Fundamental aspects of beryllium compound formation and erosion and hydrogen retention in beryllium

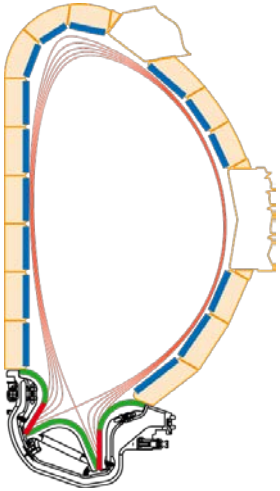
Christian Linsmeier

P. Goldstraß, A. Wiltner, F. Kost, M. Reinelt, M. Oberkofler,
M. Köppen, R. Piechoczek
A. Allouche, Y. Ferro *(Aix-Marseille Université)*

Overview

1. **Processes at the ITER first wall**
2. **Investigated Be-based systems**
3. **Thermally induced reactions (examples)**
   - C/Be, Be/C
   - W/Be, Be/W
4. **Ion-induced reactions (examples)**
   - $C^+ \rightarrow$ Be, $CO^+ \rightarrow$ Be
   - $N^+ \rightarrow$ Be
   - $O^+ \rightarrow Be_2W$/W
5. **Modeling of surface reactions**
6. **Hydrogen isotope retention and release**
7. **Surrogates for Be?** (separate presentation)
8. **Outlook**

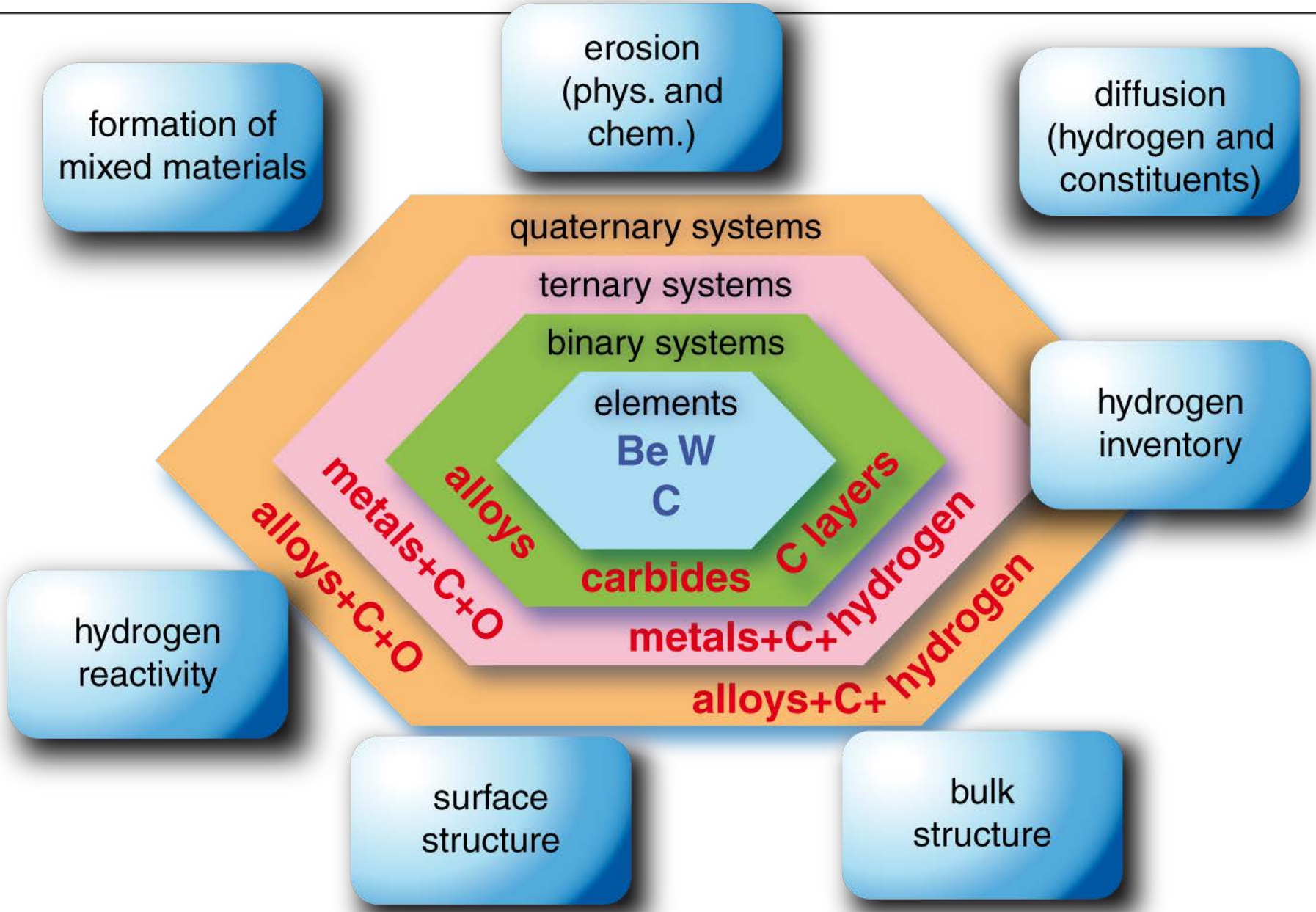
Surface chemistry on first wall materials



