An attempt to predict oligomer sputtering with binary collision approximation simulations

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DS 20.21
Poster D: DS 152 Thu

see also DS 144 Thu
see also:
Poster B DS 147 Wed

Motivation

- Development of a versatile Monte Carlo (MC) binary collision approximation (BCA) simulation program for MeV ion scattering, as well as low energy and ultra-low energy ion-solid interactions[1,2,3]. **Here: Prediction of oligomer sputter yields**
- **Fast simulation comparable to duration of an experiment**
- Follow up dynamic stoichiometry changes
- **Capability of parallel processing using MPI routines**
- Upgrade and extension of the MC-BCA code SDTrimSP [4]

➔ **I**on **M**atter **I**nteraction **D**ynamic IMINTDYN

- Complementary to SIMNRA [5], POTKU [6], CORTEO [7] simulation software

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

Upgrades and new features of IMINTDYN

New simulation options:

- **Table of thermodynamic data for binary and ternary compounds**
- **Improved energy loss options up to 2 GeV**
- SRIM-2013 stopping data
- **New bulk binding energy model**
- **Vacancy as a "new" target atom**
- Modelling of generation and annihilation of vacancies

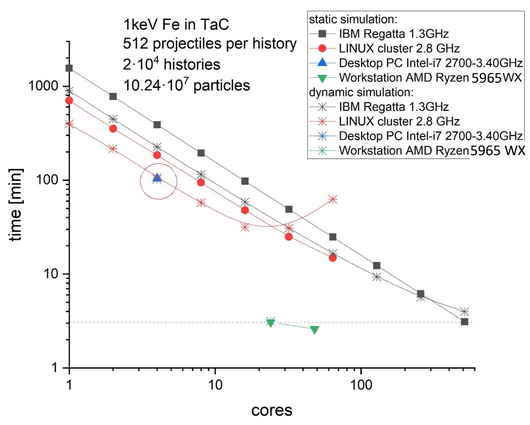
- **DELL Precision 7865 Desktop Tower**
- **AMD Ryzen Threadripper Pro 5965WX**, 24 cores, 48 threads, 3.8-4.5 GHz
- oneAPI FORTRAN Compiler
- parallel processing using message passing interface (MPI)

New Input/Output options:

- Improved projectiles angular / energy distributions
- Improved target layer structure definition
- Includes target isotopic properties
- Oligomer formation enthalpy table
- **Oligomer sputter yield output table**

- **Enhanced book keeping**
- Coincident events mapping
- Scattering angle distributions
- Collision counters
- Logbook and debugging

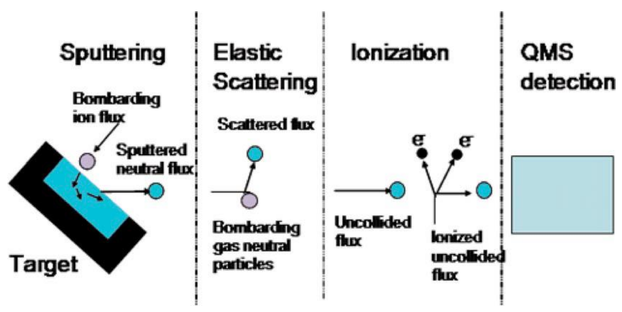
Benchmark from SDTrimSP

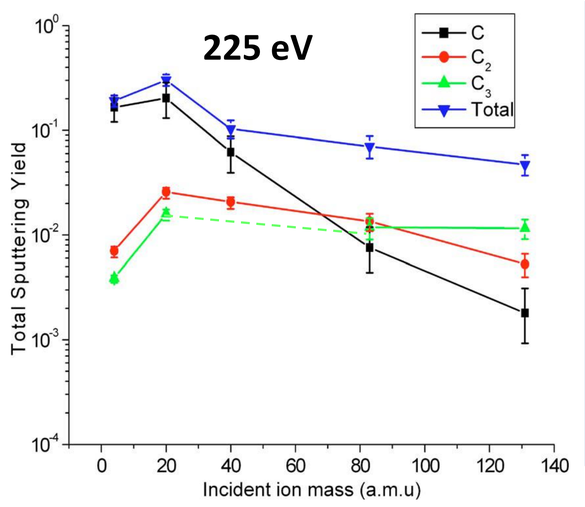


- **If you have an SDTrimSP 6.0 license (500€ single user, 1000€ up to 5 users) , you may obtain the IMINTDYN code**

