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Conductivity for the site-percolation problem by an improved effective-medium theory

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The effective-medium theory has been presented by many authors and widely applied. In particular, the theory is accepted as a very good first approximation for the conductivities of inhomogeneous continuous media, of random-resistor networks, and of the bond-percolation problem. But the discrepancy between the conductivity given by theory and that of the site-percolation problem is substantial. In this Brief Report we improve the theory for this problem and propose three equations for the effective conductivity in the site-percolation problem. Although the three equations are empirical, the conductivities given by these equations agree well with data from computer simulations and actual experiments for the site-percolation problem except for the (extreme) vicinity of the critical percolation probability.

The effective-medium theory[1-3] (EMT) was applied to the problem of the conductivities of random-resistor networks by Kirkpatrick,[4] and the effective conductivity given by the EMT agrees well with the conductivities of random-resistor networks and of the bond-percolation problem except for the vicinity of the critical percolation probability. For the site-percolation problem, however, the conductivity given by the EMT disagrees substantially with the conductivity of random-resistor networks, and the EMT has been improved for this case.[5-8] Recently, we presented another way of improving the EMT.[9] In this Brief Report we derive, using the improved EMT, three empirical equations for the conductivity of the site-percolation problem, and compare the results with data from computer simulations or from actual measurements. The equation for the effective conductivity σ^* for a binary system is given by the EMT[4,5,10] in the form

$$\frac{\sigma^*-\sigma_1}{\sigma_1+(1/p_c-1)\sigma^*}p+\frac{\sigma^*-\sigma_2}{\sigma_2+(1/p_c-1)\sigma^*}(1-p)=0 \ , \quad (1)$$

where σ_1 and σ_2 are the conductivities of the components, p is the volume fraction of the component with σ_1 ($>\sigma_2$), and p_c is the critical percolation probability when $\sigma_2=0$. For the percolation problem in which $\sigma_2=0$, the normalized effective conductivity σ^*/σ_1 is obtained from (1) as follows:

$$\frac{\sigma^*}{\sigma_1}=\frac{p-p_c}{1-p_c}, \quad p\geq p_c \ . \quad (2)$$

Equation (2) is known to be a very good first approximation for the bond-percolation problem, but it cannot be applied to the site-percolation problem. For the purpose of extending the applicability of the equation even to the site-percolation problem, we presented an improved EMT[9] by replacing σ_i ($i=1,2$) in (1) with a certain conductivity σ_i^a ($i=1,2$) which includes not only the property of σ_i itself but also an averaged property of the medium in some form. Then Eq. (1) becomes

$$\frac{\sigma^*-\sigma_1^a}{\sigma_1^a+(1/p_c-1)\sigma^*}p+\frac{\sigma^*-\sigma_2^a}{\sigma_2^a+(1/p_c-1)\sigma^*}(1-p)=0 \ . \quad (3)$$

As a trial to determine suitable σ_i^a, it is effective to set σ_1^a and σ_2^a to an upper and a lower bound on σ^*, respectively, because the bounds were derived by the spatial average of some physical properties of the medium.[11,12] The upper bound is close to the more conductive conductivity σ_1 and the lower bound is close to the less conductive conductivity σ_2. The Wiener[11] and the Hashin-Shtrikman (HS)[12] bounds are representative bounds. The Wiener upper bound is the conductivity when the two components of the material are put in parallel to the applied field, and the lower bound is the conductivity when the two components are put in series to the applied field. The arrangements of the components are, respectively, the most conductive and the most resistive geometrical configuration. The HS bounds are the most restrictive ones that can be given only in terms of σ_1, σ_2, and p. Then σ_1^a and σ_2^a are given by

$$\sigma_1^a=p\sigma_1+(1-p)\sigma_2 \ , \quad (4)$$

$$\sigma_2^a=\frac{\sigma_1\sigma_2}{(1-p)\sigma_1+p\sigma_2} \quad (5)$$

for the Wiener bounds, and

$$\sigma_1^a=\sigma_1+\frac{d(1-p)\sigma_1(\sigma_2-\sigma_1)}{d\sigma_1+p(\sigma_2-\sigma_1)} \ , \quad (6)$$

