Low energy ion-solid interactions: a quantitative experimental verification of binary collision approximation simulations

Hans Hofsäss, Felix Junge, Patrick Kirscht, Koen van Stiphout

2nd Institute of Physics, University Göttingen, Germany

hans.hofsaess@phys.uni-goettingen.de

DPG spring meeting 2024

DS 20.21

Poster D: DS 144 Thu

see also DS 152 Thu

see also:

Poster B DS 147 Wed

Abstract

The new dynamic Monte Carlo program IMINTDYN based on the binary collision approximation allows a reliable prediction of low energy implantation profiles and target compositional changes, as well as efficient simulation of high energy light ion scattering. **To demonstrate the quality of these predictions and simulations, we present a model case experiment where we implanted W ions into tetrahedral amorphous carbon with low (10 keV) and ultra-low (20 eV) ion energies and analyzed the W implantation profiles with high resolution Rutherford backscattering spectrometry (HR-RBS). This experiment is compared with a complete simulation of all aspects of ion-solid-interactions of the experiment using the new IMINTDYN program.** A unique novel simulation option is the inclusion of the vacancy as target species with dynamic vacancy generation and annihilation. Whereas simulations neglecting vacancy formation cannot reproduce the measured implantation profiles, we find excellent agreement between simulated and measured HR-RBS spectra. We also demonstrate the important role of simultaneous weak collisions in the binary collision approximation.

Upgrades and new features of IMINTDYN

Simulation options:

- **Improved energy loss options up to 2 GeV**
  - Ziegler/Biersack stopping model
  - SRIM-2013 stopping data
- **New bulk binding energy model**
- **Flexible mean free path of projectiles**
  - To speed up light ion high energy collisions
- **Vacancy as a "new" target atom**
  - Modelling of generation and annihilation of vacancies
- **Enforce large angle scattering**
  - Tunable for backscattering and forward scattering
  - Includes multiple scattering
  - Use of statistical weights
- **Enhanced book keeping**
  - Coincident events mapping
  - Scattering angle distributions
  - Collision counters
  - Logbook and debugging

- **DELL Precision 7865 Desktop Tower**
- **AMD Ryzen Threadripper Pro 5965WX**, 24 cores, 48 threads, 3.8-4.5 GHz
- oneAPI FORTRAN Compiler
- parallel processing using message passing interface (MPI)

New Input/Output options:

- Improved projectiles angular / energy distributions
- Improved target layer structure definition
- Includes target isotopic properties
- Non-Rutherford IBANDL library cross section data
- Post processing programs for ERDA, EBS, RBS, LEIS, ERCS, C-ERDA
- Creates input files for SIMS simulations

- **If you have an SDTrimSP 6.0 license (500€ single user, 1000€ up to 5 users) , you may obtain the IMINTDYN code**

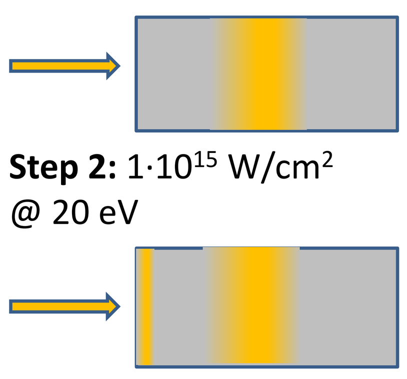
Experiment:

1. **Sample: ta-C film on Si**
2. **1st Implantation of ta-C with 10 keV W 10^{15} cm^{-2}**
3. **2nd Implantation of ta-C with 20 eV W 10^{15} cm^{-2}**
4. **High Resolution RBS ion beam analysis with 446 keV He$^+$ @ 127° and resolution $\Delta E/E = 0.005$**
5. **Simulation of implantation profiles and HR-RBS spectra with IMINTDYN**
6. **Calibration sample: sputtered W film on Si**

