pysrim: Automation, Analysis, and Plotting of SRIM Calculations

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Summary

The behavior of ions traveling through a material is of great interest to many fields. For instance nuclear materials and ion beam modification are most concerned with the bulk of the material and understanding the damage formation and evolution of defects along the ion path (Was 2016). Some of the important properties that can be gleaned from investigating the initial damage from the ion include: number of vacancies produced, energy deposited per unit length, track diameter, and implantation profile. These properties enable further simulations and allow computing a common radiation damage unit, displacements per atom (DPA), which can be used to compare experiments (Backman et al. 2013) (Stoller et al. 2013). Additionally the ejection of materials near the surface due to incident ions is important to techniques such as RBS, SIMS, and sputtering (Vickerman and Gilmore 2011). The interaction of ions within a material can be broken into two parts: electronic and nuclear stopping. Electronic stopping is the energy lost from the ion due to inelastic collisions with electrons along its path. Nuclear stopping is the energy lost due to elastic collisions between the ion and atomic nuclei within the material.

The Stopping and Range of Ions in Matter (SRIM) is a well known software in the nuclear community that allows the simulation, via Monte Carlo, of ions through a material by modeling the energy transfer through electronic and nuclear stopping (Ziegler, Ziegler, and Biersack 2010). SRIM was originally developed in 1985 and has had numerous updates on the electronic stopping powers since then with the nuclear stopping well explained by the ZBL potential (Ziegler 1988). The executable SRIM is free to use for non-commercial use but the source code is not available to the community despite requests. While SRIM is a scientifically accurate code it does not get updated frequently and has many bugs from a usability standpoint.

Pysrim

`pysrim` is a python library for automating srim calculations, analysis, and for publication quality plotting. It is a continuously delivered, tested, and fully-documented module. In addition, the documentation includes several jupyter notebooks for getting started.

The first pain point that `pysrim` aims to solve is running the SRIM calculation. SRIM has some well known limitations such as crashing with large simulations and bad input values, only running on Windows, and needing to be run interactively with user input. `pysrim` solves this by having an api compatible with windows, linux, and OS X, having support for chunking of large calculations, and recovering from SRIM crashes. All of these features allow SRIM to be fully automated via `pysrim`.

After running these calculations SRIM will produce many output files all of which are not convenient to parse. Traditionally research groups have copy and pasted sections into excel for analysis. `pysrim` hopes to solve this by providing parsers for all the major output files. These output files include: IONIZ.txt, VACANCY.txt, NOVAC.txt, E2RECOIL.txt, PHONON.txt, RANGE.txt, and COLLISON.txt. Once the output file is parsed the data is available in `numpy` arrays. From here the user is free to create plots of interesting relationships in their data. `pysrim` additionally provides plotting utilities for producing figures commonly needed in nuclear materials. This software has been used for the SRIM calculations, analysis, and plotting in two publications (Zhang et al. 2017) (Zhang et al. 2014).

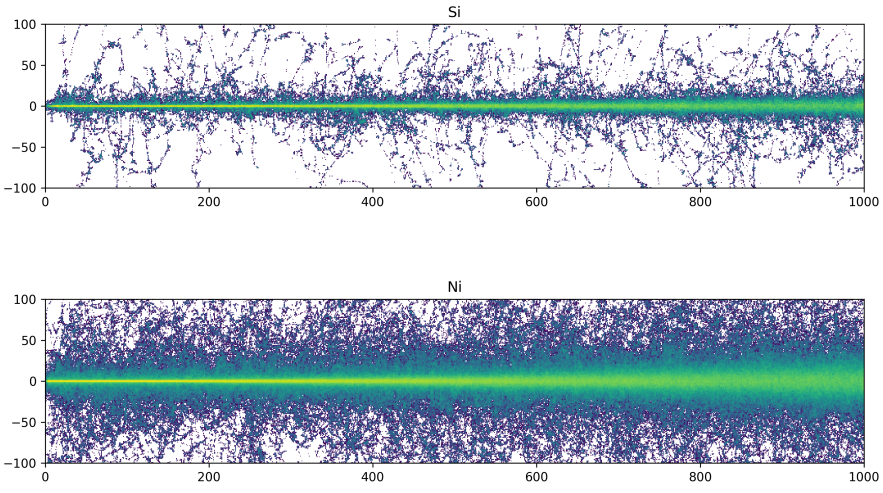

Figure 1: Plots produced by `pysrim` of vacancies for ions traveling through SiC material. (top) Si ion (bottom) Ni ion

Acknowledgements

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