Abstract:

Multicrystalline informatics: A methodology to advance materials science

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The question of how to improve the macroscopic performance of multicrystalline materials is a common one in materials science. We aim to address this issue by utilizing a methodology called “multicrystalline informatics”, which combines experimental, theoretical, computational, and data sciences. While most data science-assisted materials development is targeted towards new materials with multiple elements, we have chosen to focus on silicon as a model, a material composed of a single element. This choice allows us to narrow the scope to the complex microstructures and grain boundaries that are inherent in multicrystalline materials and require data science. As an example of the usefulness of mutlicrystalline informatics, we show a root cause analysis of dislocation generation. [1] A 3D digital model of multicrystalline silicon can be created using a combination of image processing and machine learning techniques. Photoluminescence and optical images obtained from practical wafers for solar cells are used to develop this model. Finite element stress analysis can then be performed on the model, coupled with crystal growth simulation, to reveal the distribution of stress. Multiscale structural characterizations and ab initio calculations are used to understand specific nanostructures that generate dislocations and underlying physics. This approach can be extended to other materials, and by accumulating such advances in materials science, the establishment of universal guidelines for developing high-performance multicrystalline materials becomes possible.

References:

[1] K. Yamakoshi, Y. Ohno, K. Kutsukake, T. Kojima, T. Yokoi, H. Yoshida, H. Tanaka, X. Liu, H. Kudo, N. Usami, Multicrystalline Informatics Applied to Multicrystalline Silicon for Unraveling The Microscopic Root Cause of Dislocation Generation, Advanced Materials, 2308599 (2023).