

Cellulose aerogel porous nanostructure modelling with Bezier curves

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At present, cellulose aerogels are increasingly used in the medical field. Due to their biocompatibility, they are applied for tissue engineering, as artificial skin, in dental implants, in spine and joint replacement operations.

Producing aerogels with the required properties is associated with a large number of experimental studies. This increases the cost of the product. This problem can be solved by developing mathematical and computer models that allow to generate digital aerogel structures corresponding to experimental samples and predicting their properties — creating “digital twins”. To generate digital structures of cellulose aerogels, a model for creating a fibrous nanostructure using Bezier curves is proposed. A computer model that allows to generate three-dimensional cellulose aerogels digital structures corresponding to experimental samples and a visualization module for displaying the obtained structures were developed. Computational experiments on the generation of cellulose aerogels digital structures and their comparison with experimental samples by structural characteristics were carried out. The generated digital structures can be used in the calculations of the cellulose aerogels properties, such as adsorption, thermal conductivity and mechanical properties. Thus, the number of full-scale experiments which is necessary to obtain cellulose aerogels with the required properties can be reduced by partially replacing them with the computational experiments.