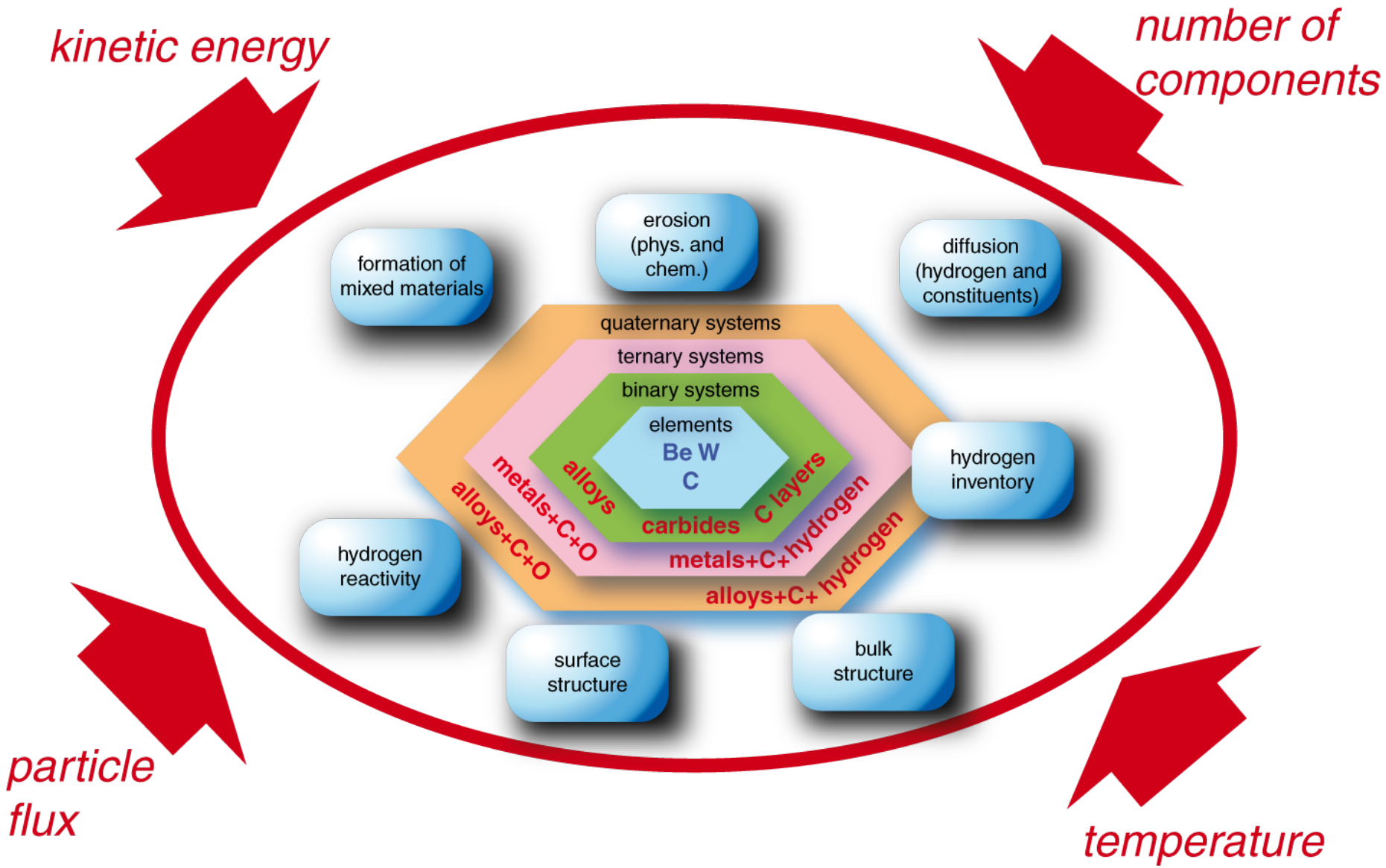
- First wall on ITER
  - → carbon 55 m^2
  - → tungsten 140 m^2
  - → beryllium 690 m^2
- Variable local conditions (temperature, fluence, species…)
- Erosion and redeposition, impurities:
  - → mixed phases (e.g. carbides, oxides, nitrides, alloys)
- Layers on metals influence hydrogen (isotope) inventory:
  - → reaction, diffusion, desorption
- Goal: qualitative and quantitative description of fundamental processes
  - → formation and erosion of multi-component layers
  - → influence of layers on hydrogen inventory

