ACTUAL PROBLEMS OF SOLID STATE PHYSICS



Estimation of the percolation threshold for mixed site-bonds problems using polynomial mappings

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Many properties of composite materials such as electrical conduction, dielectric response and others are closely related to the geometrical arrangement of the constitutive phases. Percolation theory, whose objective is to characterize the connectivity properties in random geometries and to explore them with respect to physical processes, thus provides a natural frame for the theoretical description of random composites.

In recent years, great progress has been made in the field of numerical methods of percolation theory; however, analytical descriptions for many important cases still remain open. In particular, mixed problems, in which both nodes and bonds can be removed from the lattice, are resource-demanding for numerical experiments and require at least rough methods of analytical estimates.

In this work we propose applying the generalized renormalization group method to obtain the position of the percolation threshold for a mixed problem. The work considers mixed percolation problems on square and cubic lattices. Polynomial mappings were constructed for the relationship between the probability p_{n+1} of a renormalized cell conductance at n+1 iteration and p_n at the n-th iteration. The percolation threshold was calculated as the position of the real-space fixed points of the mentioned polynomial mapping.

The estimates were verified using a numerical method based on the construction of regular graphs of the corresponding lattices for different probabilities (Figure) of filling with conducting nodes and connections.

Two direct modelling approach for mixed percolation studies were developed and tested on square and cubic lattices. Time complexity of both algorithms increases no faster than $O(V^{1.04})$, which means good scalability. New analytical estimation approach was developed for mixed percolation problem on the basis of fixed-points analysis of polynomial maps. It was established that there is an imaginary fixed point, which limits the percolation threshold from below and real fixed point, which limits the percolation threshold from above.

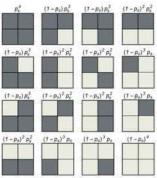


Figure. Probabilities of different configurations of 2x2 cell

References

[1] Gould, H., Tobochnik, J., Christian, W., 2007. An introduction to computer simulation methods: applications to physical systems, 3rd ed. ed. Pearson Addison Wesley, San Francisco.