
Microstructural Characterization of Aerogel through Deep Symbolic Regression

Rajesh Chandrasekaran*¹, Rasul Abdusalamov¹, and Mikhail Itskov¹

¹Department of Continuum Mechanics, RWTH Aachen University – Germany

Abstract

Aerogels are renowned for their unique properties, including low density, high surface area, and excellent thermal insulation. Two prominent modeling approaches—diffusion-limited cluster-cluster aggregation (DLCA) for silica aerogels and Laguerre-Voronoi tessellation for nanoporous open-cell aerogels—offer frameworks for studying the influence of fractal morphology and network structure on mechanical behavior. This contribution presents a novel methodology for advancing microstructural characterization in the modeling of aerogels using deep symbolic regression (DSR). Unlike black-box neural networks, DSR yields interpretable, algebraic expressions that elucidate the relationship between input parameters and structural outputs. Applying DSR in aerogel modeling enables a deeper understanding of how parameters such as particle radius and pore size distribution influence the material's structural and mechanical behavior. By integrating the microstructural insights, the proposed approach facilitates the development of material models that directly incorporate the structural effects within strain energy functions, providing a significant step forward in accurately modeling and optimizing aerogels for advanced applications.

Keywords: Microstructural characterization, Aerogel modeling, Particle radius, Pore size distribution, Deep symbolic regression

*Speaker