→ **Include surface reactions in global integrated PWI model**

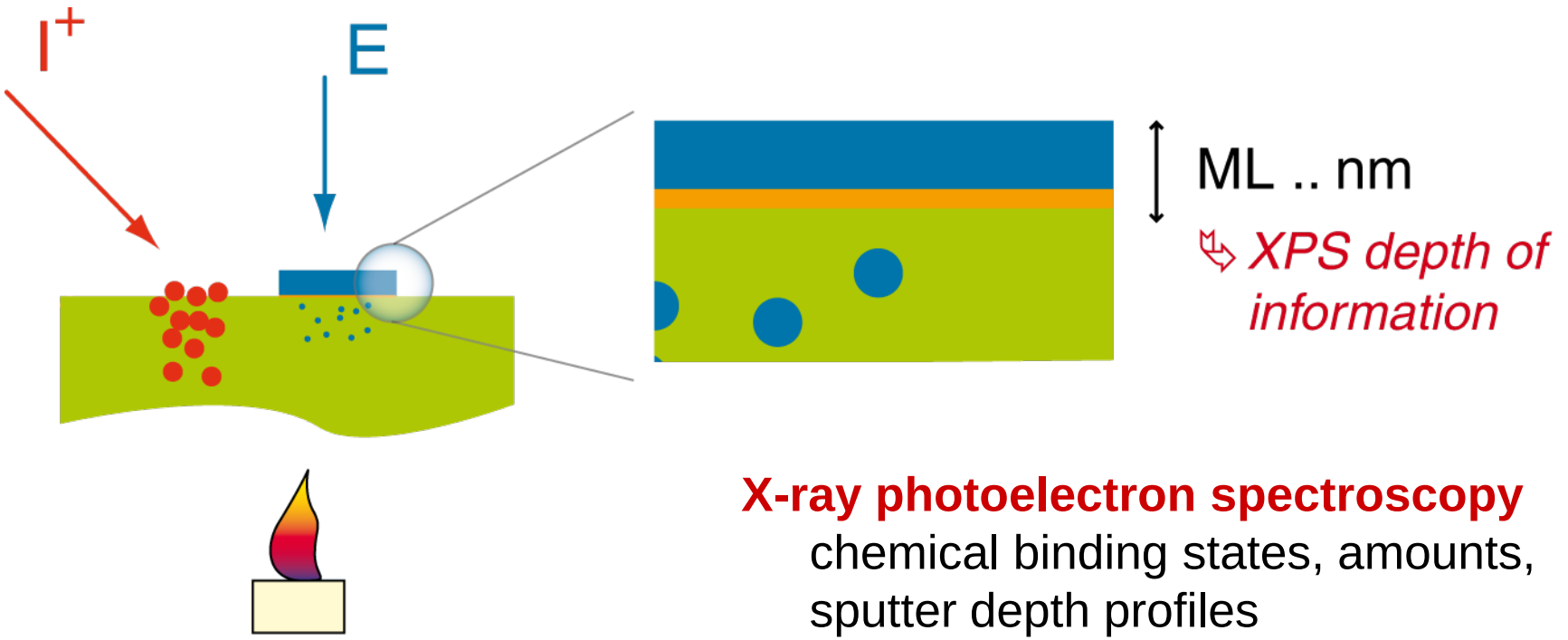
Components and processes



Components, processes and parameters



Experimental approach



X-ray photoelectron spectroscopy

chemical binding states, amounts, sputter depth profiles
synchrotron: chemical depth profiles

Accelerator-based techniques

amounts, depth profiles
hydrogen isotope analysis (amounts, profiles)

Preparation and treatment conditions

base pressure ≥ 2 x 10^{-9} Pa

Modeling approach: Description of chemistry

1. Define all substances

Be
W
C
Be_2C
W_2C
WC
Be_2W
$Be_{12}W$
Be_{gas}
BeO
O_{ads}
WO_3
$WO_{3,gas}$

+ Initial areal densities [#/m²]

2. Elementary reactions

$2\,Be + C \rightarrow Be_2C$
$Be_2C \rightarrow 2\,Be + C$
$W + C \rightarrow WC$
$WC \rightarrow W + C$
$2\,W + C \rightarrow W_2C$
$W_2C \rightarrow 2\,W + C$
$W + 2\,Be \rightarrow Be_2W$
$Be_2W \rightarrow W + 2\,Be$
$W_2C \rightarrow WC + W$
$WC + W \rightarrow W_2C$
$Be + O \rightarrow BeO$
$BeO \rightarrow Be + O$
$W + 3\,O \rightarrow WO_3$
$WO_3 \rightarrow W + 3\,O$

Sublimation:
$Be \rightarrow Be_{gas}$
$WO_3 \rightarrow WO_{3,gas}$

O-Adsorption:
$O_{2,gas} \rightarrow O_{ads}$
$O_{ads} \rightarrow O_{2,gas}$

3. Define equations for reaction fluxes

$$\Gamma_1\left[\tfrac{1}{m^2 s}\right] = [Be]^2[C]k_1 \exp\frac{-\Delta E_1}{kT} \quad \text{with} \quad k_1\left[\tfrac{m^4}{s}\right]$$

$$\Gamma_2\left[\tfrac{1}{m^2 s}\right] = [Be_2C]k_2 \exp\frac{-\Delta E_2}{kT} \quad \text{with} \quad k_2\left[\tfrac{1}{s}\right]$$

4. Define balances

Change of areal density of substance =
+ all formation reaction fluxes
– all destruction reaction fluxes
± all "non-chemical" fluxes

$$\frac{d[Be]}{dt} = -2\Gamma_1 + 2\Gamma_2 + \ldots \qquad \frac{d[Be_2C]}{dt} = +\Gamma_1 - \Gamma_2 + \ldots$$

→ Set of ordinary differential equations

$$y'(t) = f(t, y(t)), \quad \text{with initial value} \quad y(t_0) = y_0$$

Overview: investigated systems

1. Binary Be-based systems

- **C/Be, Be/C** lab., DFT
- **$C^+ \rightarrow$ Be** lab.
- Be/W, W/Be lab., DFT
- **$N^+ \rightarrow$ Be** lab., DFT
- O_{at}, $O_2 \rightarrow$ Be lab.

3. Ternary Be-based systems

- **$CO^+ \rightarrow$ Be** lab.
- **$O^+ \rightarrow Be_2W$/W** synchr.
- C/BeO/W synchr.
- Be/C/W, C or Be excess lab.
- C/Be/W, C or Be excess lab.
- Be/WO_2, Be/WO_3 lab.
- C/W/Be synchr.
- WO_x/Be synchr.

