OPTIMIZATION OF NANOPOROUS METALLIC ACTUATORS BY COMBINING MULTISCALE CALCULATIONS AND MACHINE LEARNING

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Abstract

Nanoporous materials (NMs) in electrolytes have demonstrated the ability to achieve approximately 1% deformation under low operating voltages of about 1 V, making them promising for use in artificial muscles and micro-robotics. Optimizing the performance of these electrochemical actuators requires careful design of the nanopore and ligament structure and size. However, the multi-field and multi-scale nature of the NM electrochemical actuator makes simulation-based optimization extremely challenging. To address this, a computational framework was developed that combines joint density functional theory (JDFT), surface eigenstress model, symbolic regression, finite element methods (FEM), and surrogate modeling to perform both concurrent and sequential multi-scale calculations. Specifically, JDFT calculations were performed on Au thin films to obtain in-plane strain as a function of charge density and film thickness. The surface eigenstress and surface Young's modulus of the Au nanofilm were then determined by fitting the surface eigenstress model to the JDFT data. Additionally, symbolic regression was used to obtain the constitutive equation of surface eigenstrain as a function of surface charge density. These material parameters were used to conduct macroscale FEM evaluations of electrochemical actuation performance. Finally, a mapping scheme was established between a given sequence of numbers and a particular structure of nanoporous Au, which allowed for the employment of Gaussian process regression surrogate models. These surrogate models were trained to accelerate the evaluation of actuation strain and effective Young's modulus, and hence enable the exploration of the entire design space, facilitating the identification of the best nanoporous Au electrochemical actuator. This computational framework provides a valuable reference for other multi-scale optimization problems.

Acknowledgements

The work is supported by the National Natural Science Foundation of China (No. 12072179 and 11672168), and the Key Research Project of Zhejiang Lab (No. 2021PE0AC02).