

Reciprocity as a criterion of reliability of SRIM and MSTAR low energy electronic stopping power calculation.

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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 investigating various properties of matter but also substantially changing them. These are of great importance for modern and future industries. Ion beam technologies are key elements of wide variety of applications ranging from semiconductor to aero-space and bio-medical technologies including nano-technologies.

As technology is shrinking more and more high demands for accuracy of theoretical predictions are made. Although the history of the problem began at the beginning of the last century, there is still a great need in reliable theory of stopping of slow heavy ions. This quantity determines a profile of implanted ions that in many respects defines 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. Although there have not been made improvements in scientific basics since 2003, the overall accuracy of stopping power calculations with the last implementations of the ZBL 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 a few keV and of about 1 MeV.

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 modern 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. Basic knowledge of Fortran or C computer languages is highly desirable.

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.

M. Behar, P.F.P. Fichtner, P.L. Grande, F.C. Zawislak, Mat. Sci. Eng. R 15 (1995) 1-83.

V. Kuzmin, Nucl. Instr. and Meth. B 267 (2009) 2657–2661.

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

V. Kuzmin, P. Sigmund, Nucl. Instr. and Meth. B 269 (2011) 817-823.

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”, Nucl. Instr. and Meth., B 267, pp. 2657–2661, 2009.
- V. Kuzmin, P. Sigmund, “Exploring reciprocity as a tool in low-energy electronic stopping”, Nucl. Instr. and Meth., B 269, pp.817-823, 2011.
- V. Kuzmin, “Recent progress in evaluation of low-energy electronic stopping: What we can expect from use of reciprocity?”, Proceedings of 9th International Conference on Interaction of Radiation with Solids, 2011, Sept. 20-22, Minsk, Belarus, pp. 20-22.

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).
- 8th International Conference on Interaction of Radiation with Solids, Sept., 2009, Minsk, Belarus, (plenary talk).
- 24th International Conference on Atomic Collisions in Solids, July, 2010, Krakow, Poland, (talk).
- 9th International Conference on Interaction of Radiation with Solids, Sept., 2011, Minsk, Belarus, (talk).