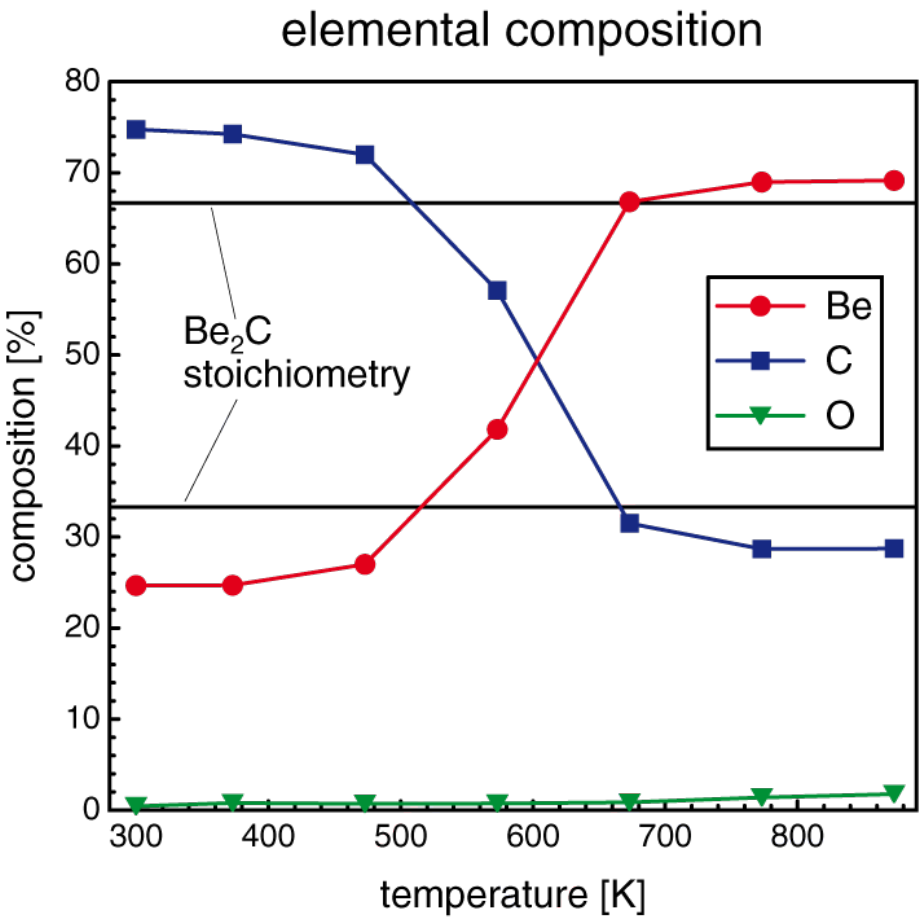
2. Hydrogen isotope retention and release

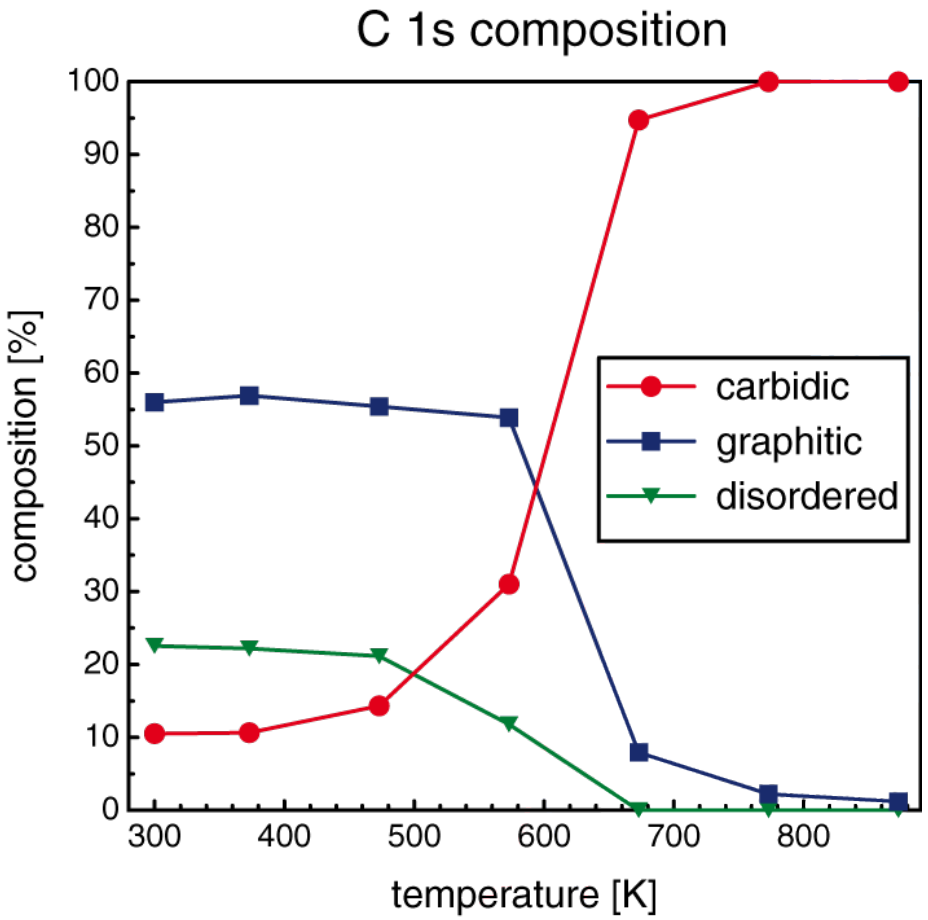
- **$D^+ \rightarrow Be_{poly}$, Be(0001), Be(1 1 -2 0)** lab., DFT
- $D^+ \rightarrow$ O/Be, BeO lab., DFT