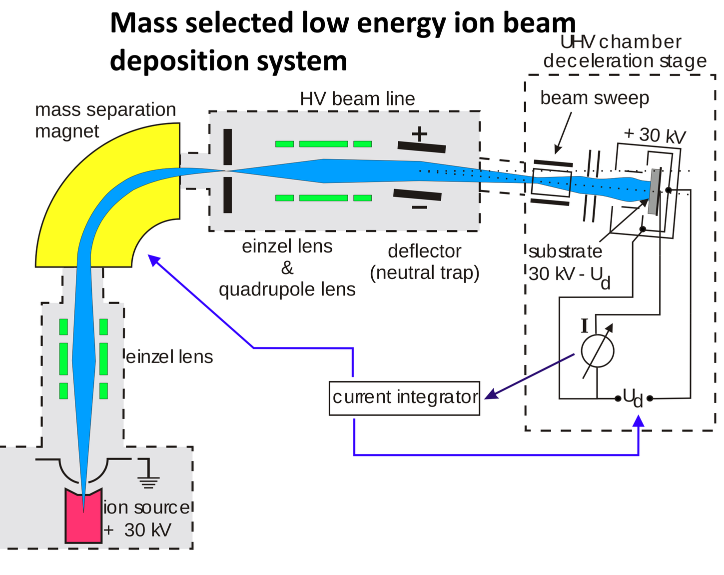
Experiment:

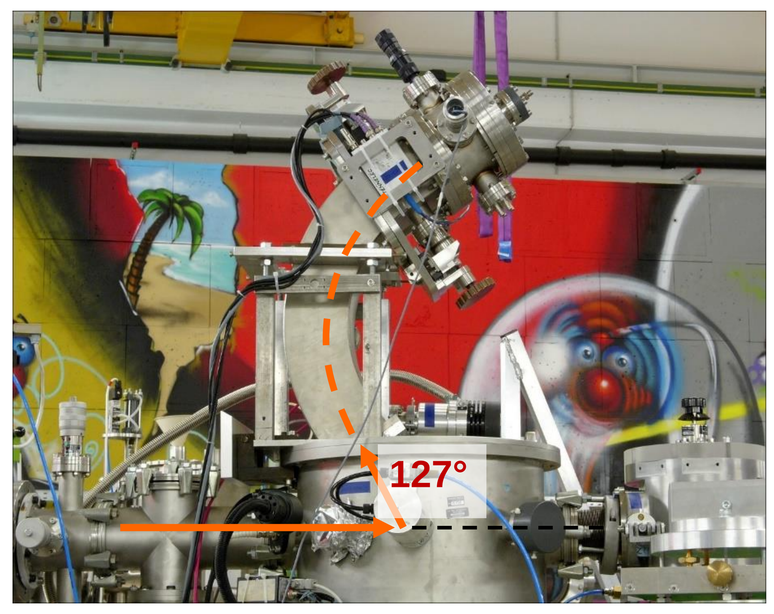
Step 1: $1{\cdot}10^{15}$ W/cm^2 @ 10 keV

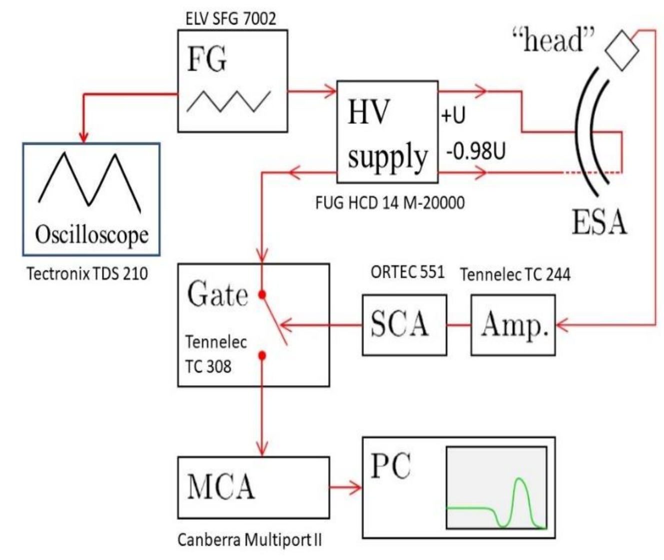
Step 2: $1{\cdot}10^{15}$ W/cm^2 @ 20 eV



