Fisher 1971)

$$P = L^{-\beta/\nu} F((p_c - p)L^{1/\nu}) \tag{A3}$$

where β is the critical exponent for the percolation probability P. Conditions under which $p_c - p$ approaches zero as L increases are sought because then the three-dimensional result, p, converges on the two-dimensional infinite-system result. The form of $F(z)$ is unknown, but if a power law dependence z^q is postulated, it is clear that not all values of q will ensure the desired convergence or, more generally, there is no guarantee that extrapolating the three-dimensional results for the percolation threshold to infinite system size will yield the two-dimensional value. Indeed, plots of the percolation threshold against either the reciprocal of system size, or system size raised to $-1/\nu$, gave infinite-system results inconsistent with the correct value.

References

Bevington P R 1969 *Data Reduction and Error Analysis for the Physical Sciences* (New York: McGraw-Hill)

da Silva L R, Almeida N S and Tsallis C 1985 *Phys. Rev.* B **32** 4725-31

Derrida B, Stauffer D, Herrmann H J and Vannimenus J 1983 *J. Physique Lett.* **44** L701-6

Durand P P 1989 *PhD thesis* University of Pennsylvania

Farrington G C and Briant J L 1969 *Science* **204** 1371-9

Fisher M E 1971 *Critical Phenomena* (*Proc. Enrico Fermi Int. School of Physics*) ed M S Green (New York: Academic) pp 1-99

Frisch H L and Hammersley J M 1963 *J. Soc. Ind. Appl. Math.* **11** 894-918

Gaunt D S, Whittington S G and Sykes M F 1981 *J. Phys. A: Math. Gen.* **14** L247-50

Green M S (ed) 1971 *Critical Phenomena* (*Proc. Enrico Fermi Int. School of Physics*) (New York: Academic)

Guttmann A J and Whittington S G 1982 *J. Phys. A: Math. Gen.* **15** 2267-71

Hammersley J M and Welch D J A 1980 *Contemp. Phys.* **21** 593

Heermann D W and Stauffer D 1981 *Z. Phys.* B **44** 339-44

Johnson P M 1987 *MSE thesis* University of Pennsylvania

Landauer R 1978 *Electrical Transport and Optical Properties of Inhomogeneous Media* (*AIP Conf. Proc.* **40**) ed J C Garland and D B Tanner (New York: American Institute of Physics) pp 2-45

Levinshtein M E, Shklovskii B I, Shur M S and Efros A L 197 *Sov. Phys.-JETP* **42** 197-200

Lobb C J and Frank D J 1984 *Phys. Rev.* B **30** 4090-2

Middlemiss K M, Whittington S G and Gaunt D S 1980 *J. Phys. A: Math. Gen.* **13** 1835-40

Nakanishi H, Reynolds P J and Redner S 1981 *J. Phys. A: Math. Gen.* **14** 855-71

Pandey R B and Stauffer D 1983 *Phys. Rev. Lett.* **51** 527-9

Redner S and Stanley H E 1979 *J. Phys. A: Math. Gen.* **12** 1267-83

Stauffer D 1985 *Introduction to Percolation Theory* (London: Taylor and Francis)

Torrie G M, Gaunt D S, Guttmann A J and Whittington S G 1982 *J. Phys. A: Math. Gen.* **15** 2259-66

Tozer S W, Kleinsasser A W, Penney T, Kaiser D and Holtzberg F 1987 *Phys. Rev. Lett.* **59** 1768-71

Zhang X-W 1984 *J. Phys. A: Math. Gen.* **17** 3067-71

Ziff R M and Sapoval B 1986 *J. Phys. A: Math. Gen.* **19** L1169-72