# Fast simulation of ion beam analysis spectra using binary collision approximation

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DPG spring meeting 2024
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]
- **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 [3]

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

- Complementary to SIMNRA [4], POTKU [5], CORTEO [6] 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

**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:**

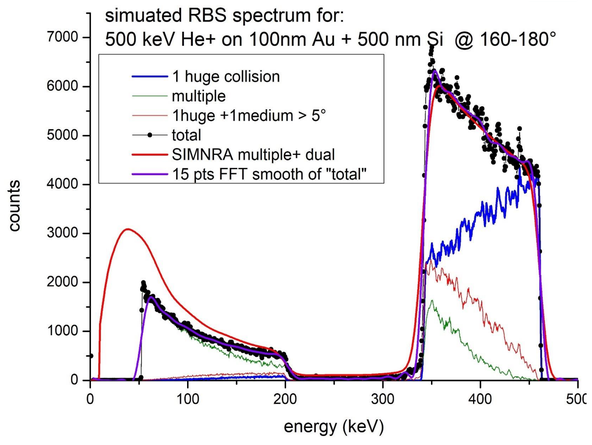
- Improved projectiles angular / energy distributions
- Improved target layer structure definition
- Includes target isotopic properties
- Non-Rutherford IBANDL library cross section data
- Post processing programs for ERDA, EBS, RBS, LEIS, ERCS, C-ERDA
- Creates input files for SIMS simulations

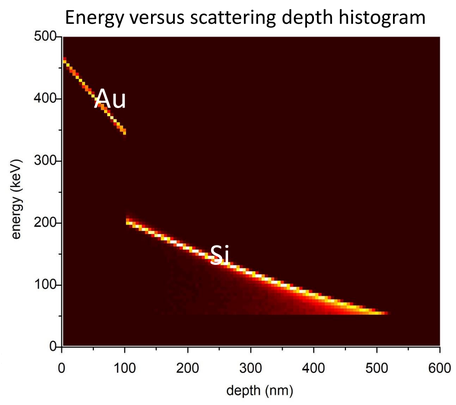
- **If you have an SDTrimSP 6.0 license (500€ single user, 1000€ up to 5 users) , you may obtain the IMINTDYN code**