Be—C
thermally induced reactions

C / Be: chemical compound formation

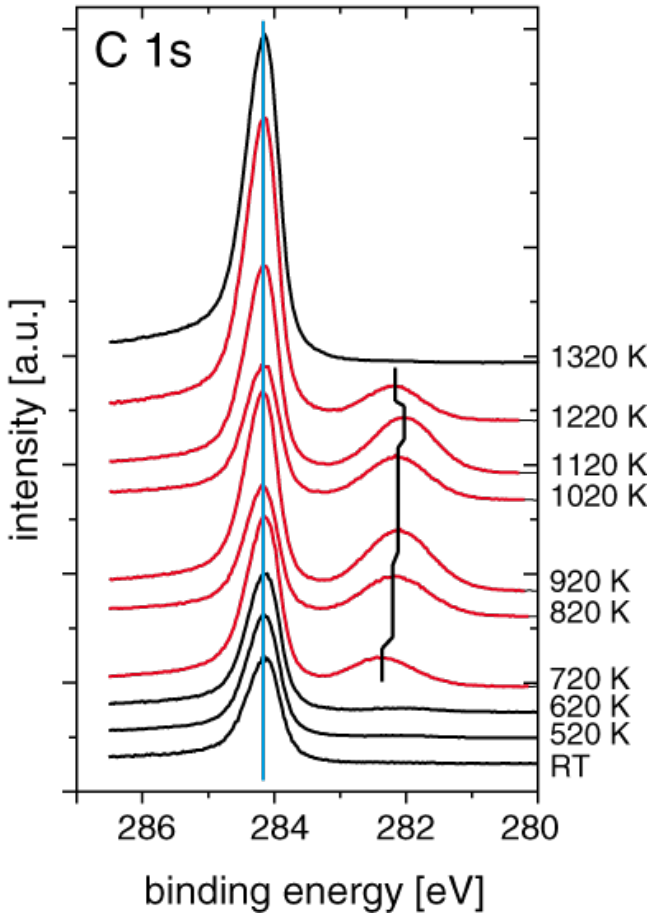
C amount: 4.86×10^{16} cm^{-2} ($\approx$ 5.3 nm)



