Solid target extensions in TRAX

C. Wälzlein[*1,2], *M. Krämer*[1], *E. Scifoni*[1], *and M. Durante*[1,2]
[1]GSI, Darmstadt, Germany; [2]FIAS, Frankfurt, Germany

The GSI track structure Monte Carlo (MC) code TRAX [1], whose main purpose is to properly describe creation and transport of low-energy electrons, has been further extended. TRAX is intended to be suitable for a variety of different target materials and projectiles. In ion irradiation the distribution of produced secondary electrons is dominated by energies below 100 eV. Therefore electrons with initial energies in this range are the most relevant for radiation damage.
One of our goals is to reproduce the data from the GSI Toroid experiment [2] to gain further insight on low-energy electron creation and transport in solids. Therefore our cross section database was extended to account for electron induced excitations. Consideration of excitation reduces the cut-off energy, below which electrons are considered to be stopped, as no further cross sections for inelastic interactions are available below. Cross sections for electron induced ionization can be easily calculated for all target materials using a simplified formula based on binary encounter theory according to Kim and Rudd [3]. With a few input parameters like the binding and kinetic energy of electrons in any target atom or molecule, we can easily access ionization cross sections. For electron induced excitation neither a complete database nor a simple model exists which could calculate all desired cross sections. With the Toroid experiment in mind we consider the target materials carbon, nickel, silver and gold.

Carbon

The cross section database for low energy electrons incident on carbon has been extended to account for electronic excitations. Collision strengths from a review of Suno [4] have been used to calculate cross sections for 21 individual excitation channels. Considered are excitations from 2s to 2p states (6 channels), 2p→3s (2 ch), 2p→3p (6 ch), 2p→3d (5 ch) and 2p→2p (2 ch). Below ≈ 100 eV the excitation cross sections exceed the ionization cross sections. and below the ionization threshold (11.26 eV) excitation is the only source of energy deposition in our simulation. With the newly introduced excitation cross sections, the cut-off energy is reduced from 11.26 eV to 1.26 eV. More details are given in [5].

Gold

We consider 3 single excitation channels (6s-6p and 5d-6s excitations) by using experimental cross sections from Maslov and Zatsarinny et al. [6, 7]. The cross sections were extrapolated to higher energies using the Bethe-Born approximation [8]. We also consider plasmon excitation by using the formula given by Quinn [9]. This reduces the cut-off energy from 9.23 eV to 2.7 eV. More details are given in [10].

Nickel and Silver

For excitations in Nickel and Silver we used the ACE code [11] which is a collision code based on distorted wave methods by Mann [12]. We account for 9(Ni) and 11(Ag) dielectric excitation channels. For Ni we have transitions with energy losses down to 0.12 eV (4s-3d) and for Ag down to 3.28 eV (5s-5p).

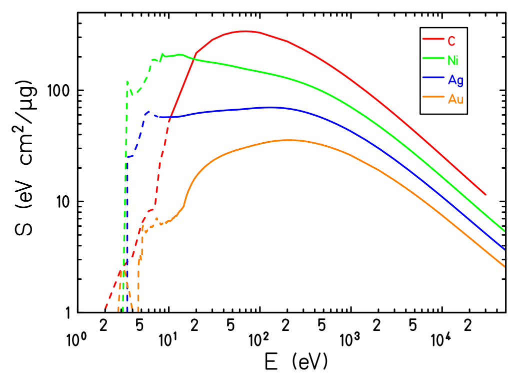

Figure 1: Energy dependent electron stopping power for target materials used in the Toroid experiment. The stopping powers were calculated using the ionization and excitation cross sections and the corresponding energy losses.

* Work supported by Beilstein Institute (NanoBiC project). Work is part of HGS-HIRe.

References

[1] M. Krämer and M. Durante, Eur. Phys. J. D, 60 (2010) 195.
[2] N. Lineva et al., NIM B 267 (2009) 891.
[3] Y.K. Kim and E. Rudd, Phys. Rev. A 50 (1994) 3954.
[4] H. Suno et al., At. Data and Nucl. Data Tabl. 92 (2006) 407.
[5] C. Wälzlein et al., Phys. Rev. E., submitted.
[6] M. Maslov et al., Phys. Rev. A 77 (2008) 062711.
[7] O. Zatsarinny et al., Phys. Rev. A 78 (2008) 042713.
[8] G.W. Bransden et al., Int. J. Radiat. Biol. Stud. Phys. Chem. Med. 10 (1966) 317.
[9] J.J. Quinn, Phys. Rev. 126(4) (1962) 1453.
[10] C. Wälzlein et al., Appl. Rad. and Isot., in press.
[11] R.E.H. Clark et al., Manual LA-11436-M, Los Alamos Laboratory (1988).
[12] J.B. Mann, At. Dat. Nuc. Data Tables 29 (1983), 407.