$$\sigma_2^a=\sigma_2+\frac{dp\sigma_2(\sigma_1-\sigma_2)}{d\sigma_2+(1-p)(\sigma_1-\sigma_2)} \quad (7)$$

for the HS bounds, where d is the dimensionality. For the percolation problem ($\sigma_2=0$) we denote by σ_{I}^* and σ_{II}^* the normalized conductivities obtained from (3), (4), and (5) and (3), (6), and (7), respectively. Then σ_{I}^* and σ_{II}^* are given, respectively, by

$$\sigma_{\mathrm{I}}^*=\frac{p(p-p_c)}{1-p_c}, \quad p\geq p_c \quad (8)$$

and

$$\sigma_{\mathrm{II}}^*=\frac{(d-1)p(p-p_c)}{(1-p_c)(d-p)}, \quad p\geq p_c \ . \quad (9)$$

Next we use

$$\sigma_1^a=\frac{p+p_c}{1+p_c}\sigma_1 \quad (10)$$

and

$$\sigma_2^a=0 \quad (11)$$

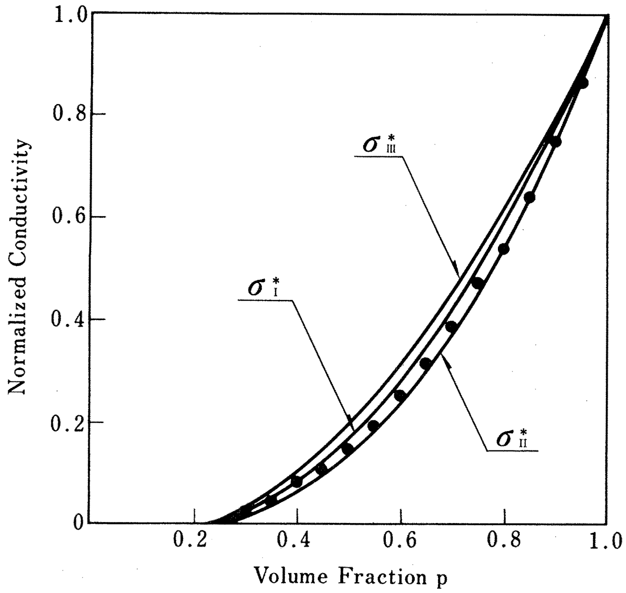

FIG. 1. Normalized conductivity against p for $p_c = 0.24$. The data points are results from a computer simulation for a body-centered-cubic network (Ref. 13).

to obtain Watson-Leath's (WL) result.[6] When we express by $\sigma_{III}{}^*$ the normalized conductivity obtained from (3), (10), and (11), σ^*_{III} is

$$\sigma_{III}{}^* = \frac{p^2 - p_c^2}{1 - p_c^2}, \quad p \geq p_c \ . \tag{12}$$

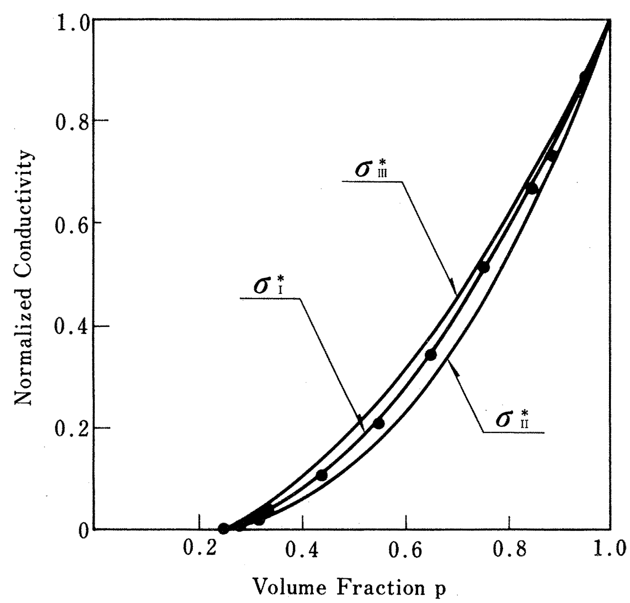

FIG. 2. Normalized conductivity against p for $p_c = 0.251$. The data points are results from an actual measurement for a mixture of hard, insulating, and conducting particles (Ref. 14).

