MattPy

MattPy v0.1 User Manual

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https://github.com/mcaroba/MattPy.git

written by

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MattPy is a collection of **Mat**erial **t**ensor **Py**thon routines designed to help in the manipulation and analysis of material tensors. Currently, it can handle elastic (4-rank) and piezoelectric (3-rank) tensors. Among other functionalities, the user can rotate the tensors or transform from Cartesian to Voigt forms. ***MattPy***'s main capability, and the one for which it was originally designed, is to project and align material tensors of arbitrary symmetry onto a higher (or lower) symmetry tensor. The method was originally proposed by Moakher and Norris [1] in the context of elastic tensor analysis, and I introduced a straightforward angle dependence that allows to optimize the projection [2]. ***MattPy*** is particularly useful in the context of computational materials science involving calculation of alloy properties, where results are typically obtained for supercells where alloying disorder reduces the lattice symmetry from the macroscopic average to the supercell's symmetry (often triclinic). For the scientific details the reader is referred to the original work [1] and my implementation paper [2]. Here I give guidelines for the practical use of the ***MattPy*** library and present sample scripts to perform some of the most usual tasks. For bug reports and (reasonable) feature requests I can be contacted directly on my email.

Contents

[1] M. Moakher and A. N Norris, "The closest elastic tensor of arbitrary symmetry to an elasticity tensor of lower symmetry", *J. Elasticity* **85**, 215 (2006).

[2] M. A. Caro, "Extended scheme for the projection of material tensors of arbitrary symmetry onto a higher symmetry tensor", *arXiv:1408.1219* , (2014).