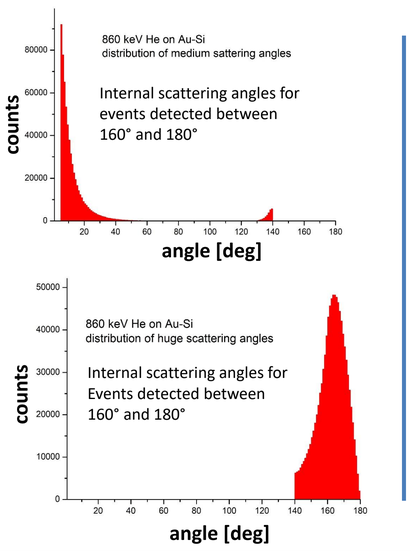
## Example: RBS and EBS simulations

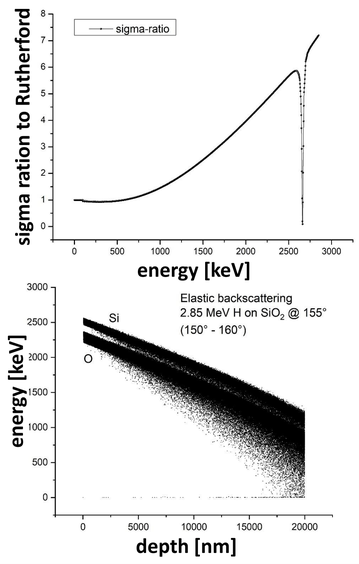

160-180°
500 keV He+
860 keV He+

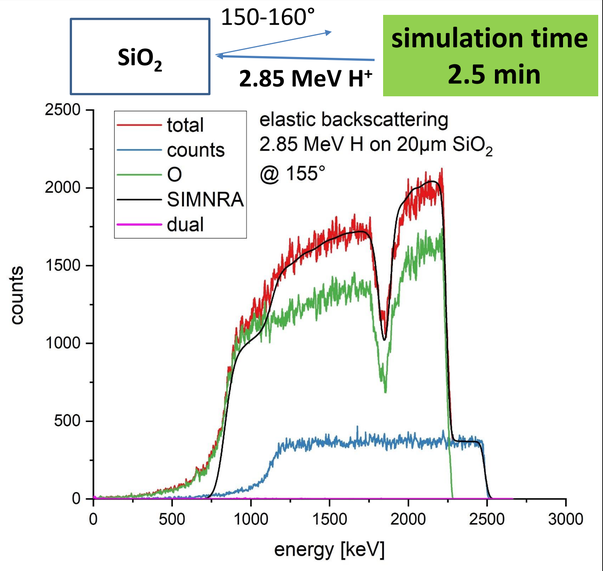
**simulation time 19 min**



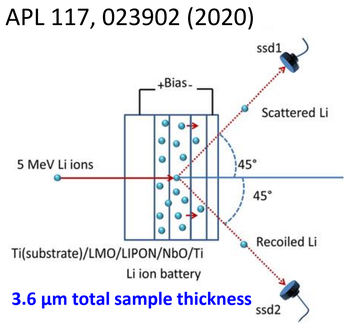

## Example: coincidence ERDA simulations

**Experiment done in Uppsala:**

**In-operando observation of Li depth distribution and Li transport in thin film Li ion batteries**

Vairavel Mathayan, Marcos V.Moro, Kenji Morita, Bun Tsuchiya, Rongbin Ye, Mamoru Baba, Daniel Primetzhofer

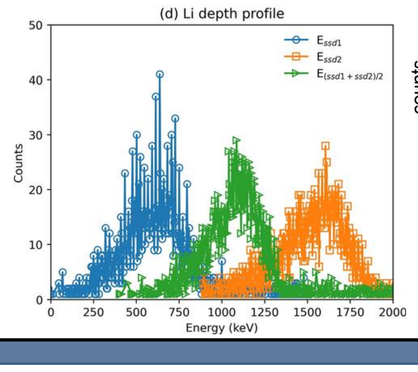
APL 117, 023902 (2020)



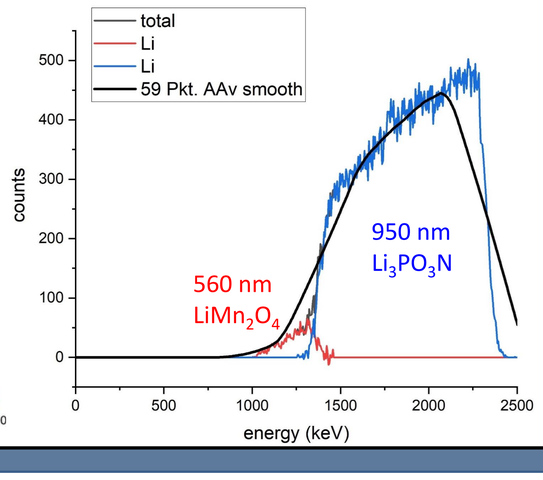

3.6 µm total sample thickness

**simulation time 7 min**

Measured Li depth profile by coincident detection of scattered and recoiled Li atoms:



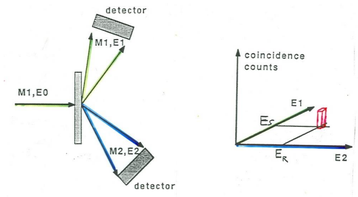

**IMINTDYN simulation of Li-Li C-ERDA spectrum**




## Example: Elastic recoil coincidence spectroscopy ERCS simulations

**2 MeV He on 2 µm Polycarbonate**

**simulation time 7 min**

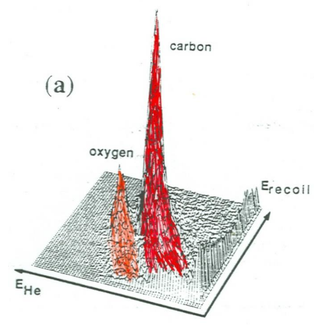



$[E_S,E_R] \rightarrow [d,M_2]$

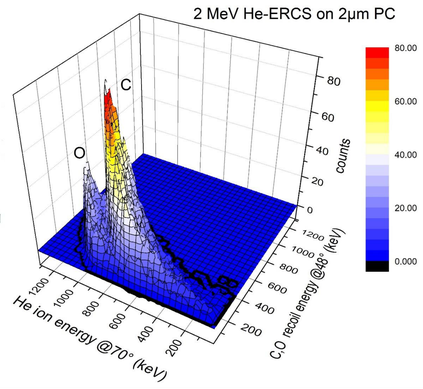
Each pair of energies [ES,ER] is related to the mass $M_2$ of the recoiled atom and the depth d where scattering/recoil has taken place

H.C. Hofsäss, N.R. Parikh, M.L. Swanson and W.K. Chu, Nucl. Instr. Meth. B58 (1991) 49

**Experimental data**




**IMINTDYN simulation**



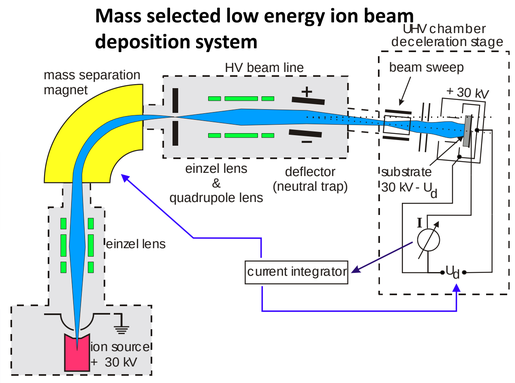

## Example: High Resolution RBS analysis of low energy implantation of W into tetrahedral amorphous carbon (ta-C)

**Experiment:**

Step 1: $1 \cdot 10^{15}$ W/cm² @ 10 keV

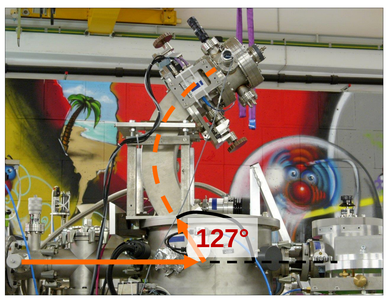
Step 1: $1 \cdot 10^{15}$ W/cm² @ 20 eV

**Mass selected low energy ion beam deposition system**




High resolution electrostatic energy analyzer for $He^+$, $He^{2+}$ ions < 1 MeV.

$$\frac{\Delta E}{E} < 0.005$$

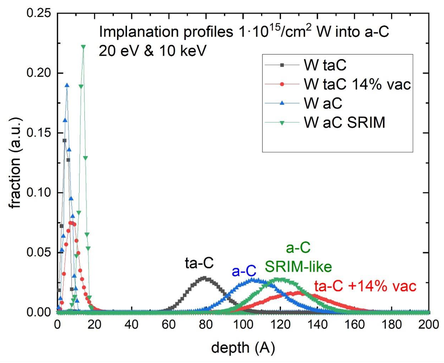



Cylindrical capacitor r=30 cm, d = 6 mm

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

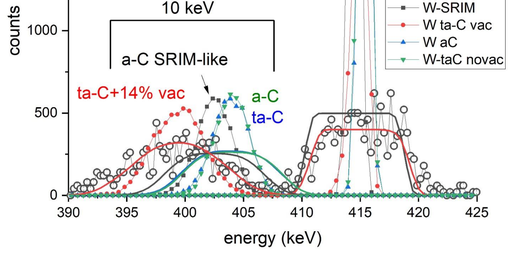
**total simulation time: 1 min**

- W ta-C: Fixed ta-C density of 3 g/cm³
- W a-C : Implantation in a-C with 2.263 g/cm³
- W aC SRIM: Implantation in a-C with 2.263 g/cm³ ZBL potential, magic integration, no weak collisions (SRIM-like)
- W taC + 14% vac : dynamic vacancy generation in ta-C 2.6 g/cm³