Mass selected low energy ion beam deposition system



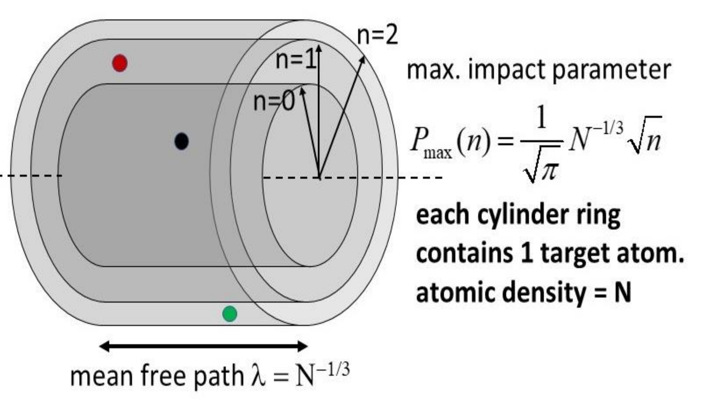




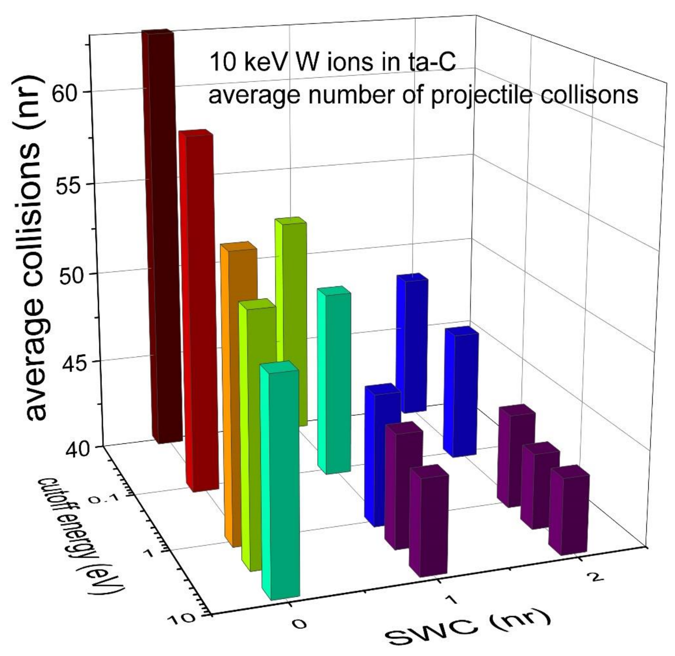
View of the HR-RBS chamber with cylindrical electrostatic analyzer with 90° deflection. The He$^+$ ion beam from our 500 kV ion accelerator enters through the beamline on the left side. The acceptance angle of the analyzer is 127° with respect to the beam direction. At the top of the 90° capacitor are extraction collimators and the surface barrier detector ion counter.

Schematic signal processing diagram of the ESA System.

