ISSN: 2834-4928

Research Article

Journal of Electrical Electronics Engineering

Model of Local Stiffness Enhancement in Porous Composite Materials with Low Dielectric Constant via Breaking of "Soft" Bonds

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Submitted: 2025, Nov 04; **Accepted:** 2025, Dec 08; **Published:** 2025, Dec 16

Citation: Arkhincheev, V. E. (2025). Model of Local Stiffness Enhancement in Porous Composite Materials with Low Dielectric Constant via Breaking of "Soft" Bonds. *J Electrical Electron Eng, 4*(6), 01-03.

1. Introduction

As is known, to increase computer speed during the transition to the nanoscale, modern electronics utilize dielectrics with low dielectric constant (low-k dielectrics) [1-5]. The use of materials with low dielectric constant helps solve a number of problems: reducing RC signal delay, reducing power losses, and reducing noise. An important property of low-k materials is their porosity, which ensures the low value of the dielectric constant. However, the presence of pores, in turn, reduces the stiffness of the materials. The mechanical properties of low-k materials are crucial for their integration into semiconductor devices, as they must withstand manufacturing stresses (e.g., CMP, thermal cycling) and prevent delamination or cracking during operation.

The most straightforward way to increase the stiffness of a material and, accordingly, its Young's modulus is to increase the Young's modulus of the original dielectric matrix Eo, which is based on SiO_2 molecules. Therefore, attempts have been made to replace oxygen bonds with carbon bonds to enhance the stiffness of the matrix [6-9]. However, it turned out that "rigid" fragments do not provide sufficient stiffness due to their low concentration and because they are embedded in a "soft" matrix. The improvement of elastic characteristics (Young's modulus) in low-k materials through the strengthening of local bonds is described in detail in [10].

The aim of this article is to investigate the influence of porosity, an increase of which leads to the breaking of additional atomic bonds, on the stiffness of the system. A model of a two-dimensional lattice with a random arrangement of stiff springs with stiffness coefficient K1 and soft springs with stiffness coefficient K2 was studied. (In relation to low-k materials, soft springs model oxygen bonds in the original matrix, while stiff springs correspond to carbon bonds.) It is shown that the random breaking of springs in a composite medium of randomly arranged stiff and soft springs leads to an unexpected result—a local increase in the stiffness of the system.

2. Model of Elastic Disordered Media

Consider a 2D planar lattice shown in Fig. 1. Here, stiff springs with stiffness coefficient K_1 are shown in red, and soft springs with stiffness coefficient K_2 are shown in black. The concentration of stiff springs is 1/3 of the total number of springs in the considered simple model.

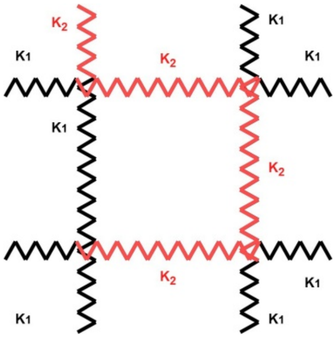

Figure 1: A Lattice of Randomly Arranged Stiff and Soft Springs

Next, we randomly break 1/4 of the bonds; one of the possible configurations is shown in Figure 2 as an example.

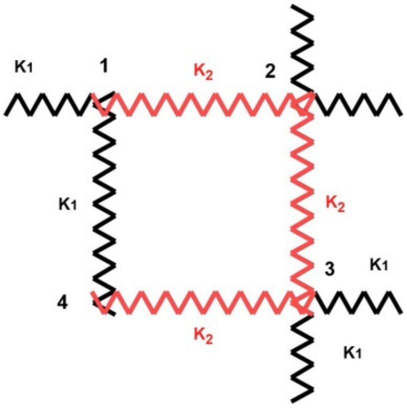

Figure 2: A Lattice Configuration with Broken Bonds

According to the known rules for series (and parallel) connections of springs, we calculate the stiffness of springs 1-4 and 4-3 connected in series: $K_{13} = \frac{K_1 K_2}{K_1 + K_2}$. We obtain the connection scheme shown in Figure 3a.

