

bem: Modeling for Neutron Bragg-Edge Imaging

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1 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 of 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 even archaeology [1].

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 [2, 3]. 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 [4]. Also implemented are algorithms that take into account the March-Dollase texture model, and the Jorgensen peak profile [4].

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References

- [1] M Strobl, I Manke, N Kardjilov, A Hilger, M Dawson, and J Banhart. Advances in neutron radiography and tomography. *Journal of Physics D: Applied Physics*, 42(24):243001, 2009.
- [2] Lidiya Josic, Axel Steuwer, and E Lehmann. Energy selective neutron radiography in material research. *Applied Physics A*, 99(3):515–522, 2010.
- [3] Hirotaka Sato. Deriving quantitative crystallographic information from the wavelength-resolved neutron transmission analysis performed in imaging mode. *Journal of Imaging*, 4(1):7, 2017.
- [4] Sven Vogel. *A Rietveld-approach for the analysis of neutron time-of-flight transmission data*. PhD thesis, Verlag nicht ermittelbar, 2000.