The Proton induced Displacement Cross Section: SRIM comparison with DXS

(calculations by Benjaminas Marcinkevicius, NDS, May 2015)

The SRIM [1] code is often used for the calculations of the ion induced damage production, sputtering, the ions range and stopping power. The details of the practical use of code and correct interpretation of its results was discussed recently [2, 3].

The alternative approaches use the up-today nuclear reaction models for rather precise nuclear cross sections calculations in combination with NRT model [4] to estimate the displacements in materials. This was implemented, e.g. in the advanced database of the protons and neutrons induced displacement and gas production cross sections (DXS) for several materials [5, 6], [7].

Here we present a results of calculation of the proton induced displacement cross sections by the SRIM-2013 code and comparison with DXS database.

The atom displacement cross sections were calculated by SRIM-2013 with Kinchin-Pease option (SRIM/K-P) and the NRT model taking the damage energy T_{dam} from SRIM (SRIM/T_{dam}/NRT predicts). The displacement energies for Zr, Fe, Cu, Ni, Cr and Al were selected as 40, 40, 30, 40, 40 and 27 eV, consequently, as recommended by [8].

It worthwhile to note that proton energy distribution inside the elementary space bin of material (used by SRIM) has a Gaussian shape with low energy tail, Fig. 1, which also contributes to the number of displacements.

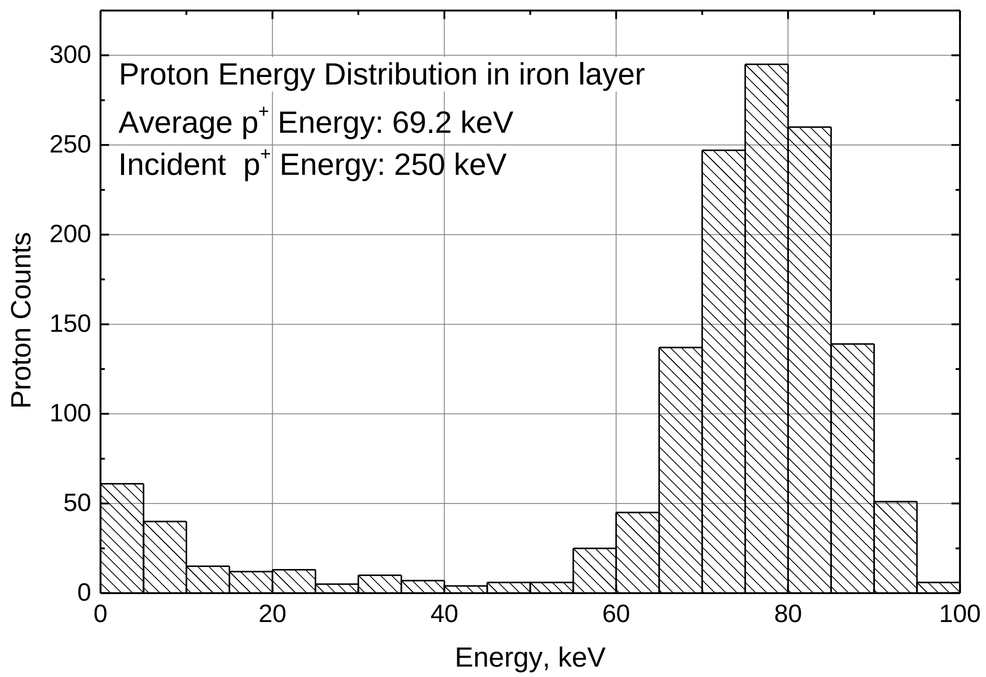

Fig. 1. Proton energy distribution in the Iron bin #50 (where mean energy is 69.2 MeV) for the incident protons with energy 250 keV.

The comparison between SRIM and DXS for Fe, Zr, Ni, Cr, Cu and Al is displayed in Figs. 2 to 7.