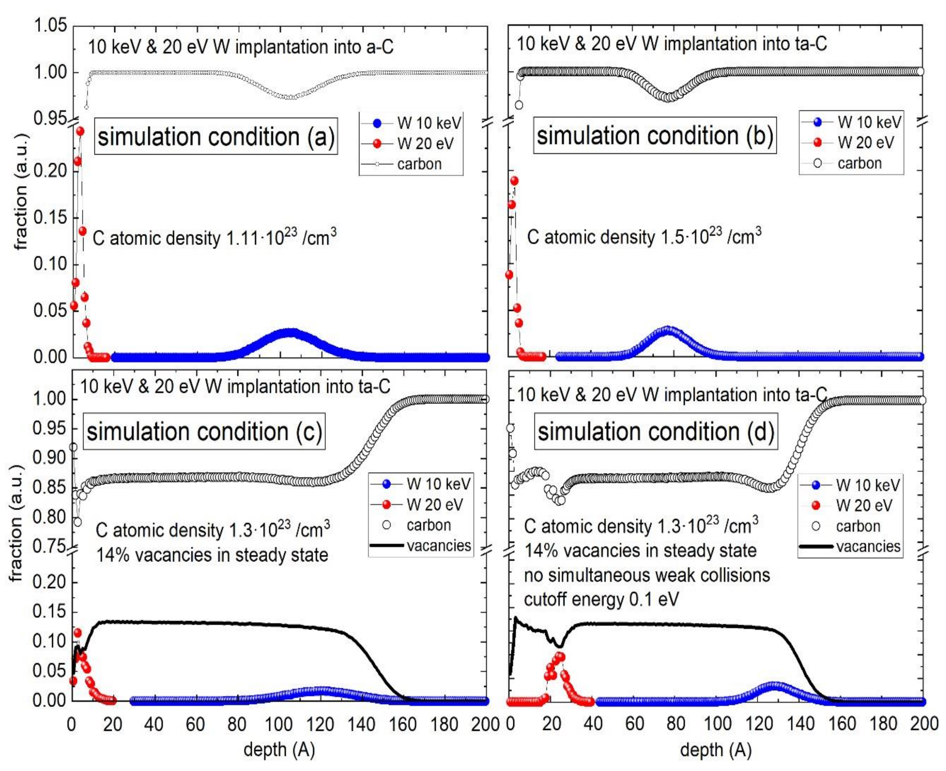
Simultaneous weak collisions

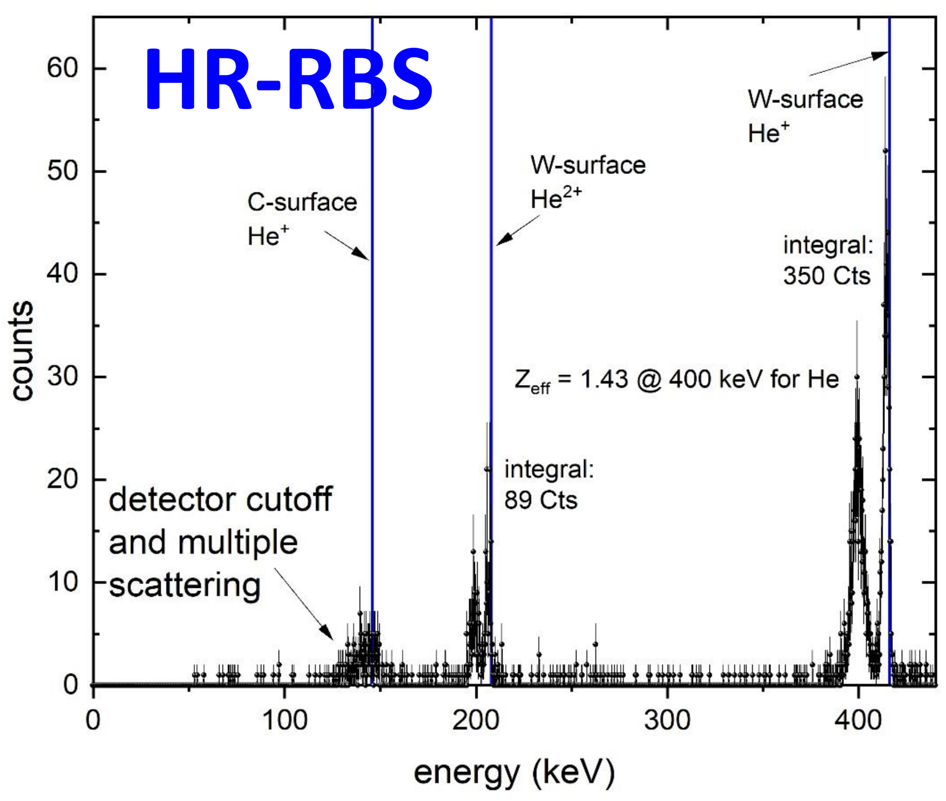


Above: Concept of simultaneous weak collisions with coaxial ring cylinder volumes containing one target Atom each at random position.