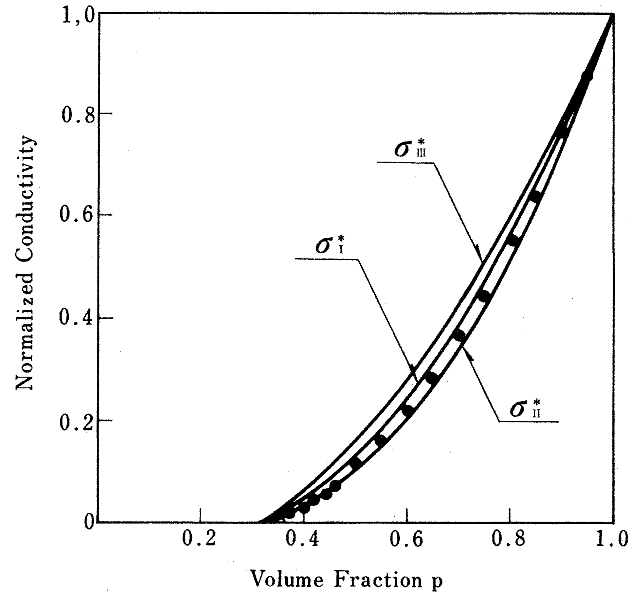

FIG. 3. Normalized conductivity against p for $p_c = 0.32$. The data points are results from a computer simulation for a simple cubic network (Ref. 13).

When

$$p_c = \sqrt{(\pi - 2)/\pi} \ , \tag{13}$$

Eq. (12) becomes WL's equation[6,7]

$$\frac{\sigma^*}{\sigma_1} = \frac{\pi}{2} p^2 - \frac{\pi - 2}{2}, \quad p \geq \sqrt{(\pi - 2)/\pi)} \ . \tag{14}$$

In Figs. 1–6 we compare $\sigma_I{}^*$, $\sigma_{II}{}^*$, and $\sigma_{III}{}^*$ with data from computer simulations and actual experiments. In all the figures the solid lines are $\sigma_{III}{}^*$, $\sigma_I{}^*$, and $\sigma_{II}{}^*$ against p in order of decreasing conductance, and the data points are results from computer simulations or actual measurements for six types of site percolation. Figures 1, 2, and 3 illustrate

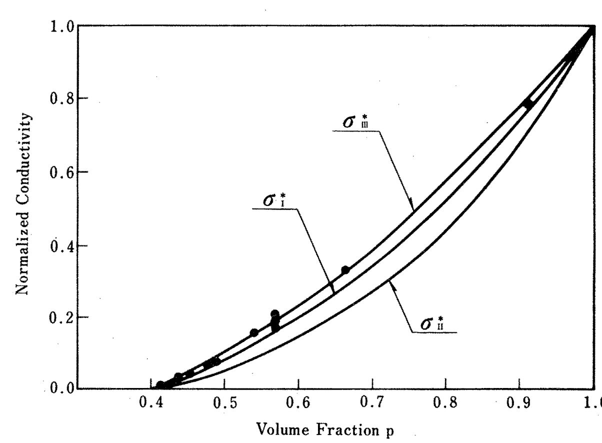

FIG. 4. Normalized conductivity against p for $p_c = 0.407$. The data points are results from an actual measurement for a two-dimensional continuum system (Ref. 15).

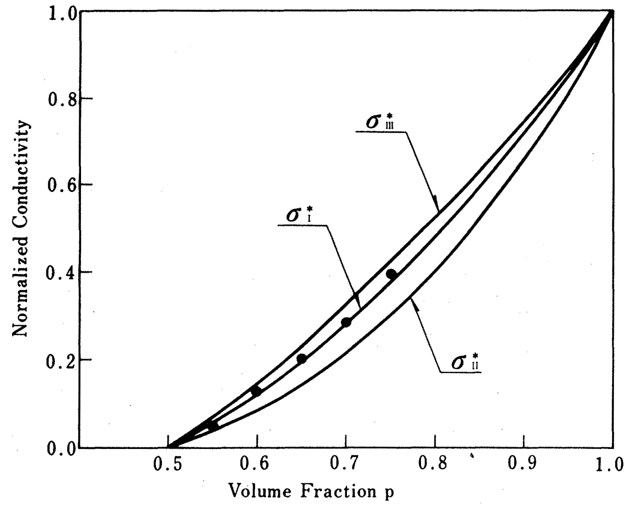

FIG. 5. Normalized conductivity against p for $p_c = 0.5$. The data points are results from a computer simulation for a two-dimensional Voronoi tessellation (Ref. 16).

