The Journal of Open Source Software

ImagingReso: A Tool for Neutron Resonance Imaging

Yuxuan Zhang[1] **and Jean Bilheux**[1]

1 Oak Ridge National Laboratory

DOI: 10.21105/joss.00407

Software

- Review
- Repository
- Archive

Summary

ImagingReso is an open-source Python library that simulates the neutron resonance signal for neutron imaging measurements. By defining the sample information such as density, thickness in the neutron path, and isotopic ratios of the elemental composition of the material, this package plots the expected resonance peaks for a selected neutron energy range. Various sample types such as layers of single elements (Ag, Co, etc. in solid form), chemical compounds (UO3, Gd2O3, etc.), or even multiple layers of both types can be plotted with this package. Major plotting features include display of the transmission/attenuation in wavelength, energy, and time scale, and show/hide elemental and isotopic contributions in the total resonance signal.

The energy dependent cross-section data used in this library are from National Nuclear Data Center, a published online database. Evaluated Nuclear Data File (ENDF/B) (Chadwick et al. 2011) is currently supported and more evaluated databases will be added in future.

Python packages used are: SciPy (Oliphant 2007), NumPy (Walt, Colbert, and Varoquaux 2011), Matplotlib (Hunter 2007), Pandas (McKinney 2010) and Periodictable (Kienzle 2017).

The energy dependent cross-section data used in this library are from National Nuclear Data Center, an online database published by Brookhaven National Laboratory. Evaluated Nuclear Data File (ENDF/B) is currently supported and more evaluated databases will be added in the future.

The neutron transmission calculation algorithm of neutron transmission $T(E)$, is base on Beer-Lambert law (Ooi et al. 2013; A. S. Tremsin et al. 2017; Zhang et al. 2017):

Ni : number of atoms per unit volume of element i,

di : effective thickness along the neutron path of element i,

$ij(E)$: energy-dependent neutron total cross-section for the isotope j of element i,

Aij : abundance for the isotope j of element i.

For solid materials the number of atoms per unit volume can be calculated from:

NA : Avogadro's number,

Ci : molar concentration of element i,

i : density of the element i,

mij : atomic mass values for the isotope j of element i.

Acknowledgements

This work is sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle LLC, under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy. The United States Government retains and the publisher, by accepting the article for publication, acknowledges that the United States Government retains a non-exclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this manuscript, or allow others to do so, for United States Government purposes. The Department of Energy will provide public access to these results of federally sponsored research in accordance with the DOE Public Access Plan(http://energy.gov/downloads/doe-public-access-plan).

References

Chadwick, M.B., M. Herman, P. Obložinsk' y, M.E. Dunn, Y. Danon, A.C. Kahler, D.L. Smith, et al. 2011. "ENDF/B-Vii.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data." *Nuclear Data Sheets* 112 (12): 2887–2996. doi:10.1016/j.nds.2011.11.002.

Hunter, John D. 2007. "Matplotlib: A 2d Graphics Environment." *Computing in Science & Engineering* 9 (3). IEEE COMPUTER SOC: 90–95. doi:10.1109/MCSE.2007.55.

Kienzle, P. A. 2017. "Periodictable V1.5.0." doi:10.5281/zenodo.840347.

McKinney, Wes. 2010. "Data Structures for Statistical Computing in Python." In *Proceedings of the 9th Python in Science Conference*, edited by Stéfan van der Walt and Jarrod Millman, 51–56.

Oliphant, Travis E. 2007. "SciPy: Open source scientific tools for Python." doi:10.1109/MCSE.2007.58.

Ooi, M, M Teshigawara, T Kai, M Harada, F Maekawa, M Futakawa, E Hashimoto, et al. 2013. "Neutron Resonance Imaging of a Au-In-Cd Alloy for the JSNS." *Physics Procedia* 43: 337–42. doi:http://dx.doi.org/10.1016/j.phpro.2013.03.040.

Tremsin, A. S., A. S. Losko, S. C. Vogel, D.D. Byler, K. J. McClellan, M. A. M. Bourke, and J. V. Vallerga. 2017. "Non-Contact Measurement of Partial Gas Pressure and Distribution of Elemental Composition Using Energy-Resolved Neutron Imaging." *AIP Advances* 7 (1): 015315. doi:10.1063/1.4975632.

Walt, Stéfan van der, S. Chris Colbert, and Gaël Varoquaux. 2011. "The Numpy Array: A Structure for Efficient Numerical Computation." *Computing in Science & Engineering* 13 (2): 22–30. doi:10.1109/MCSE.2011.37.

Zhang, Y, K S Ravi Chandran, M Jagannathan, H Z Bilheux, and J C Bilheux. 2017. "The Nature of Electrochemical Delithiation of Li-Mg Alloy Electrodes: Neutron Computed Tomography and Analytical Modeling of Li Diffusion and Delithiation Phenomenon." *Journal of the Electrochemical Society* 164 (2): A28–A38. doi:10.1149/2.0051702jes.