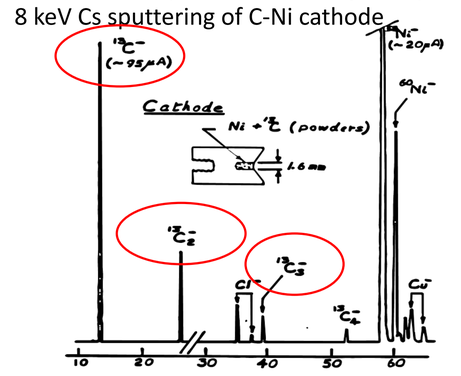
Sputtering of Dimers and Trimers

Carbon atom and cluster sputtering under low-energy noble gas plasma bombardment
E. Oyarzabal, R. P. Doerner, M. Shimada, and G. R. Tynan, J. Appl. Phys. **104**, 043305 (2008)





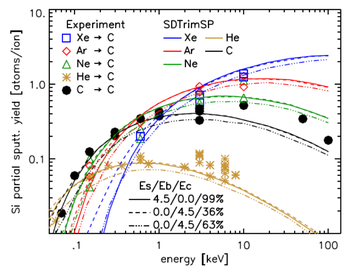
Roy Middleton
Department Of Physics, University of Pennsylvania
Philadelphia, PA 19104
October 1989 (Revised February 1990)
8 keV Cs sputtering of C-Ni cathode



Spectrum of ^{13}C. The cathode was prepared from about a 1 to 1 atom mixture of very fine nickel

SDTrimSP: C ➔ C

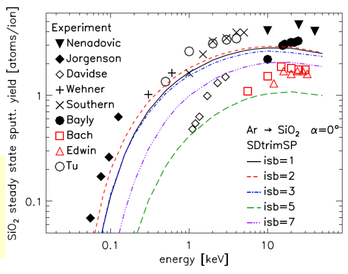
surface binding energy 4.5 eV, not 7.4 eV !!



SDTrimSP: Ar ➔ SiO_2

surface binding energy 1.0 eV, not 2.58 eV !!

SDTRimSP users see the surface binding energy as fit parameter

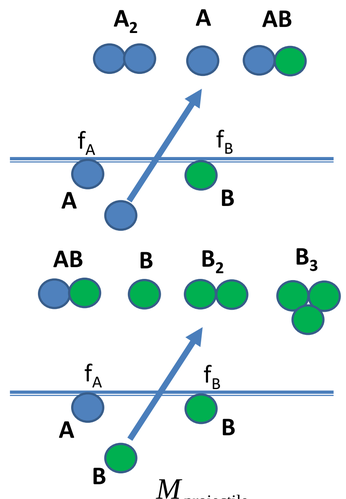


Oligomer sputtering model

Sputter yield is based on thermodynamic properties like monomer, dimer and trimer **formation enthalpies H** and local surface atomic concentrations **f**

Data base:
NIST chemistry WebBook

Z1-Z2	Z1	Z2	Z1-Z1	Z1-Z2	Z2-Z2	Z2-Z2-Z2
	monomer	monomer	dimer	dimer	dimer	trimer
	eV/atom	eV/atom	eV /molecule	eV /molecule	eV /molecule	eV /molecule
C = C	7.4	7.4	8.68	8.68	8.68	8.51
Si = O	4.7	2.58	6.11	-1.04	0.0	1.48
Ta = O	8.1	2.58	-----	1.99	0.0	1.48
Ba = O	1.86	2.58	3.71	-1.28	0.0	1.48
Na = Cl	1.11	1.25	1.47	-1.88	2.31	-----
Li = F	1.65	0.82	2.24	-3.53	0.0	-----