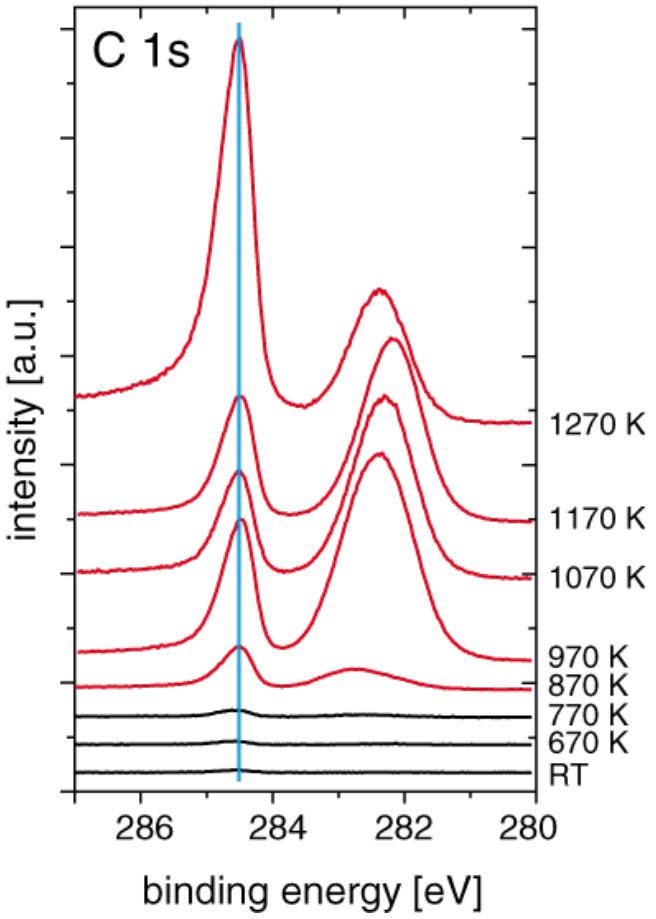


Phases during annealing

1.35 nm Be on PG



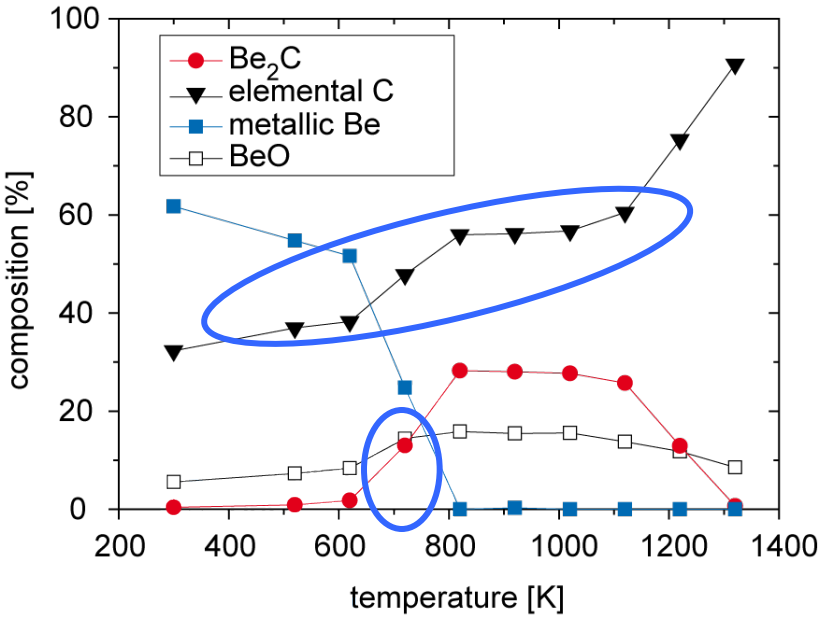
4.6 nm Be HOPG



- PG: carbide formation at lower temp.
- Be_2C peak position: shift due to island size

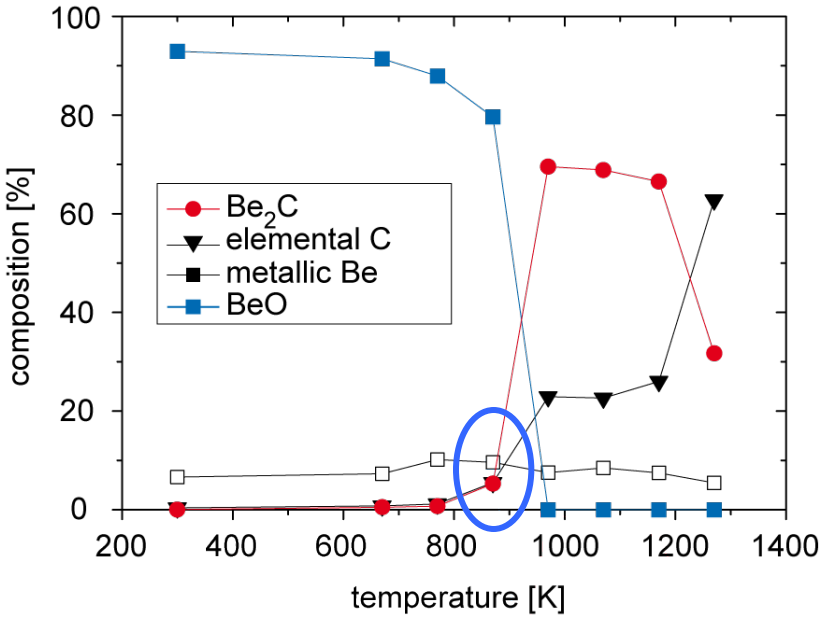
Phases during annealing

1.35 nm Be on PG



- Additional Be_2C: >720 K
- Be_2C loss starts at 1170 K, no carbide above 1330 K
- Island growth

4.6 nm Be HOPG



- Additional Be_2C: >870 K
- Be_2C loss starts at 1270

Carbide formation kinetics: Be on PG

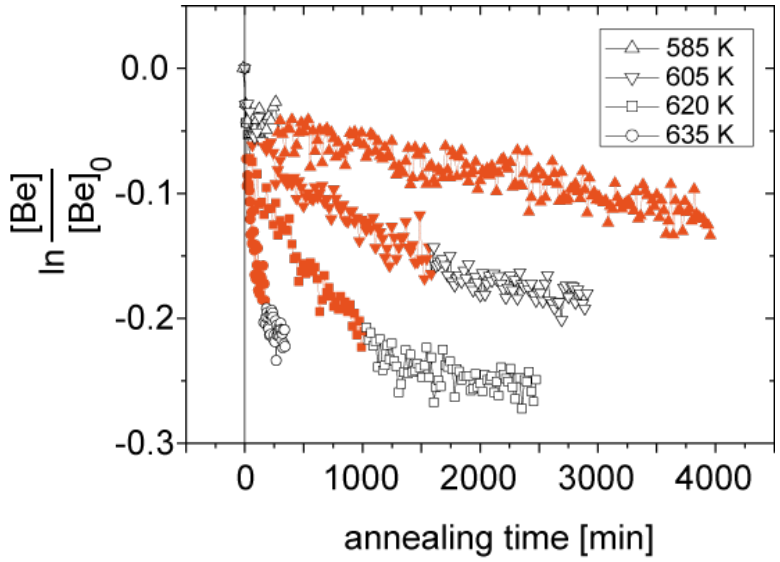
1st order reaction:

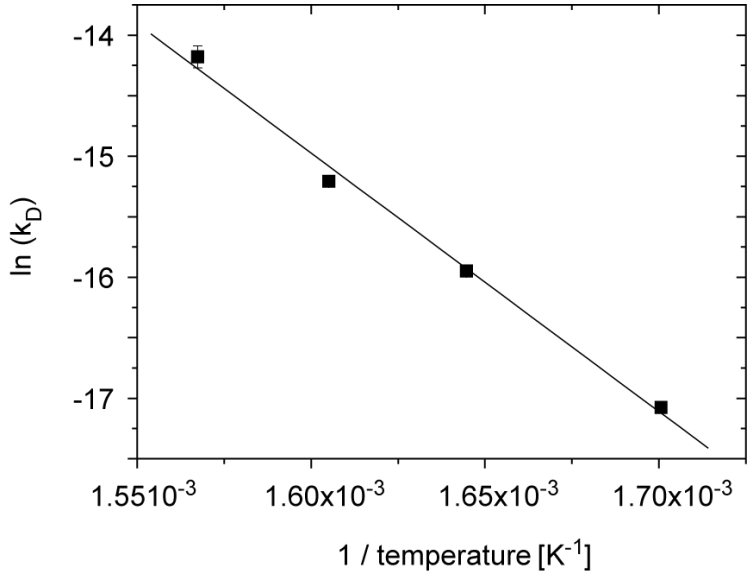
$$\ln \frac{[Be]}{[Be]_0} = -k_D(T) \cdot t$$

