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Dear Editor,

On behalf of my co-authors and myself, I am hereby submitting our manuscript, entitled “Modeling of silver transport in cubic SiC: Integrating molecular dynamics, bounds averaging, and uncertainty quantification”, for publication in Physical Review Materials.

In this paper, we present a physics-informed model for estimating the effective diffusivity of silver in polycrystalline 3C–SiC. Molecular dynamics (MD) simulations yield diffusivities for Σ3 and Σ9 grain boundaries (GBs), while literature values are used for other GB types and the bulk. These are combined using a bounds-averaging approach accounting for distinct GB transport properties. Bayesian inference of experimental data provides credible intervals for effective Arrhenius parameters and reveals a correlation between activation energy and pre-exponential factor. Although the homogenized model captures GB-mediated transport mechanisms, it overpredicts silver diffusivity relative to experiments. To resolve this, a multiplicative correction based on reversible trapping at nano-pores is introduced. It is derived from first principles and is shown to reproduce observed transport behavior. Sensitivity analysis identified trap desorption energy and Σ9 GB diffusivity as dominant factors influencing Ag transport. The resulting framework provides a mechanistic description of Ag transport suitable for integration into higher-scale fuel performance models.

To the best of our knowledge, this study is the most comprehensive attempt at holistically describing the mechanisms of silver transport in SiC. We believe our research offers valuable insights into the behavior of SiC and grain boundary transport and adds greatly to the scientific community.

Sincerely,

Benjamin Beeler