Conduction in inhomogeneous materials: Hot and high-field spots

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Consider electrical conduction in a macroscopically inhomogeneous material with two randomly distributed phases of different conductivity. There will be regions with a particularly high generation of Joule heat (hot spots) and regions with a particularly high electric field (high-field spots). These spots are determined both by the conductivity at the spots themselves (local effects) and by the phase composition in the region surrounding the spots (long-range effects). We have studied the local and long-range effects in two and three dimensions, using analytical models with one and two inclusions in a uniform matrix and numerical calculations on random resistor networks. Hot and high-field spots are favored by long-range compositional fluctuations with borderlines similar to an hourglasslike double cone and with the cone axes along the applied field and the hot or high-field spot at the point where the apexes of the cones meet. The well-conducting phase dominates inside the cones, and the poorly conducting phase dominates outside. The opening angle of the cones is 90° in two dimensions and $2\arccos(1/\sqrt{3})=109°$ in three dimensions.

I. INTRODUCTION

In an inhomogeneous material, subject to an external field, a breakdown may occur. Mechanical and electrical breakdown has been modeled using two-dimensional regular networks of springs or resistors.[1–5] In the case of resistor models, initiation of the breakdown process has been attributed to resistors with high electric field strength[1–4] (high-field spots) or high generation of Joule heat[5] (hot spots). The resistor distributions giving rise to these spots are called "critical defects." Duxbury *et al.*[2] considered the random resistor network, i.e., a regular network with some resistors absent. They assumed that the most critical defect is when the missing resistors form a line. The more general problem of describing and predicting hot and high-field spots in a random two-component system where both components are conducting, is still largely unsolved. In this paper we model such systems by two- and three-dimensional two-component square and cubic networks and study those spatial fluctuations which give rise to high fields or hot spots. In particular we shall find how the field and Joule heat in a single resistor depend on the resistor itself (local effect) and on its surrounding network (long-range effect). We also use analytical results for inclusions in a matrix to study weakly inhomogeneous materials.

II. ANALYTICAL RESULTS

A. A single inclusion

Consider a uniform matrix of conductivity σ_m with a single circular inclusion (spherical in three dimensions) of conductivity σ_i. An electric field is applied, the field being E_0 far from the inclusion. Let R be the radius of the inclusion, r the distance to its center, and θ the angle between r and E_0 (Fig. 1). The exact results for the field **E** are well known.[6] Inside the inclusion it is uniform, directed along the external field. In two dimensions, let

$$f=(\sigma_i-\sigma_m)/(\sigma_i+\sigma_m)\ , \tag{1}$$

i.e., $1>f>-1$. Inside the circle ($E=|\mathbf{E}|$)

$$E=(1-f)E_0\ , \tag{2}$$

and outside the circle

$$E=[1+2f(R/r)^2\cos(2\theta)+f^2(R/r)^4]^{1/2}E_0\ . \tag{3}$$

In three dimensions, let

$$g=(\sigma_i-\sigma_m)/(\sigma_i+2\sigma_m)\ , \tag{4}$$

i.e., $1>g>-0.5$. The fields inside and outside the sphere are, respectively,

$$E=(1-g)E_0\ , \tag{5}$$

$$E=[1+2g(R/r)^3(3\cos^2\theta-1)+g^2(R/r)^6(3\cos^2\theta+1)]^{1/2}E_0\ . \tag{6}$$

From expressions above we get the local generation of Joule heat per area (volume), $P=\sigma E^2$. In two dimensions, and inside the circle

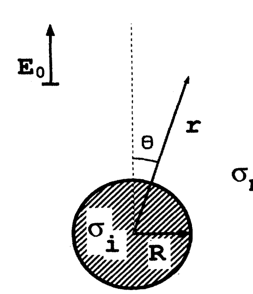

FIG. 1. Coordinates used to define the field $\mathbf{E}(r,\theta)$.

$$P=(1-f^2)\sigma_m E_0^2 \ . \quad (7)$$

In three dimensions, and inside the sphere,

$$P=(1+g-2g^2)\sigma_m E_0^2 \ . \quad (8)$$

Outside the circle (sphere) P is immediately obtained as $\sigma_m E^2$, with E given by Eqs. (3) or (6).