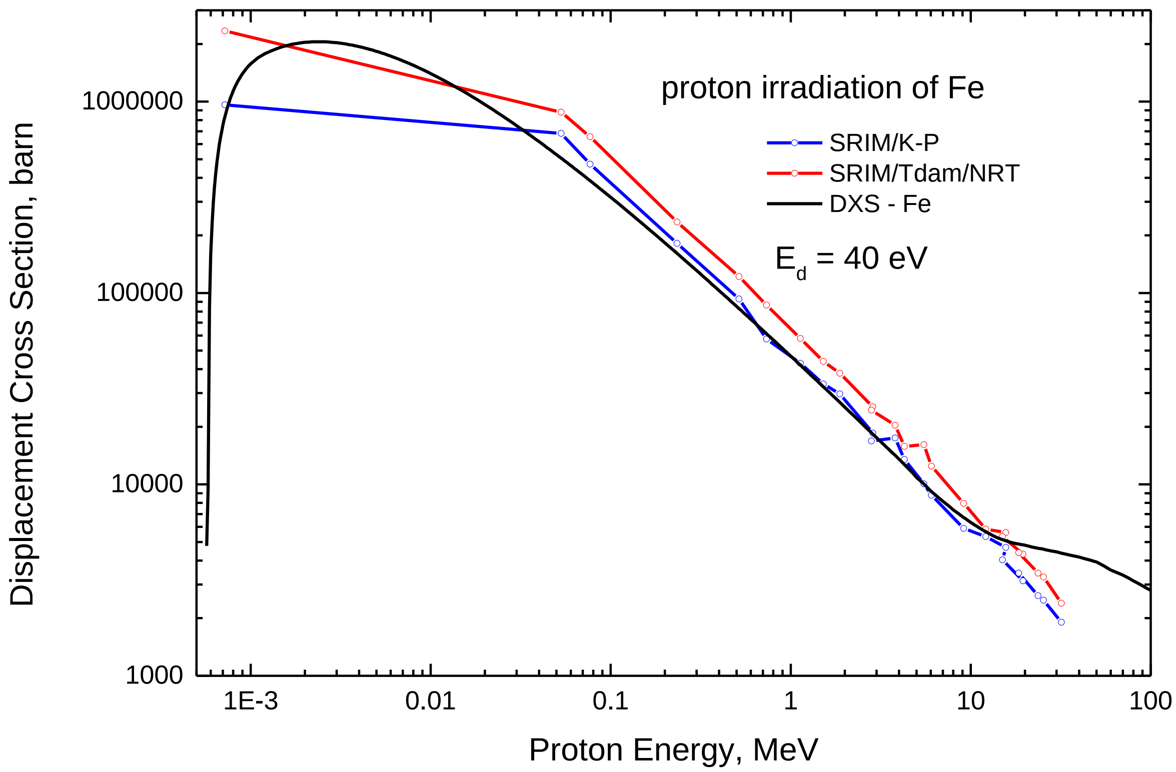

Fig. 2. Proton induced displacement cross section for Iron: comparison of SRIM K-P and SRIM/T_{dam}/NRT with recommended values from DXS.