Activation energy:

$$\ln k_D(T) = -\frac{E_{act}}{k_B \cdot T} + \ln k_0$$

~1.9 nm Be on PG:





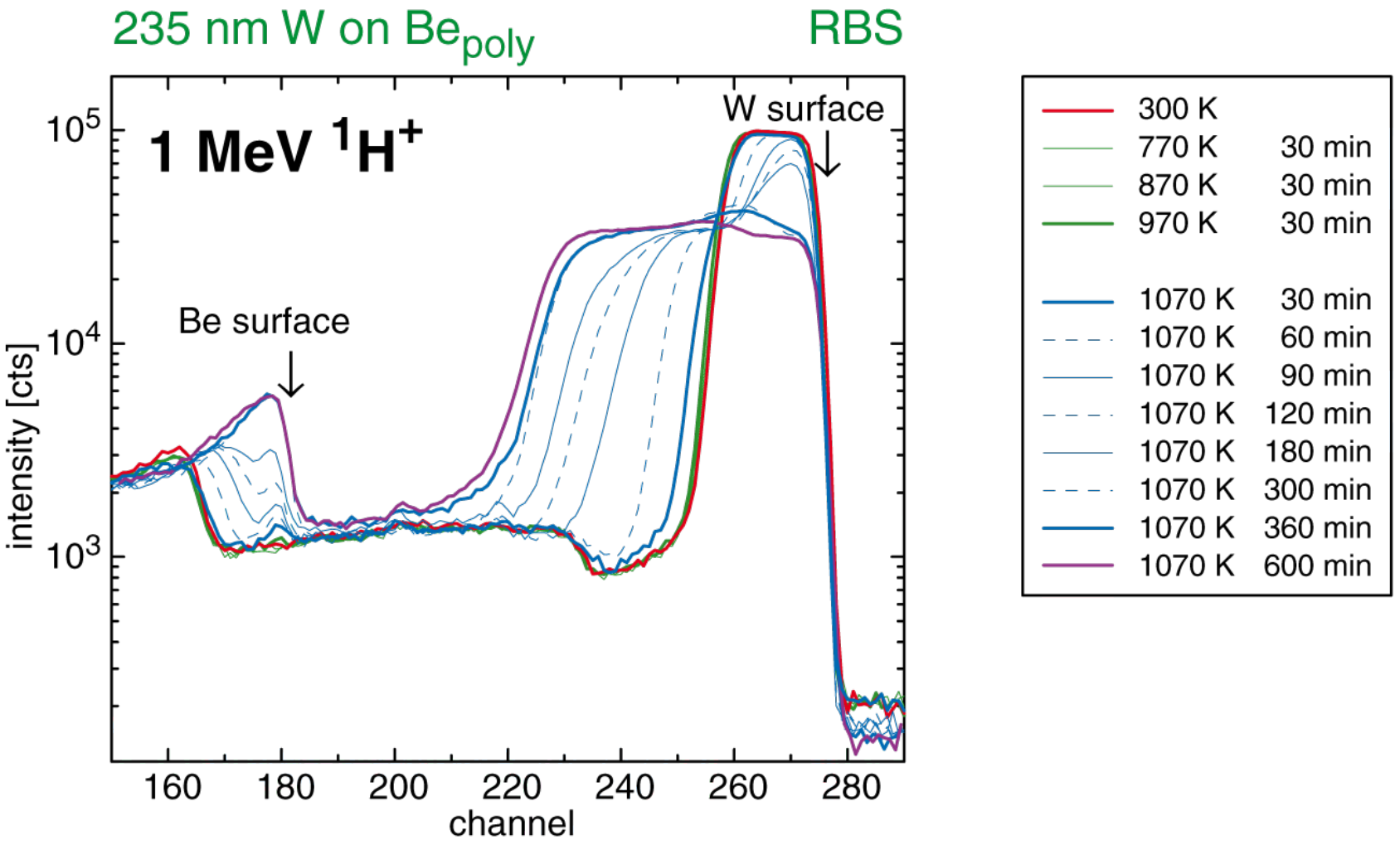
- Activation energy for pyrolytic graphite: 1.8 ± 0.1 eV

Summary: C—Be binary systems

- Be_2C at interface at 300 K deposition
- Be/graphite: Initially, island growth mode for Be on PG, above 0.6 nm layer growth
- <0.7 nm: carbide formation >570 K (surface diffusion)
- additional Be_2C: C/Be: >570 K
  Be/PG: >720 K HOPG: >870 K
- loss of Be (Be_2C decomp.): both: >1330 K
- Activation energy for Be_2C formation due to diffusion: PG: 1.8 eV HOPG: 2.1 eV (structural change?)