B. Influence of a neighboring inclusion

Let A be an inclusion with conductivity σ_A in a matrix of conductivity σ_m, and determine how it affects the field at another point B, where a "test inclusion" of conductivity σ_B is placed. The distance between the centers of A and B is r. B is assumed so small that it does not affect the field at A. In two dimensions, with θ as in Fig. 2, Eqs. (2) and (3) imply that the new field at B is

$$[1+2f_A(R/r)^2\cos(2\theta)+f_A^2(R/r)^4]^{1/2}(1-f_B)E_0 \ , \quad (9)$$

where

$$f_A=(\sigma_A-\sigma_m)/(\sigma_A+\sigma_m) \ . \quad (10)$$

As a lowest-order correction to mutual interactions between inclusions, we now let A and B have the same radius R, consider small R/r and let the field at A be changed due to the presence of B. Neglecting terms of the sixth order and higher in (R/r), and with f_B from Eq. (1) and $\sigma_i=\sigma_B$, the field at B is obtained as

$$[1+2f_A(R/r)^2\cos(2\theta)+2f_Bf_A(R/r)^4+f_A^2(R/r)^4]^{1/2} \times(1-f_B)E_0 \ . \quad (11)$$

Now, consider the lowest-order prefactor in Eqs. (9) and (11), i.e. $[1+2f_A(R/r)^2\cos(2\theta)]^{1/2}$. The locus of inclusions A which have the same influence on the field at B is given by $2f_A(R/r)^2\cos(2\theta)=C'$, or

$$r^2=C_2\cos(2\theta) \ , \quad (12)$$

where C' and C_2 are constants. Eq. (12), which has the mathematical form of a lemniscate, defines the locus of equal influence of an inclusion A on the field at B, cf. Figs. 4 and 5 below. Similarly, in three dimensions and from Eq. (6), the locus of equal influence is given by

$$r^3=C_3(3\cos^2\theta-1) \ , \quad (13)$$

where C_3 is a constant.

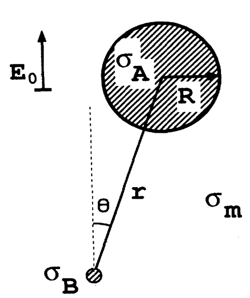

FIG. 2. Geometry used in the calculation of the influence of an inclusion A on the electric field at another inclusion B.

C. Hot and high-field spots: Local, boundary, and long-range effects

With local effects on hot spots we mean how the Joule heat P generated at a certain point (a hot spot) depends on the conductivity σ_i at the point itself. Inside a circular (spherical) inclusion in a uniform matrix, P is constant. It follows from Eqs. (7) and (8) that the maximum P is obtained when $\sigma_i=\sigma_m$ (two dimensions) and $\sigma_i=2\sigma_m$ (three dimensions). We next consider the Joule heat P in the matrix, just outside the boundary of a single circular (spherical) inclusion, i.e., at $r=R$. Joule heat maxima occur at $\theta=0°$ and $\theta=180°$ for $\sigma_i>\sigma_m$ and at $\theta=\pm 90°$ for $\sigma_i<\sigma_m$. We note that in these geometries there is always a point outside the inclusion with a P that is higher than inside the inclusion.

Long-range effects here refer to how the Joule heat at a certain point is affected by the phase composition away from that point. We rely on the discussion in Sec. II B. To get an enhanced field at B, and hence an enhanced Joule heat, we should have f_A positive in the regions where $\cos(2\theta)$ is positive and f_A negative where $\cos(2\theta)$ is negative cf. Eq. (9). Similarly, in three dimensions a hot spot at B is favored if g_A is positive where $\cos^2\theta>\frac{1}{3}$ and negative where $\cos^2\theta<\frac{1}{3}$ cf. Eq. (6). Thus, in three dimensions, hot spots are favored by compositional fluctuations such that there is an excess of the well-conducting phase inside two cones, with touching apexes and placed in an hourglasslike way with the cone axes along the external field. Outside these cones there should be an excess of the poorly-conducting phase. The opening angle of the cones is $2\arccos(1/\sqrt{3})=109°$. In two dimensions we get the analogous geometry, but with a cone opening angle of 90°. These angles were obtained also by Machta and Guyer.[7] They used a variational method to discuss the current distributions in double-cone geometries, emphasizing how the maximum current scales with the specimen size. The cone-shaped distributions of the phases can be considered as the central part of the lemniscate (12) and its three-dimensional counterpart (13).