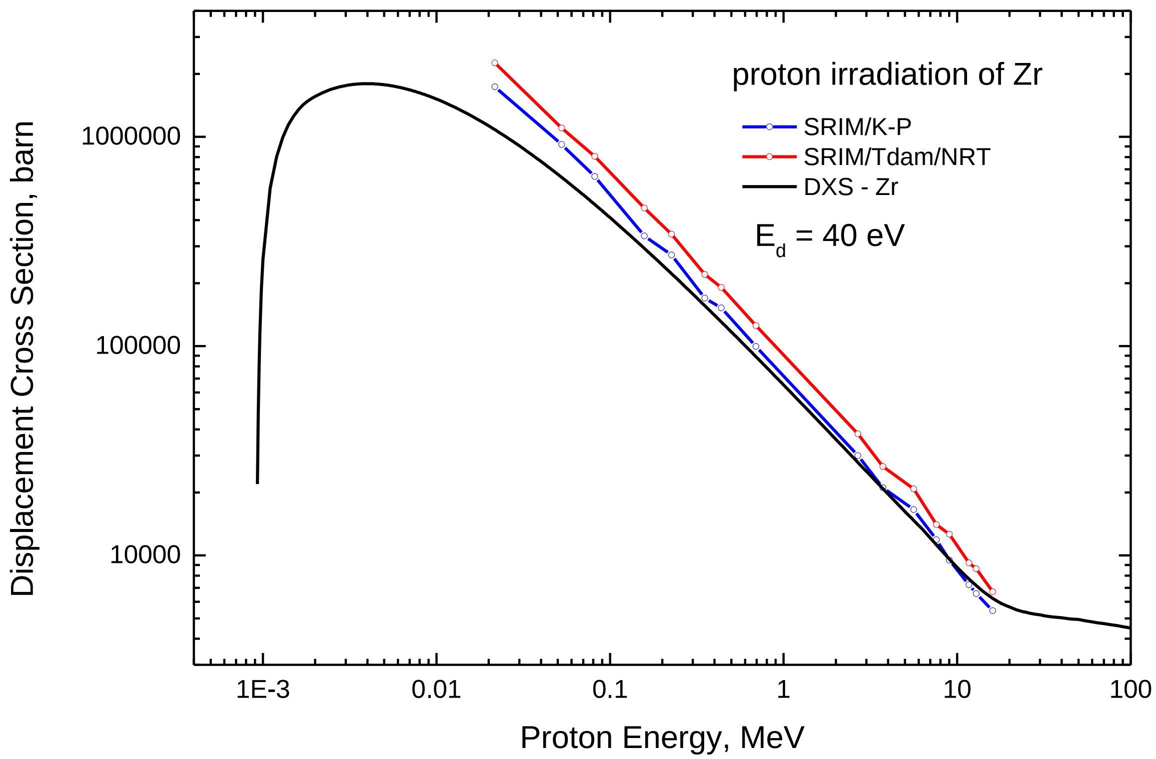

Fig. 3. Proton induced displacement cross section for Zirconium: comparison of SRIM K-P and SRIM/T_{dam}/NRT with recommended values from DXS.

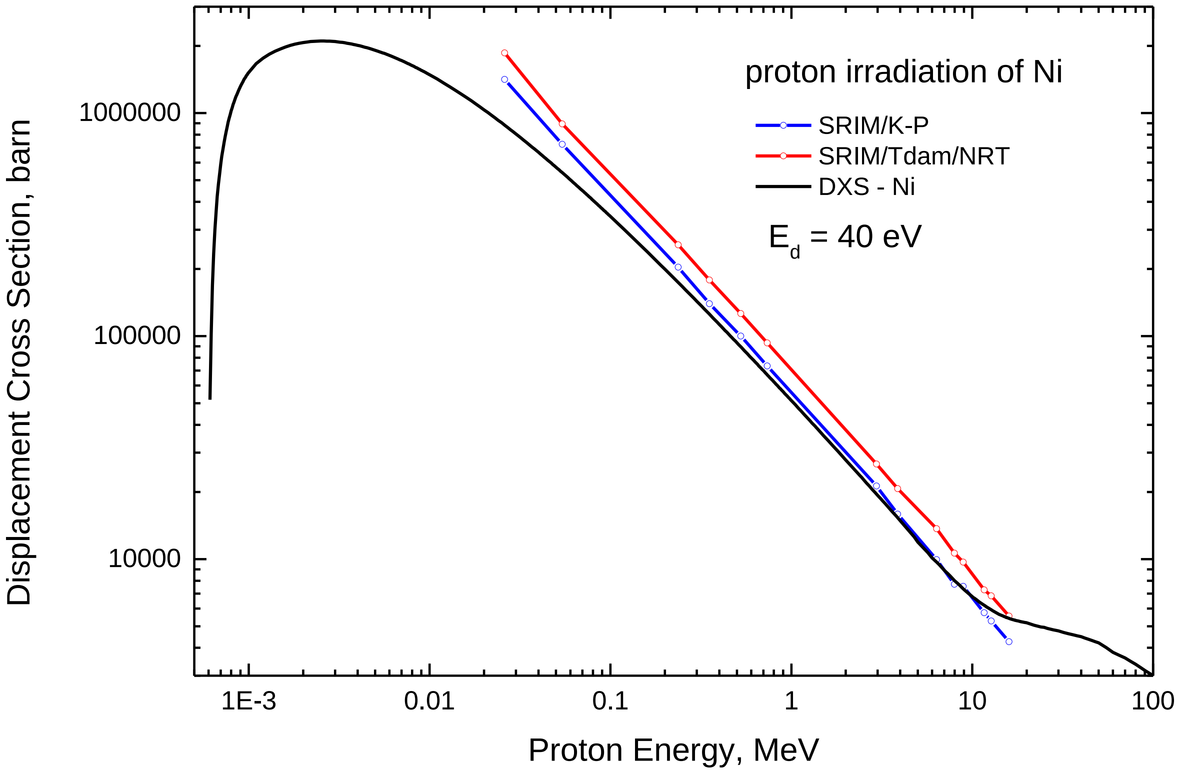

Fig. 4. Proton induced displacement cross section for Nickel: comparison of SRIM K-P and SRIM/T_{dam}/NRT with recommended values from DXS.

