# Impacts of polycrystalline microstructures on effective ionic conductivity of ceramic electrolytes: computational homogenization and machine learning

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**Abstract**

Polycrystalline ionic conducting oxide ceramics can be applied as solid electrolytes in all-solid-state batteries and solid fuel cells. In these application scenarios, high effective (macroscopic) ionic conductivity is demanded. Many oxide ceramics exhibit high intrinsic ionic conductivity in the grain bulk. However, the ionic conductivity at grain boundaries (GBs) is much lower than the bulk one, which results in low effective conductivity. In this contribution, we explore how to enhance ionic conductivity in these materials by microstructure engineering. To this end, we reveal the correlation between microstructural characteristics and ionic conductivity by investigating a large number of polycrystalline samples with different grain and GB features. Polycrystalline microstructures with controllable features represented by Voronoi diagrams are computationally generated. Theoretical models are proposed to characterize the ionic conducting behavior in the bulk and at GBs. Based on these models, the computational homogenization method is employed to calculate their macroscopic ionic conductivities. The influence of different microstructural features on the effective ionic conductivity is systematically studied. The revealed microstructure-property relationships are encapsulated into a graph neural network-based machine learning model. The ML model trained by the data from simulations can accurately predict the effective ionic conductivity for a given polycrystalline microstructure. This work provides crucial quantitative guidelines for optimizing the ionic conducting performance of oxide ceramics by tailoring microstructures.

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