The Journal of Open Source Software

bem: modeling for neutron Bragg-edge imaging

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DOI: 10.21105/joss.00973

Software

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Submitted: 28 August 2018
Published: 18 October 2018

Summary

Due to its zero net charge, neutron is a unique probe of materials. Low neutron absorption and scattering cross sections by most nuclei make it suitable for studying bulk samples. Unlike X-ray scattering, neutron form factors are not monotonically dependent on atomic numbers; the fact that the neutron scattering cross section of hydrogen is large makes neutron a useful tool in biology. In the past half century, neutron imaging has seen growing applications in various scientific fields including physics, engineering sciences, biology, and archaeology (Strobl et al., 2009).

With energy-resolved neutron imaging techniques, neutron Bragg-edge imaging has recently found applications for materials science in phase mapping, stress/strain mapping, and texture analysis (Josic, Steuwer, & Lehmann, 2010, Sato (2017)). To model Bragg-edge neutron imaging data, it is necessary to calculate the total neutron cross section of a sample. This open-source python package provides easy-to-use functions to calculate coherent elastic (diffraction), incoherent elastic, coherent inelastic, and incoherent inelastic scattering cross sections, as well as absorption cross sections based on approximations and formulas in (Vogel, 2000). Also implemented are algorithms that take into account the March-Dollase texture model, and the Jorgensen peak profile (Vogel, 2000).

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Acknowledgements

This work is sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle LLC, for DOE. Part of this research is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, User Facilities under contract number DE-AC05-00OR22725.

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