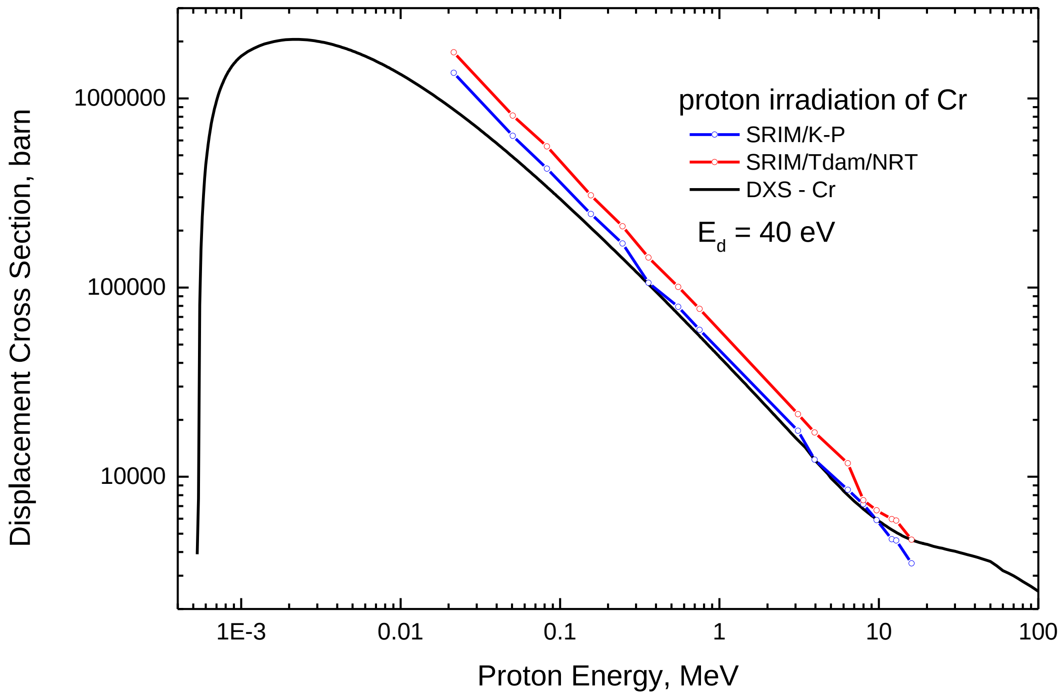

Fig. 5. Proton induced displacement cross section for Chromium: comparison of SRIM K-P and SRIM/T_{dam}/NRT with recommended values from DXS.