Left: Average number of collisions as function of number of simultaneous weak collisions (SWC) and as function of the cutoff energy.





Simulation of vacancy generation and annihilation

formation probability:

$$p_{formation} = q_{vac} \cdot (1 - c_{vac})^2$$

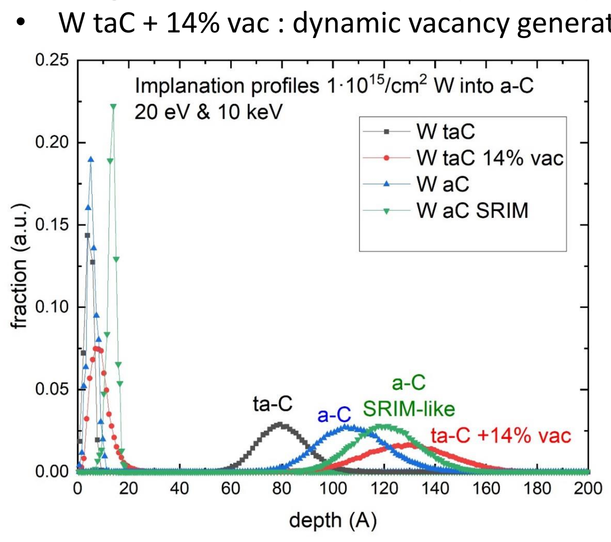
annihilation probability:

$$p_{annihilation} = \min\left[1, n_{coord} \cdot c_{vac}\right]$$

- **probability per collision:** $q_{vac} = 1$
- **dependence on local vacancy concentration c_{vac} and atomic coordination number n_{coord} =3,…,6**

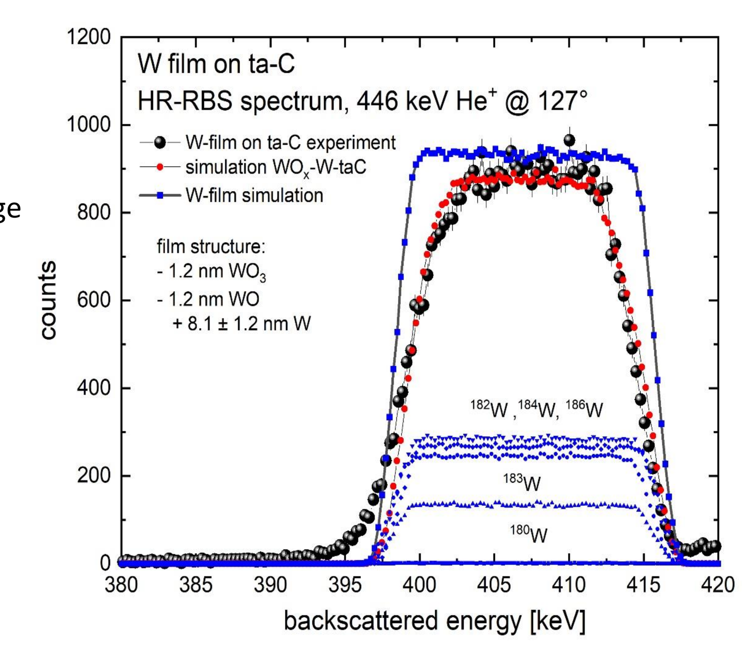
IMINTDYN simulation of implantation profiles for 20 eV & 10 keV W in to ta-C:

- W ta-C: Fixed ta-C density of 3 g/cm^3
- W a-C : Implantation in a-C with 2.263 g/cm^3
- W a-C SRIM: Implantation in a-C with 2.263 g/cm^3 ZBL potential, magic integration, no weak collisions (SRIM-like)
- W taC + 14% vac : dynamic vacancy generation in ta-C 2.6 g/cm^3

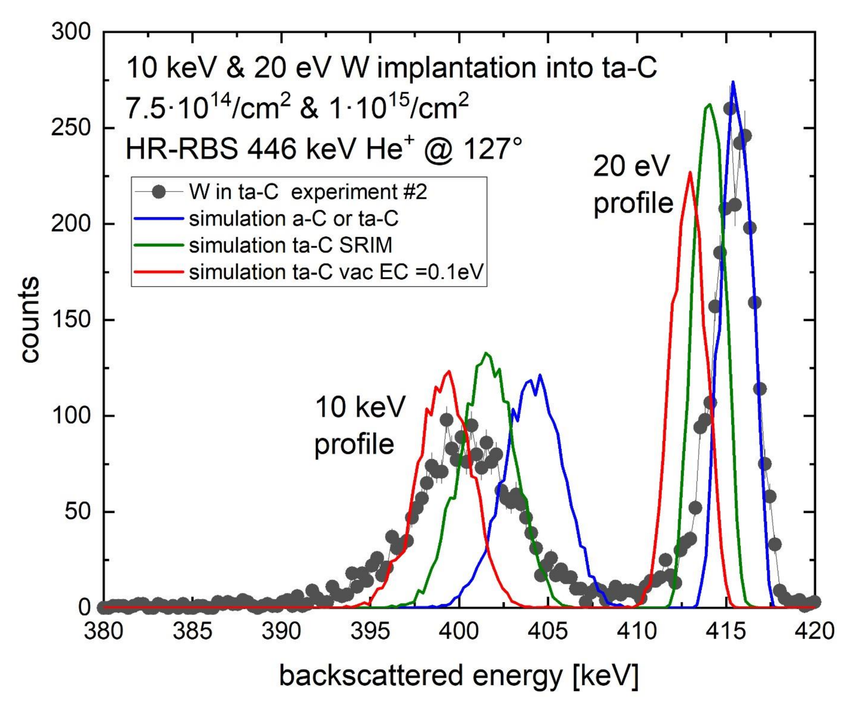


- Up to 60 % variation in ion range depending on simulation conditions
- Small fraction of voids or vacancies (14%) increase the range significantly
- Voids cannot be simulated by assuming a lower density.