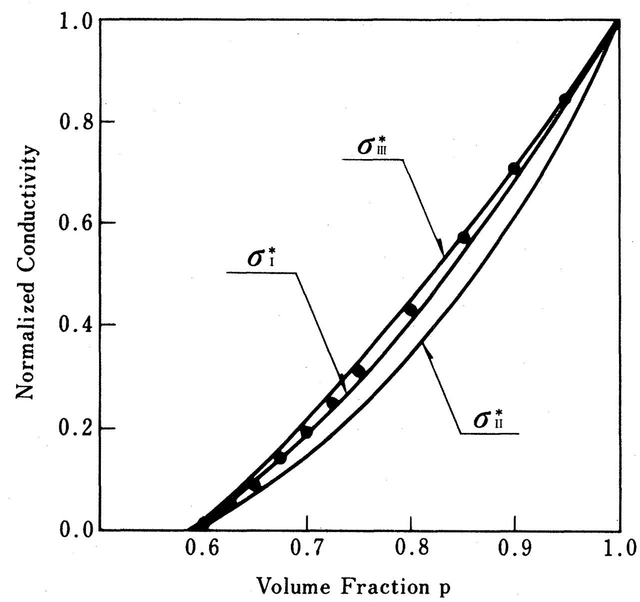

FIG. 6. Normalized conductivity against p for $p_c = 0.591$. The data points are results from a computer simulation for a square network (Ref. 17).

three-dimensional (3D) problems and Figs. 4, 5, and 6 denote two-dimensional (2D) problems. In 3D, $\sigma_{\rm I}{}^*$ and $\sigma_{\rm II}{}^*$ agree well with the data; so do $\sigma_{\rm I}{}^*$ and $\sigma_{\rm III}{}^*$ in 2D. For the vicinity of p_c the behaviors of the three equations are linear with the increase of $p - p_c$. However, except for a narrow region near p_c, the three equations can be well applied to the conductivities of the site-percolation problem.

In this Brief Report we empirically derived the conductivities for the site-percolation problem, and the conductivities agree well with data from computer simulations and from actual measurements. More theoretical and deductive methods are left open for future work.

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[1]R. Landauer, J. Appl. Phys. 23, 779 (1952).

[2]R. Landauer, in *Electrical Transport and Optical Properties of Inhomogeneous Media,* edited by J. C. Garland and D. B. Tanner (AIP, New York, 1978).

[3]M. Nakamura, Phys. Rev. B 28, 2216 (1983).

[4]S. Kirkpatrick, Rev. Mod. Phys. 45, 574 (1973).

[5]A. Davidson and M. Tinkham, Phys. Rev. B 13, 3261 (1976).

[6]B. P. Watson and P. L. Leath, Phys. Rev. B 9, 4893 (1974).

[7]J. Bernasconi and H. J. Wiesmann, Phys. Rev. B 13, 1131 (1976).

[8]C. G. Granqvist and O. Hunderi, Phys. Rev. B 18, 1554 (1978).

[9]M. Nakamura, J. Phys. C 15, L749 (1982).

[10]J. Koplik, J. Phys. C 14, 4821 (1981).

[11]M. Beran, Nuovo Cimento 38, 771 (1965).

[12]Z. Hashin and Shtrikman, J. Appl. Phys. 33, 3152 (1962).

[13]A. B. Harris and S. Kirkpatrick, Phys. Rev. B 16, 542 (1977).

[14]H. Ottavi, J. Clerc, G. Giraud, J. Roussenq, E. Guyon, and C. G. Mitescu, in Ref. 2.

[15]L. N. Smith and C. J. Lobb, Phys. Rev. B 20, 3653 (1979).

[16]P. H. Winterfeld, L. E. Scriven, and H. T. Davis, J. Phys. C 14, 2361 (1981).

[17]Y. Yuge and K. Onizuka, J. Phys. C 11, L763 (1978).