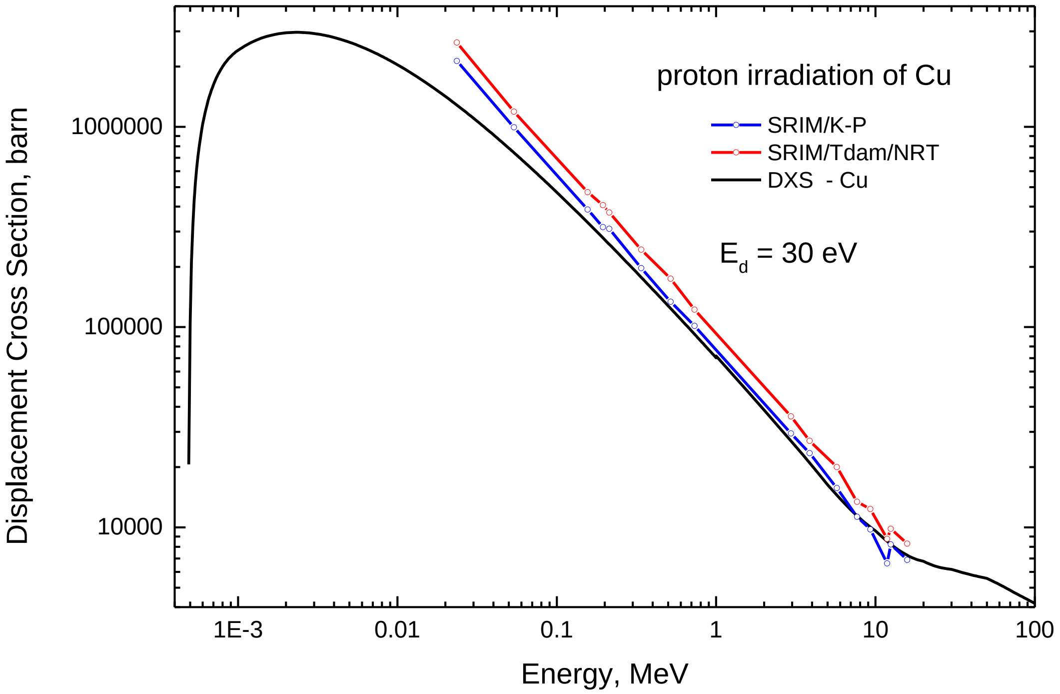

Fig. 6. Proton induced displacement cross section for Copper: comparison of SRIM K-P and SRIM/T_{dam}/NRT with recommended values from DXS.

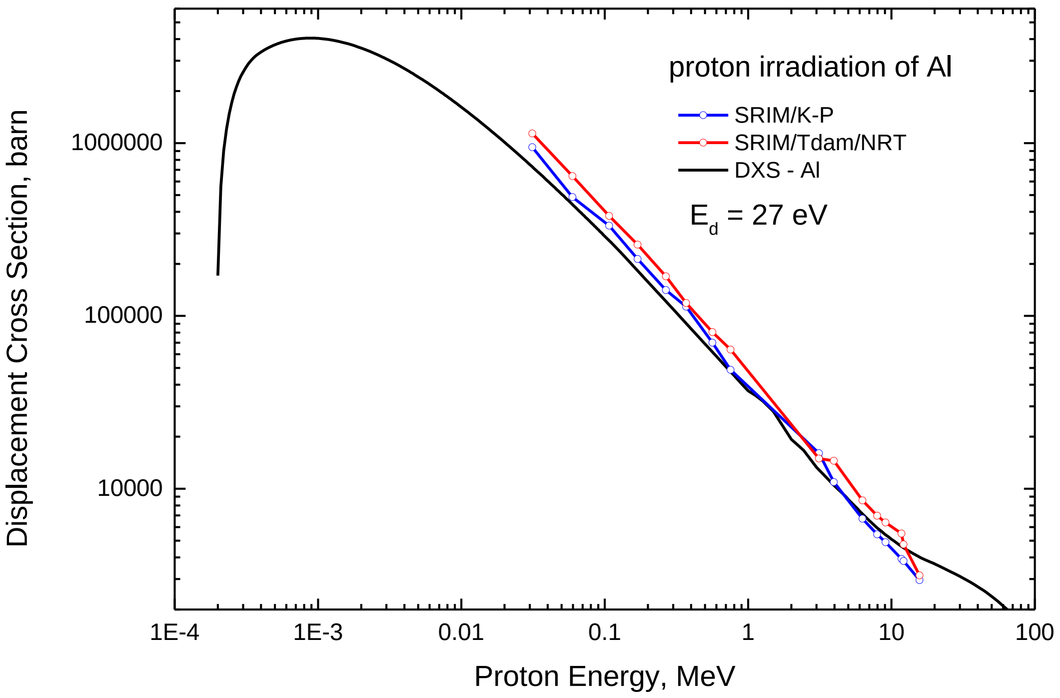

Fig. 7. Proton induced displacement cross section for Aluminium: comparison of SRIM K-P and SRIM/T_{dam}/NRT with recommended values from DXS.

Conclusions

The simulation of the proton induced atom displacements (vacancies production) was done with two options (K-P) and (T_{dam}/NRT) available in the SRIM code.

The comparison with DXS has shown:

- below 20 - 50 keV the binning used in the SRIM results to broad energy bins;
- from 100 keV to 10 MeV the SRIM/K-P model reasonably agrees with DXS (deviations increase up to 20 - 30% at low energy), while SRIM/NRT/Tdam is systematically larger than DXS by factor up to 2;
- above 10 - 20 MeV the SRIM code omits contributions of the opening nuclear reaction channels that results to the underestimation of displacement in comparison with DXS.

Bibliography

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