A discussion of high-field spots parallels that of hot spots. The high-field spot is always favored by a low local conductivity, $\sigma_i<\sigma_m$. The largest possible field inside the inclusion is $2E_0$ in two dimensions and $1.5E_0$ in three dimensions, in both cases when $\sigma_i \ll \sigma_m$. Just outside the inclusion, and in two dimensions, the largest field is $2E_0$ at points $\theta=0°$ and $\theta=180°$ (for $\sigma_i \gg \sigma_m$) or at points $\theta=\pm 90°$ (for $\sigma_i \ll \sigma_m$), cf. Eq. (3). In three dimensions and for $\sigma_i \gg \sigma_m$, the largest field is $3E_0$ at points $\theta=0°$ and $\theta=180°$, while for $\sigma_i \ll \sigma_m$ the largest field is $1.5E_0$, at points $\theta=\pm 90°$.

III. DIMENSIONALITY

In one dimension, the current through each link is the same, and the hot and high-field spots always occur at the regions of largest resistivity, i.e. it is an entirely local effect. In the mathematical abstraction of a dimensionality tending to infinity, a resistor network has infinitely many parallel paths of a given length connecting two lattice nodes. Then the potential between two neighboring nodes is a constant. The hot spots arise at the links with the largest conductance. Thus, we have again an entirely local effect. In the case of a continuous medium we get similar results. The largest Joule heat is generated in an inclusion of conductivity[8] $\sigma_i=(N-1)\sigma_m$, where N is the dimension and σ_m refers to a uniform matrix.

In two dimensions there are important duality theorems. Dykhne[9] has defined a transform in which the Joule heat generation in each link is unchanged if all the phases are interchanged and the external field is turned 90°. For $c_1=0.5$, the square network is self-dual. This means that if there is a spatial fluctuation which gives a hot spot, the transformed network has a hot spot in the same position.[10] Since this is in a link of the other type, there is no preferred resistor type for the hot spot itself. For $c_1=0.2$ the corresponding dual network has $c_1=0.8$ and those two systems give equivalent results for hot spots. High-field spots become high-current spots when transformed.

IV. NUMERICAL CALCULATIONS

A. Network models

Numerical calculations are performed on resistor networks, following procedures used earlier.[11] Consider a square network with 200×200 nodes. The resistors are randomly assigned a high conductance s_1 or a low conductance s_2 so that their concentrations are c_1 and $c_2=1-c_1$. The potential in each node of the lattice is calculated by the Gauss-Seidel method. Periodic boundary conditions connect the network sides parallel to the external field. The effective conductance s_e is obtained from the total Joule heat. To avoid boundary effects we do not analyze results for the outermost 10 layers of resistors. Similar calculations are performed for three-dimensional simple cubic $53\times53\times53$ networks, again neglecting the ten outermost resistor layers. The calculations are done for a large number of statistically independent networks, for $c_1=0.2$, 0.5, and 0.8, and our results refer to averages over them. Hot and high-field spots are here[12] chosen to be the 1.2% links which generate the highest Joule heat or have the highest potential drop between its nodes.

B. Hot spots

First, consider local effects in a two-dimensional network. When c_1 is above the percolation threshold $p_c=0.5$ hot spots almost entirely occur at the well-conducting links, while when $c_1<p_c$ they occur at poorly-conducting links. When there are equal amounts of the two resistors in the square network, $c_1=p_c$, the hot spots equally often occur in poorly- and well-conducting links.

In three dimensions and above $p_c=0.2492$, hot spots occur in well-conducting links, while for $c_1<p_c$ the situation is more complicated. For conductance ratios s_1/s_2 close to unity hot spots are found at the well-conducting links and for large s_1/s_2 they occur in the poorly-conducting links.

