Nanonocomposites and nanomaterials

Percolation in aggregated systems on elongated square lattice

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Monte Carlo simulation was applied to study the impact of aggregation on the percolation anisotropy on a square lattice in the elongated $L_x \times L_y$ geometry. An interactive cluster-growth model in which the probability of occupying a site on a lattice f_z is dependent on the number of occupied the neighboring sites z was used. The value of f_z was $1/r$ at $z = 0$ and was 1 in other cases. The degree of aggregation parameter $r \geq 1$ controls the morphology of aggregates. The transition from $r = 1$ to $r \rightarrow \infty$ corresponds to the transition from ordinary random percolation to the percolation of the compact Eden clusters.

The investigations were done on the elongated square lattices with different sizes in the horizontal x and vertical y directions: $L_x \geq L_y$. The periodical boundary conditions were used in the both x and y directions. The Hoshen-Kopelman algorithm was used for labeling of different clusters. The value of percolation threshold p_c corresponds to the minimum fraction of occupied sites at which an infinite cluster formed in the infinite lattice. For estimation of p_c the percolation probability R versus the fraction of occupied sites p was calculated. The long lattice side was varied in the interval of L_x = 64 - 2048 and the number of runs was up to 1000. Electrical conductivity of the system was calculated using the highly efficient algorithm, proposed by Frank and Lobb. We used four equivalent resistors scheme with high, $\sigma_f = 10^6$; and low, $\sigma_i = 1$, conductivity for the occupied and empty sites, respectively. The effects of the lattice aspect ratio $a=L_x/L_y$ ($L_x > L_y$) on the finite-size scaling and behavior of electrical conductivity were studied. The data evidenced that the percolation threshold p_c goes through the minimum and finite size effects are enhanced with increasing of r. The dependencies of electrical conductivity on the measuring direction (x or y) at different values of r and a are discussed.