Automation of SRIM

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Summary

The behavior of ions traveling through a material is of great interest to many fields. For instance radiation materials and ion beam modification are most concered with the bulk of the material and understanding the damage formation and evolution of defects along the ion path (Was 2016). Some of the imporant properties that can be gleaned from investigating the initial damage from the ion include: number of vacancies produced, energy deposited per unit length, and average deposition distance. These properties enables further simulations for multiscale modeling and to compute a common radiation damage unit displacements per atom (DPA) (Stoller et al. 2013). In other fields they are most concerned with the ejection of materials near the surface due to incident ions with techniques such as RBS, SIMS, and sputtering.

The interaction of ions with a material can be broken into two parts: electronic and nuclear stopping. Electronic stopping is the energy lost from the ion due to interacting with the electrons along its path. While nuclear stopping is the energy lost due to collisision between the ion and atoms within the material. The Stopping and Range of Ions in Matter (SRIM) is a well known software in nuclear community that allow the simulation via Monte Carlo of ions through a material (Ziegler, Ziegler, and Biersack 2010). SRIM was originally written in 1985 and has had updates on the electonic stopping powers since then. While the executable SRIM is free to use for non-comercial use, the source code is not available to the community. Without the source code we would like to wrap and extend the capabilities of the software with `pysrim`.

Pysrim

`pysrim` is a python library for automating srim calculations, analysis, and publication quality plotting. It is 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 calcualtion. SRIM has some well known limitations such as sporadically 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 a consistent api compatible with windows, linux, and OSX, having support for chunking large of calculations, and recovering from SRIM crashes. All of these features allow SRIM to be fully automated in python via `pysrim` with no user input needed.

After running these calculations SRIM will produce many output files all of which are not convenient to parse and require complex regular expressions. Traditionally research groups have copy and pasted sections into excel for analysis. `pysrim` hopes to solve this by providing parsers for all of the major output files. These output files incluce: IONIZ.txt, VACANCY.txt, NOVAC.txt, E2RECOIL.txt, PHONON.txt, RANGE.txt, and COLLISON.txt. Once the output file is parsed the data is in convenient numpy arrays. With the results `pysrim` provides utilities for producing plots for damage energy, ionization per unit depth, vacancies produced per unit depth, and even complex plots that require all of the collisions information. The flexibility of the parsed output files allows for additional plots to be created by the user. This software has currently been used for the SRIM calcualtions, analysis, and plotting in two publications (Zhang et al. 2017) (Zhang et al. 2014).

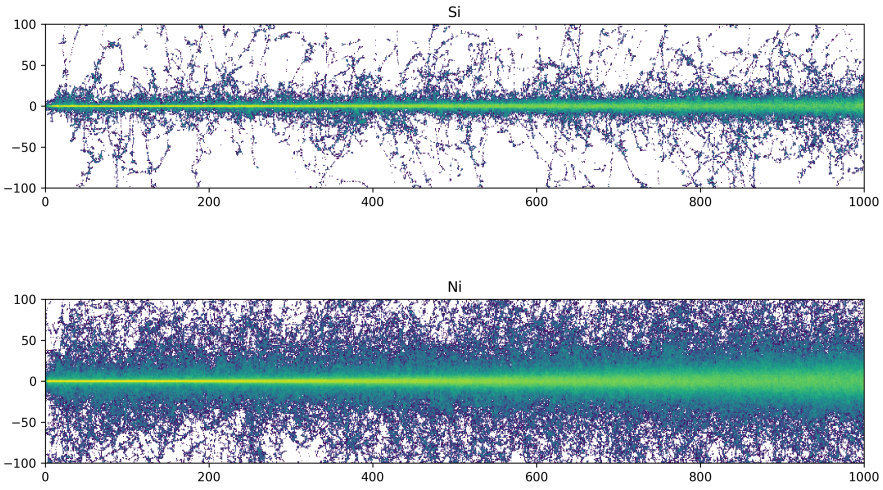

Figure 1: Plots produced by `pysrim` of vacancies produced for ions traveling through SiC material. (top) Si ion (bottom) Ni ion

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