As a further illustration of local effects on hot spots in two and three dimensions we consider square and cubic resistor networks in which each link is given any of 11 conductance values, logarithmically distributed from s to $100s$, and with equal probabilities. Figure 3 shows the distribution of the 1.2% hottest links above the conductance values. In two dimensions, the maximum in Fig. 2 is close to $s=s_e^{2D}$ and in three dimensions it is close to $s=2s_e^{3D}$, i.e. conductance values which would give a Joule heat maximum for a single inclusion in a continuum.

The long-range effect in two dimensions, related to the resistor distribution surrounding a hot spot has a characteristic double-cone shape with opening angle of 90° and cone axis along the applied field E, Figs. 4 and 5. Well-conducting links dominate inside the cone and poorly-conducting links dominate outside. This is in agreement with the findings in Sec. II B and II C for the influence of a single distant inclusion in a continuous medium. In three dimensions, our calculations show an analogous conical shape for the fluctuations in the resistor distribution, but now with an opening angle close to 109°. Since the argument about a single distant inclusion does not contain the cooperative effect of other inclusions, it should apply best to the case when the conductivities of the two phases are nearly equal. This is also found in our numerical calculations, where we have looked at the detailed resistor distribution near the hottest spot. When the conductivity ratio is 2, the distribution of the two kinds of links is rather well separated, with few links of the "wrong" type in the four sectors surrounding the hot spot in Figs. 4 and 5. With increasing conductivity ratio, the connectivity of the well-conducting phase becomes

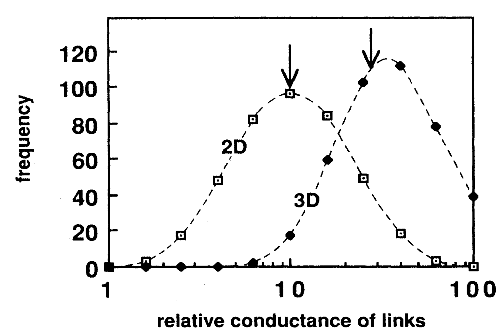

FIG. 3. Numerical calculations illustrating the local influence on the occurrence of a hot spot. In 200×200 and $53\times53\times53$ networks, each link is randomly and with equal probabilities assigned any of 11 conductance values with magnitudes s, $(100)^{1/10}s$, $(100)^{2/10}s$, , . . . , $100s$. The figure shows the distribution of hot spots (the 1.2% links with the largest Joule heat) over the 11 kinds of resistors, in two and three dimensions. Arrows indicate Joule heat maxima in the case of a single inclusion in a homogeneous matrix.

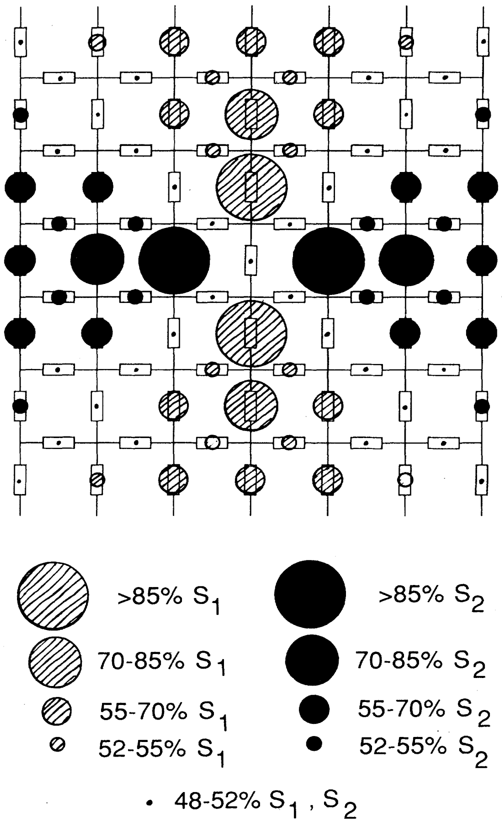

FIG. 4. Numerical calculations on resistor networks in which a resistor link takes one of two conductance values with probabilities $c_1 = c_2 = 0.5$. The figure refers to the resistor distribution surrounding hot spots, here defined as the 1.2% links with the largest generation of Joule heat. The hot spot itself is the vertical resistor in the center. Hatched circles denote an excess of well-conducting links and filled circles denote an excess of poorly-conducting links. The area of a circle is a measure of the excess concentration. The conductivity ratio is $s_1/s_2 = 10$. The figure represents an average of 40 statistically independent 200×200 networks.