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

**HR-RBS data & IMINTDYN simulation**




- **Experimental data fit best to „defective" ta-C with 14% vacancies or voids due to $sp^3$-$sp^2$ conversion.**
- **Exp. energy resolution due to accidentally poor vacuum in analyzer**

## Script file to simulate 5MeV Li-Li CERDA scattering

```
5 MeV Li in Li Battery
 &IMINT_INP
  energy_mode = „none" ! One fixed energy
  e0  = 5.0E6, 0.,0.,0.,0.,0.,0.,0.,0.,0.,0.  ! ion energy (eV)
!  set projectile and target elements
  symbol = "Li","Ti","Li","Mn","O","Li","P","O","N","Nb","O","Ti"
  target_thickness =  36400E+0  ! target depth (Angstroems)
  nqx   =  1000E+0   ! number of target intervals
  beam_fraction = 1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0
  max_atomic_fraction = 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0
  charge = 1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0   ! ion charge
  layer_input = .true.
  file_layerinp = 'battery_layer.inp'
!  set atomic densities
  dns0 = 0.05665, 0.05665, 0.0956, 0.0956, 0.0956, 0.0965, 0.0965, 0.0965, 0.0965, 0.07295, 0.07295, 0.05665
  angle_mode=„none"
  alpha0 =  0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0 ! incidence angle (deg)
  phi0 = 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0 ! azimuthal angle (deg)
  projectiles = 2.4E6   ! number of projectiles
  fluence_steps_out = 10   ! number of output  infos
  static simulation = .true.
 cascade_simulation =.true.
 fluence   = 1  ! fluence in units 1E16/cm²
 potential = "KrC"  ! 1=KrC, 2=Moliere, 3=ZBL, 4=Nakagawa-Yamamura, 5=Si-Si, 6=power
 integration_mode=2, ! 0= Magic, 1 = Gauss-Mehler, 2=Gauss-Legendre
 subthr_rec_bound =.true. ! sub threshold atoms are bound
 stopping_mode = 7,7,7,7,7,7,7,7,7,7,7 ! SRIM stopping
 free_flight_path =.true.
 ffp_accuracy= 0.015! accuracy of mean free path: fraction of electr. energy loss or x100 [deg]
 enforce_scattering =.true.
 single_scattering=.true.
 cerda_angle = 30.
 cerda_angle2 = 60.
 no_e_dependence=.false.
 num_scattering = 1
 scatt_species =  "Li"
                  out_energy_p = 5.0E5
                  out_energy_r = 5.0E5
                 out_angle_pt = 42.,48.
                 out_angle_rt = 42.,48.
 huge_angle=55.
 small_angle= 35.

 e_cutoff = 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0
 atomic_fraction   = 0.0, 1.0, 0.14, 0.28, 0.58, 0.37, 0.13, 0.38, 0.12, 0.29, 0.71, 1.0
 e_thres_r= 5e4, 5e4, 5e4, 5e4, 5e4, 5e4, 5e4, 5e4, 5e4, 5e4, 5e4, 5e4
 e_displ  = 5e4, 5e4, 5e4, 5e4, 5e4, 5e4, 5e4, 5e4, 5e4, 5e4, 5e4, 5e4
 l_threshold=.true. ! only collisions above e_displ are calculated
 lpart_pb_ed=.false.
  lpart_pt_ed=.true.
  lparticle_r = .true. ! create projectile data files
  lparticle_p = .true. ! create recoil data files
 ! number of traced particles for:
 ! stopped, backscattered and transmitted
 ! projectiles,stopped, backsputtered,
 !transmission sputtered recoils
 ioutput_part = 10, 10, 600000, 10, 600000, 600000
 /
```

## Conclusion

- **Upgraded versatile Monte Carlo BCA code applicable for:**
  - Ultra - Low energy Collisions
  - Dynamic formation of voids and vacancies
  - Sputtering with novel BBE model
  - Crater function simulation for pattern formation
  - Ion Implantation
  - High energy forward and backscattering
  - Coincidence scattering
  - Non-Rutherford scattering
  - SIMS Sputter simulations
- **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**
- **Should not replace SIMNRA but provides much more details of MeV ion scattering spectra**
- **Multiple scattering effects included**