$$E_{dimer} = \frac{M_{projectile}}{M_{projectile} + M_{target}} E_{kin}$$

$$E_{trimer} = \frac{1}{3} E_{kin}$$

$$E_{dimer,final} = E_{dimer} - H_{dimer}$$

$$E_{trimer,final} = E_{trimer} - H_{trimer}$$

BBE-model:

$$E_{dimer,final} \quad E_{trimer,final}$$

SBE-model:

$$E_{normal,dimer} = (E_{dimer,final} + H_{dimer}) \cdot \cos^2\theta \quad > H_{dimer}$$

$$E_{normal,trimer} = (E_{trimer,final} + H_{trimer}) \cdot \cos^2\theta \quad > H_{trimer}$$

partition function:

$$Z = \sum_i \gamma_i \exp\left(-\frac{H_i}{H_{C-monomer}}\right); \; oligomer\ i$$

empirical formation efficiency γ_i

oligomer fraction:

$$p_{oligomer\,i} = \frac{1}{Z}\gamma_i \exp\left(-\frac{H_{oligomer\,i}}{H_{monomer\,i}}\right)$$

probability for oligomer formation:

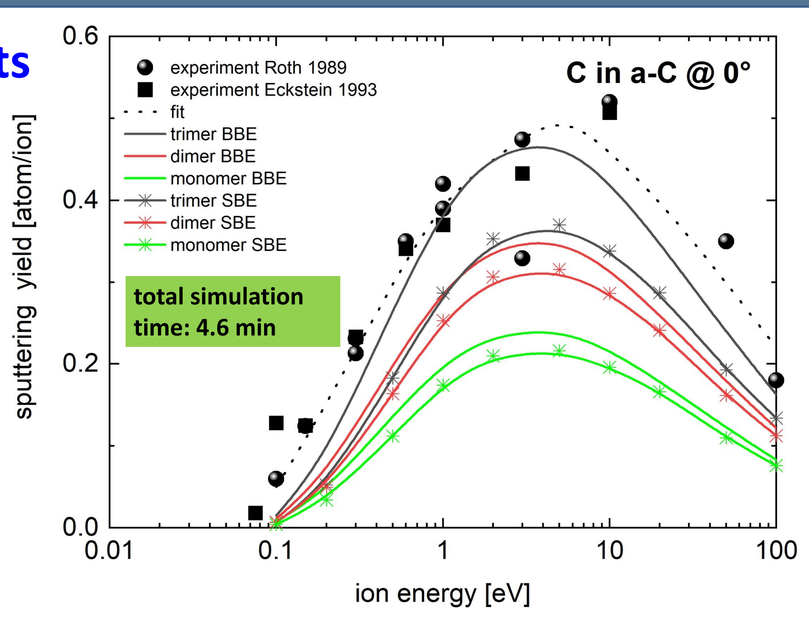
$$p_{XA} = \frac{f_A}{f_A + f_B} \quad p_{XB} = \frac{f_B}{f_A + f_B} \quad p_{BBB} = \left(\frac{f_B}{f_A + f_B}\right)^2$$

