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, radiation damage in nuclear materials and ion beam modification of materials are most concerned with understanding the 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: numbers of interstitials and vacancies produced, energy deposited per unit length to electrons and atomic nuclei, track diameter, and implanted ion profile. These properties enable further simulations and allow computing a common unit of radiation damage dose, displacements per atom (dpa), which can be used to compare irradiation experiments with different ions (Backman et al. 2013) (Stoller et al. 2013). Additionally, the ejection of materials near the surface due to incident ions is important to sputtering and ion-beam analysis techniques, such as elastic recoil detection analysis (ERDA) and secondary ion mass spectrometry (SIMS) (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) code is a well known software in the radiation damage and ion-beam communities 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: 1) having an api compatible with windows, linux, and OS X; 2) having support for chunking of large calculations; and 3) recovering from SRIM crashes. Along with cross platform support, a Docker container image using `pysrim` has been constructed that allows SRIM to run on a linux server without a display determined from benchmarks to be around 50% faster. All of these features allow SRIM to be fully automated via `pysrim` and follow best practices.

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 or other spreadsheets 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 characterizing the defect production distribution under ion irradiation for evaluating radiation damage or ion beam modification in materials. This software has been used for the SRIM calculations, analysis, and plotting in two publications (Zhang et al. 2017) (Zhang et al. 2014).

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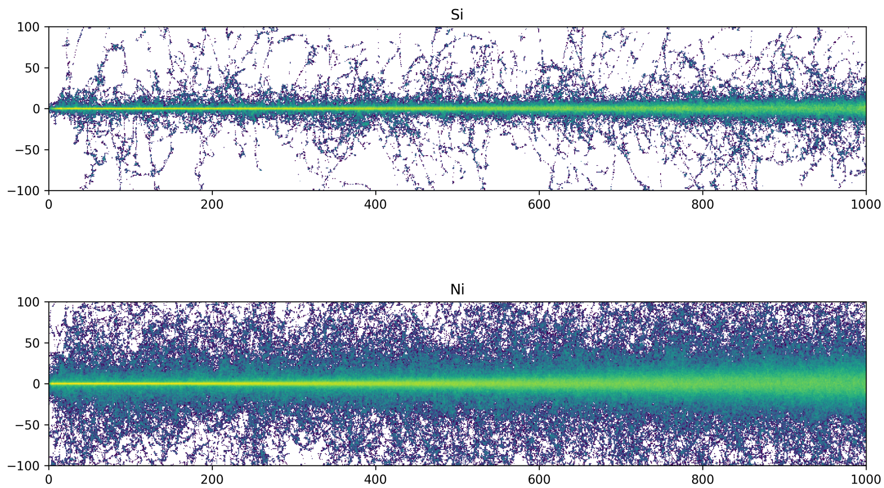

Figure 1: Plots produced by `pysrim` of vacancies for ions traveling through SiC. (top) 21 MeV Si ion (bottom) 21 MeV Ni ion

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