

Testing of SRIM 2008 and MSTAR computer codes from the point of view of the reciprocity principle

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1. Introduction

Interaction of ions with matter is of great interest from the point of view of radiation and solid state physics. Ion beams allow not only to investigate various properties of matter but substantially change it. This is of great importance for modern and future industries. Ion beam technologies have wide variety of applications ranging from semiconductor to space and bio-technologies including nano-technologies.

As technology is shrinking more rigid requirements of the accuracy of theoretical predictions are made. Although the history of the problem began at the beginning of the last century, there are still a great need in reliable theory of stopping of slow heavy ions. Profile of implanted ions in many respects determines the surface properties of the modified materials.

The semiempirical approach developed by Ziegler, Biersack and Littmark (ZBL) is perhaps the most widely used for calculation of stopping powers and ranges of energetic ions in matter. The overall accuracy of stopping power calculations with the latest implementation of the ZBL (SRIM 2008) is of order 5%. For projected range an overall agreement of ZBL predictions is of the order of 10% for a wide range of implantation energies and for a large set of ion-target combinations. However, up to 40% higher ranges in comparison with SRIM simulations have been revealed for medium-heavy ions ($29 \leq Z \leq 83$) implanted into low-Z target materials at energies between 10 and 300 keV.

Recently it was shown that the origins of the discrepancies are inaccuracies of the ZBL nuclear and electronic stopping powers. Whereas the nuclear stopping power can be calculated with a good accuracy, there is no reliable theory of electronic stopping of slow heavy ions. Relevant experimental data are rather scarce. Therefore, the recent study on reciprocity in the electronic stopping of slow ions can be very fruitful for numerous systems, where experimental data are not available.

Applicants will gain knowledge on theoretical approaches to describe penetration of ions in matter. They will acquire an experience in using of main computer codes in this field. Also, development of computer codes will improve programmer's skill.

2. Objective

Applicants are suggested to develop a computer code to test fulfillment of the reciprocity principle in the main computer codes (SRIM, MSTAR), used by overwhelming majority of specialists in radiation physics. The results computations may be presented as a colored plot, displaying the deviation from exact reciprocity for different pairs of atoms Z_1 - Z_2 .

3. Requirements

Applicants are expected to have knowledge on basics of classical and quantum mechanics, scattering theory. Knowledge of Fortran or C computer languages are necessary.

4. Literature

J.F. Ziegler, J.P. Biersack, U. Littmark, *The Stopping and Range of Ions in Solids*, Pergamon, New York, 1985.

P. Sigmund, *Particle Penetration and Radiation Effects*, Springer-Verlag, Berlin, 2006.

P. Sigmund, *Eur. Phys. J. D.* 47 (2008) 45.

V. Kuzmin, *Nucl. Instr. and Meth. B* 256 (2006) 105.

5. Number of applicants – 2

6. Supervisor

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Scientific interests:

Ion interaction with matter, ab initio calculations.

Latest publications:

- V. Kuzmin, “Range parameters of heavy ions in carbon calculated with first-principles potentials”, Nucl. Instr. and Meth. B, 249, pp. 13-17, 2006.
- V. Kuzmin, “On the correlation between nuclear and electronic stopping of heavy ions in light targets”, Nucl. Instr. and Meth. B, 256, pp. 105-108, 2007.
- V. Kuzmin, “Calculations on range parameters of heavy ions in carbon using ab initio potentials”, Surf. Coat. Tech., 201, pp. 8388-8392, 2007.
- V. Kuzmin, “Range parameters of gold ions in boron calculated with a first-principles potential”, Proceedings of 7th International Conference on Interaction of Radiation with Solids, 2007, Sept. 26-28, Minsk, Belarus, pp. 15-17.
- R. Andrzejewski, V. Kuzmin, D.O. Boerma, D. Primetzhofer, S.N. Markin, P. Bauer, “Azimuthal scans in LEIS: Influence of the scattering potential”, Nucl. Instr. and Meth. B, 267, pp. 638-641, 2009.
- V. Kuzmin, “Range parameters of slow gold ions implanted into light targets”, <http://dx.doi.org/10.1016/j.nimb.2009.05.013>, Article in Press.

Conferences:

- 17th International Conference on Ion Beam Analysis, June 2005, Sevilla, Spain; (talk)
- 14th International Conference on Surface Modification of Materials by Ion Beams, September 2005, Kusadasi, Turkey; (talk).
- 22nd International Conference on Atomic Collisions in Solids, July 2006, Berlin, Germany.
- 7th International Conference on Interaction of Radiation with Solids, Sept. 2007, Minsk, Belarus; (talk).
- 23rd International Conference on Atomic Collisions in Solids, August 2008, Phalaborwa, south Africa, (talk).