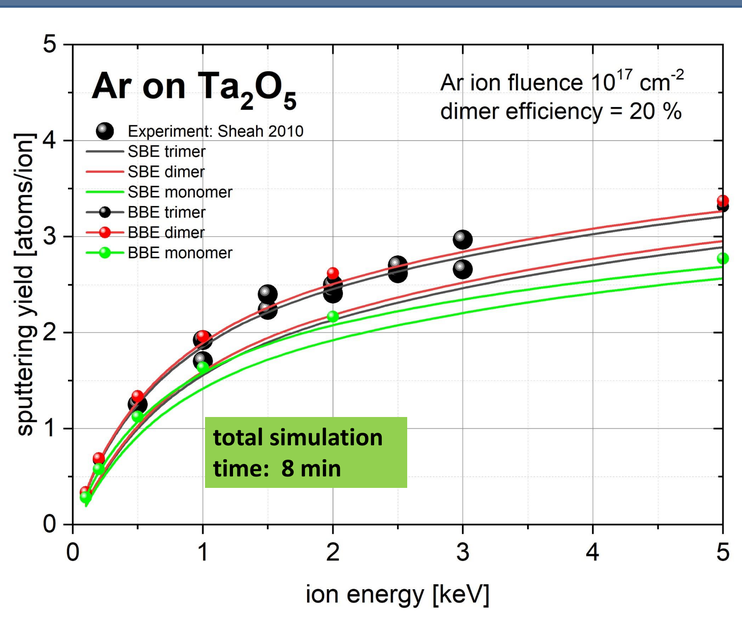
atomic fractions f_A and f_B

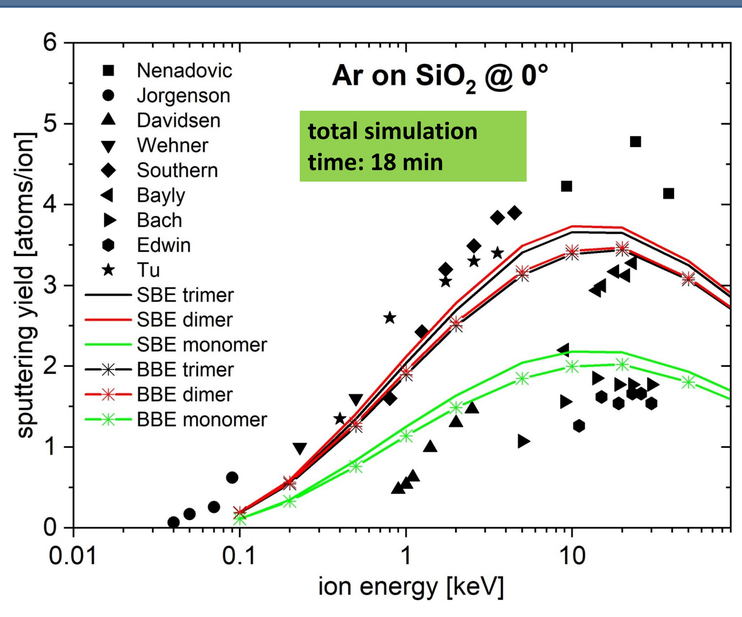
oligomer sputter yield:

$$Y_{BA} = Y_{mono,B} \cdot \left(p_{mono,B} + 2\,p_{BA}\,p_{dimer,BA}\right)$$
$$Y_{AB} = Y_{mono,A} \cdot \left(p_{mono,A} + 2\,p_{AB}\,p_{dimer,BA}\right)$$
$$Y_{AA} = Y_{mono,A} \cdot \left(p_{mono,A} + 2\,p_{AA}\,p_{dimer,AA}\right)$$
$$Y_{BB} + Y_{BBB} = Y_{mono,B} \cdot \left(p_{mono,B} + 2\,p_{BB}\,p_{dimer,BB} + 3\,p_{BBB}\,p_{trimer,BBB}\right)$$

Results







Conclusion

- **IMINTDYN = Upgraded versatile Monte Carlo BCA code applicable for:**
  - Simulation of ultra - Low energy Collisions
  - Dynamic formation of voids and vacancies
  - Sputtering simulations with novel BBE model
  - Crater function simulation for pattern formation parameters
  - **Successful Prediction of oligomer sputter yields**
  - **Output data file with detailed information on dimer and trimer sputtering**

Dimer and Trimer sputtering model quantitatively explains the sputtering yield for Carbon targets and Oxide targets (SiO_X , Ta_2O_5 , . . .

- **Fast dynamic simulations & Parallel processing**
- **FORTRAN-90 source code for compilation under Windows, LINUX and other operating systems**
- **Easy batch processing and simulation of parameter series**