total simulation time: 1 min

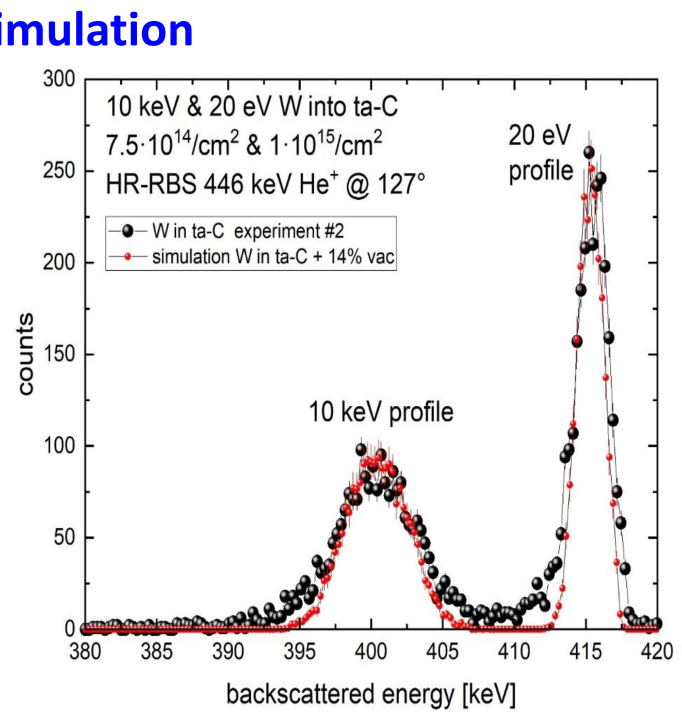


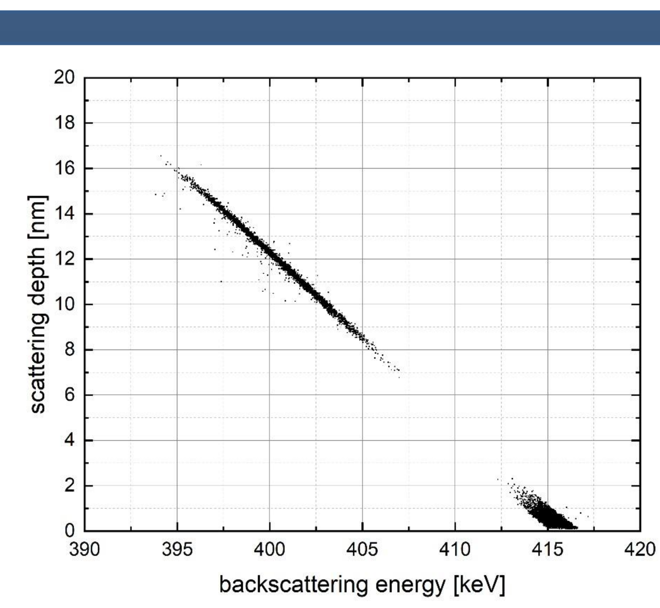
HR-RBS data & IMINTDYN simulation



HR-RBS data & IMINTDYN simulation

Comparison of the experimental HR-RBS spectrum (black data points) and a simulation (red data points) for ion implantation into ta-C with initial carbon density of $1.5{\cdot}10^{23}$ at./cm^3, allowing dynamic vacancy generation. The steady state vacancy concentration is rapidly established and is about 14%. The carbon atomic density is $1.3{\cdot}10^{23}$ at./cm^3, much higher than the atomic density of graphite.





Scatter plot of data points of the depth of backscattering at W atoms versus He+ backscattering energy for the simulated HR-RBS spectrum shown in the figure on the left.

Conclusion

- **Experimental data fit best to „defective" ta-C with 14% vacancies or voids due to sp^3-sp^2 conversion.**
- **Simultaneous weak collisions necessary**
- **Vacancy formation necessary – 14 % vacancies in steady state**

References:

[1] Low energy ion-solid interactions: a quantitative experimental verification of binary collision approximation simulations, H. Hofsäss, F. Junge, P. Kirscht, K. van Stiphout, Material Research Express (2023) DOI 10.1088/2053-1591/ace41c

[2] Binary collision approximation simulations of ion solid interaction without the concept of surface binding energies H. Hofsäss and A. Stegmaier, Nucl. Instr. Meth B 515 (2022) 49-62

[3] W. Eckstein, Computer Simulation of Ion Solid Interactions (Springer, Berlin,1991)

[4] Mutzke, A., Schneider, R., Eckstein, W., Dohmen, R., Schmid, K., Toussaint, U. v., et al. (2019). SDTrimSP Version 6.00 (IPP 2019-02). Garching: Max-Planck-Institut für Plasmaphysik. doi:10.17617/2.3026474.

[5] M. Mayer, Nul. Instr. Meth. B 332, (2014) 176

[6] K. Arstila, T. Sajavaara, J. Keinonen, Nucl. Instr. Meth. B 174 (2001) 163

[7] F. Schietekatte, Monte Carlo simulation of Ion Beam Analysis spectra using Corteo, Joint ICTP/IAEA Workshop on Advanced Simulation and Modelling for Ion Beam Analysis, 23 - 27 February 2009