Modelling of porous materials: From topology to physical properties.

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We introduce and study several kinetic models for the porous material fabrication process. All these models involve consecutive removing of pore-former particles, randomly embedded in the initially solid network. After each step of this process the system is locally adjusted to secure the connectivity: clearly, disconnected clusters can not be mechanically stable without support from the "mainland". Depending on the details of the adjustment procedure different scenarios are possible. The properties of the system can either change smoothly with the increase of porosity, or experience a second order topological phase transition to the "tree-like phase" with dramatic physical consequences. In the tree-like phase the system does not have a backbone, and, therefore, it should be non-conducting and extremely fragile. In more realistic models for the adjustment procedure the phase transition is smoothed and the high-porosity state pertains finite (though, extremely poor) conductivity and elasticity. Some principal results (e.g., the existence and characteristics of the phase transition in the simplest model) were obtained analytically, but the main instrument of our study for more sophisticated models was based on numerical simulations. Our results may give an insight for the problems, which technologists encounter, when dealing with highly porous materials.

A. S. Ioselevich, D. S. Lyubshin, "Phase transition in a self-repairing random network", JETP Letters **79**, 286 (2004).