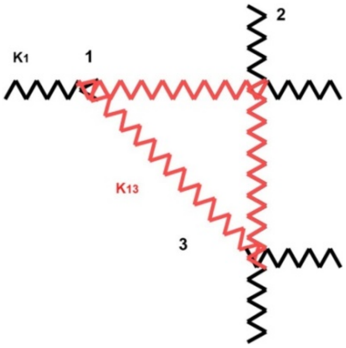

Figure 3a: “Triangle" connection scheme of springs

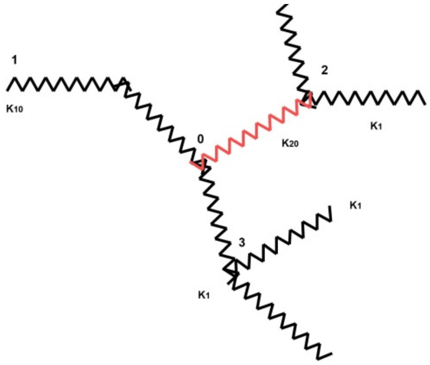

Figure 3b: "Star" connection scheme of springs

We then transform the "triangle" connection into a "star" connection with values equal to $K_{10} = K_{30} = \frac{K_2}{2}\left(1 + \frac{2K_1}{K_1 + K_2}\right)$ and $K_{20} = \frac{K_2}{2}\left(1 + \frac{2(K_1 + K_2)}{K_1}\right)$.

In the limiting case of a strong difference in spring stiffness , we obtain approximate expressions:

$$K_{10} = K_{30} \approx \frac{K_2}{2} \qquad (1)$$

$$K_{20} \approx \frac{K_2^2}{K_1} = K_2 \frac{K_2}{K_1} >> K_2 \qquad (2)$$

Thus, we obtain an interesting result—a local increase in the stiffness coefficient and, accordingly, the Young's modulus due to the breaking of "soft" bonds alongside "stiff" bonds in the newly formed elastic percolation cluster. This mechanism corresponds to experimental results—see Fig. 3.2 of the review article [10].

As is known, experimental values of the Young's modulus for the original SiO_2 matrix range from Y_1 = 5-10 GPa, while rigid inclusions such as hyperconnected 1-3-5 Benzene, 1-2-5-6-Pentalene, and 1-4-6-9-Naphthalene possess significantly higher Young's modulus values of Y_2 = 35-55 GPa [11,12]. The calculations presented above allow for a qualitative assessment of the possible contribution of hyperconnected-type inclusions and the influence of porosity on the stiffness of the entire system.

3. Conclusion

Let's discuss the obtained results. An increase in the porosity of low-k materials corresponds to the additional breaking of atomic bonds; in our model, this is the breaking of springs. With a random arrangement of "stiff" and "soft" springs, and in the case where there are fewer "stiff" springs than "soft" ones, the random breaking of any springs increases the effective proportion of "stiff" ones and, accordingly, can increase the overall stiffness of the system. The proposed mechanism of local stiffness enhancement confirms this hypothesis and, consequently, the somewhat paradoxical result—an increase in the overall stiffness of the system with an increase in broken springs (porosity). One can imagine that at a certain level of porosity, the formed elastic percolation cluster provides increased stiffness due to the proposed local stiffness enhancement mechanism. However, it is obvious that with a further increase in porosity, stiffness loss should occur due to further bokkkd breaking. Therefore, there must be an optimal value of porosity for the dielectric matrix with stiff inclusions to achieve the overall system stiffness and the maximum Young's modulus value. Thus, the task of finding this optimal porosity value arises. It should also be emphasized that for the overall stiffness of materials, global connectivity of the stiff bonds is necessary.

Acknowledgement: The author expresses gratitude to Prof. M.R. Baklanov and Mungunsuvd Gerelt-Od (MIREA) for numerous discussions on this topic.

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