

Application of Material Informatics for Tailoring Porous Ceramics: A Machine Learning Approach

MD. Nurul Karim¹, Mojtaba Mirdrikvand², Kamen Tushtev¹, Gabriel Zachmann³,
Wolfgang Dreher², Kurosch Rezwani^{1,4}

1-University of Bremen, Advanced Ceramics, Am Biologischen Garten 2, IW3, Germany

2-University of Bremen, Department of Chemistry, Leobener Str. 7, 28359 Bremen, Germany.

3-University of Bremen, Dept. of Computer Science, Bibliothekstr. 5, 28359 Bremen Germany

4-MAPEX Center for Materials and Processes, University of Bremen, 28359, Bremen, Germany

Abstract:

Characterization of porous ceramics can be performed using automated data analysis and machine learning approaches. Automated 3-Dimensional analysis of microstructure using a robust algorithm can quantify detailed geometrical properties of porous ceramics in a shorter time compared to manual techniques. Machine learning model is trained with extracted data from different porous structure, and analysis of the structural differences, to generate optimal design parameter of pores. The porous samples may be tailored based on extracted information. Therefore, the fabrication of tailored porous structures will accurately comply with the demands in dedicated applications in medicine, energy, environment, chemical, and space technology. The present work aims at developing highly automated computational and visualization tools that lead to a quantitative assessment of the morphological properties of porous materials. Special computer algorithms are developed to characterize critical morphological parameters of porous samples in detail. Various alumina-based ceramic samples were manufactured and investigated. Geometrical properties such as pore size distribution and connectivity, aspect ratios and percolation coefficients were evaluated. The algorithm developed in this work is fed by two robust analytical techniques, micro-tomography and magnetic resonance imaging. The use of the aforementioned imaging techniques allows calibrating the computer-based algorithm from micro- to cm-scale within this resolution. Accordingly, the algorithm analyzes samples with various scales and pore sizes. The exquisite outcome of this computer-based approach is consideration of hydrodynamic properties of porous ceramics such as tortuosity and diffusion coefficients.