DEPARTMENT OF
MECHANICAL ENGINEERING

Editor
Acta Materialia

February 2, 2020

Dear Editor,

I attach herewith a manuscript entitled “Five Degree-of-Freedom Property Interpolation of Arbitrary Grain Boundaries via Voronoi Fundamental Zone Octonion Framework,” by myself (Sterling G. Baird), Eric R. Homer, David T. Fullwood, and Oliver K. Johnson. We would like to submit this paper to your consideration for publication in Acta Materialia.

In this work, we present a new method for computing distances between grain boundaries (GBs) and predicting GB properties based on existing measurements (i.e. interpolation). Our approach builds on recent work by Francis, et al. who introduced the concept of grain boundary octonions. Our new approach, called the Voronoi Fundamental Zone Octonion (VFZO) framework reduces the computational cost of such distance calculations by 5 orders of magnitude. We find that scaled Euclidean distances in a Voronoi Fundamental Zone approximate the original octonion metric with reasonable enough accuracy to produce high accuracy interpolations for large datasets, and the ability to use Euclidean distances allows us to leverage many well established and highly efficient standard algorithms (e.g. Quickhull). We also develop a unique barycentric interpolation approach based on matrix transformations and hyperdimensional triangulation, which can be used for specialized applications. Validation tests and application to two GB property databases from the literature result in higher accuracy predictions than prior work. Because evaluating structure-property model surrogates resulting from our approach is highly computationally efficient, we anticipate that it will enable the incorporation of higher-fidelity GB structure-property models, based on large experimental and computational datasets, into mesoscale simulations (e.g. anisotropic grain growth, GB mobility, etc.).

We, hereby, certify that this manuscript has not been previously published nor is it under consideration for publication elsewhere. It has been approved by all co-authors and any relevant authorities at the locations where the work was performed. Below are the names and contact information for four suitable reviewers:

Dr. David J. Srolovitz (University of Pennsylvania): srol@cityu.edu.hk
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Dr. Marc De Graef (Carnegie Mellon University): degraef@cmu.edu
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We are looking forward to a review of this paper. Please advise if you require anything to proceed.

Sincerely,

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