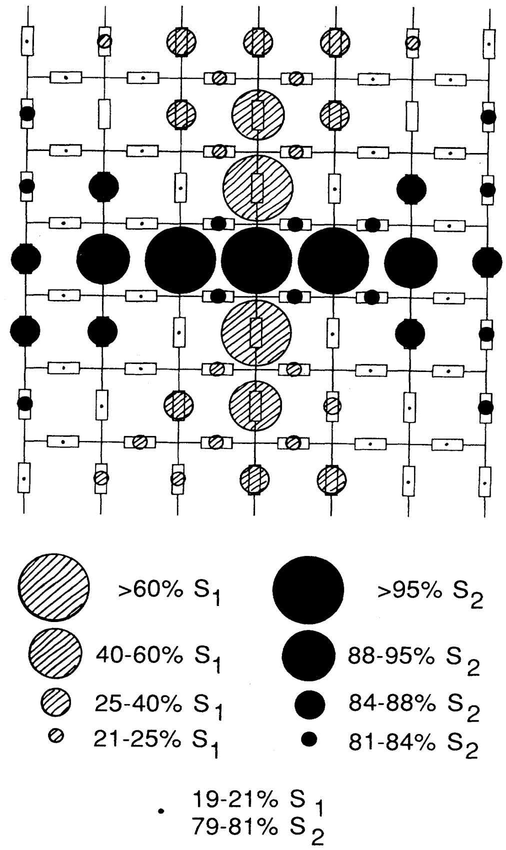

FIG. 5. As in Fig. 4 but with $c_1 = 0.2$ and $c_2 = 0.8$. (Results for $c_1 = 0.8$ agree with our discussion in the text but are not shown here.)

more important. For instance, for $s_1/s_2 = 100$, the hottest spot has a higher proportion of links of the "wrong" type in the four sectors. The well-conducting links form connected paths which are narrowed at the hot spot due to the blocking by poorly-conducting links. Then the distribution of Figs. 4 and 5 presents an average that is not necessarily realized around a specific hot spot.

C. High-field spots

The highest fields occur in the poorly-conducting phase, cf. Eqs. (2) and (3). The long-range effects are most effective in the cone-shaped geometry of the composition fluctuations found for hot spots. However, it is more important to have an excess of poorly-conducting resistors in the regions of the filled circles, than having an excess of well-conducting resistors in the regions of open circles in Figs. 4 and 5. It can be understood from Eq. (11). Note that for $\theta = 90°$ and when both f_A and f_B are negative, all terms in the large bracket have the same sign, while for $\theta = 0$, f_A positive and f_B negative, the third term in the bracket is negative.

V. CONCLUSIONS FOR REAL MATERIALS

Although our analysis has been for the idealized cases of dilute spherical inclusions in a uniform matrix and resistor networks, the results give a qualitative picture which should be valid also for real three-dimensional materials. Hot and high-field spots are due to both local and long-range effects. Let the overall effective conductivity of the material be σ_e. First, consider an average Joule heat P or electric field E over a region which contains many grains so that a local effective conductivity σ_l can be defined there. Then extreme P and E should occur in regions such that $\sigma_l = 2\sigma_e$, surrounded by compositional fluctuations of the conical (or lemniscate) shape discussed above. The same conclusion holds for a one-phase material in which the concentration of solute atoms varies spatially, leading to a continuously varying local conductivity σ_l.

If we are interested in regions small compared to the size of a single grain, the high P and E are likely to occur near phase boundaries. One still has long-range effects from compositional fluctuations of the type just mentioned, but now superimposed on the very important influence of the shape of the boundary and the precise phase distribution in its vicinity.

ACKNOWLEDGMENTS

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