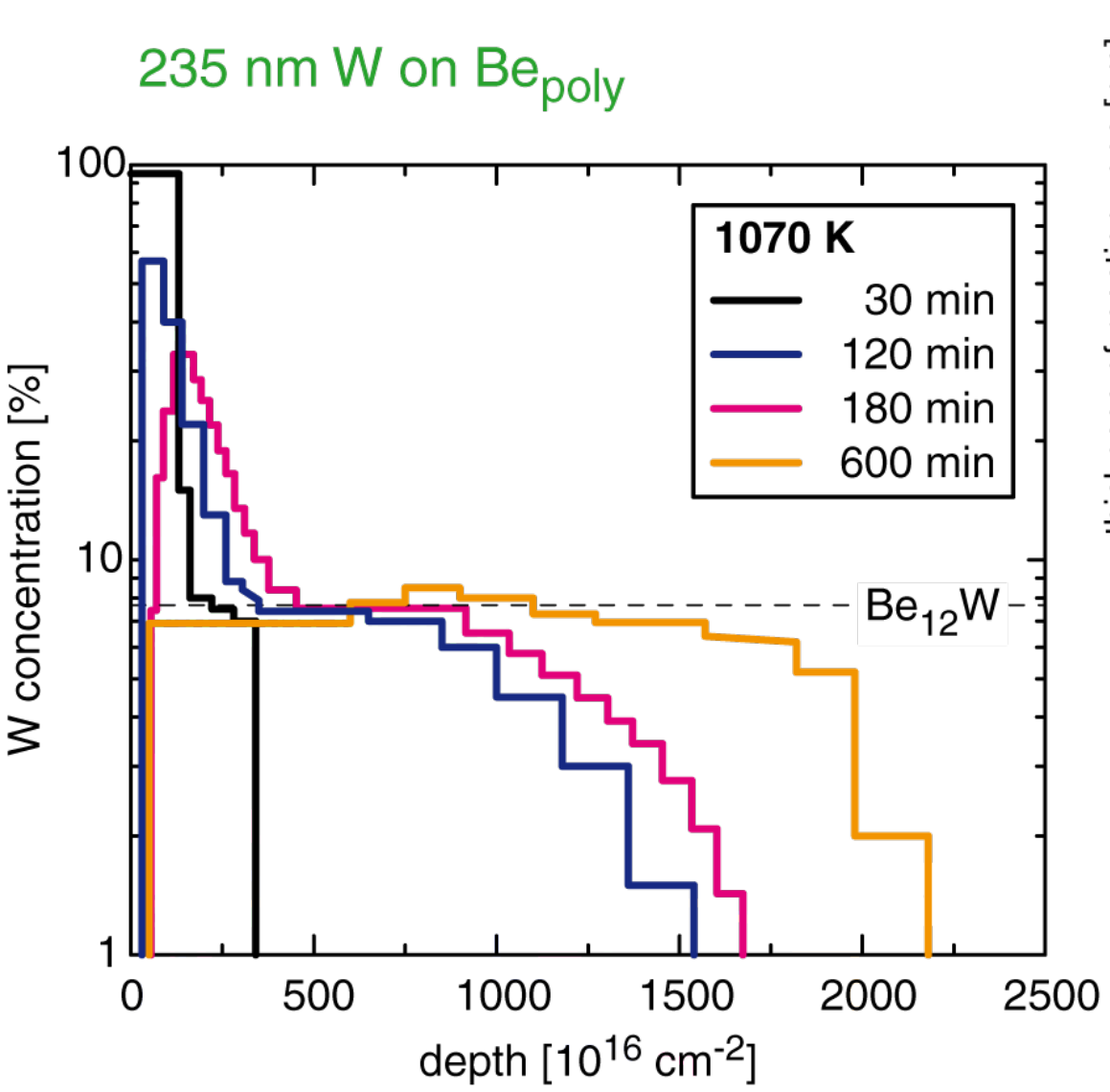
Be—W
alloy formation

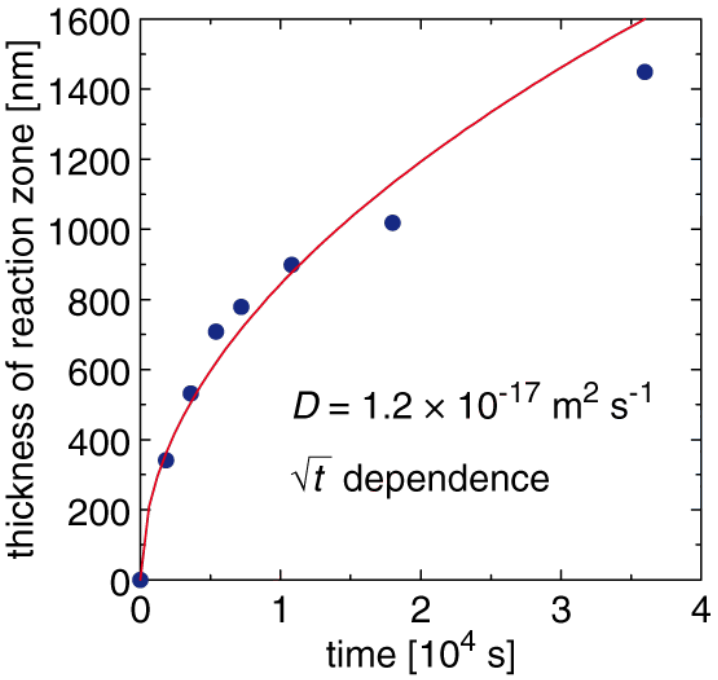
W / Be: ion beam analysis



- no visible reaction up to 970 K
- alloy formation starts at 1070 K
- 600 min at 1070 K: constant Be/W phase

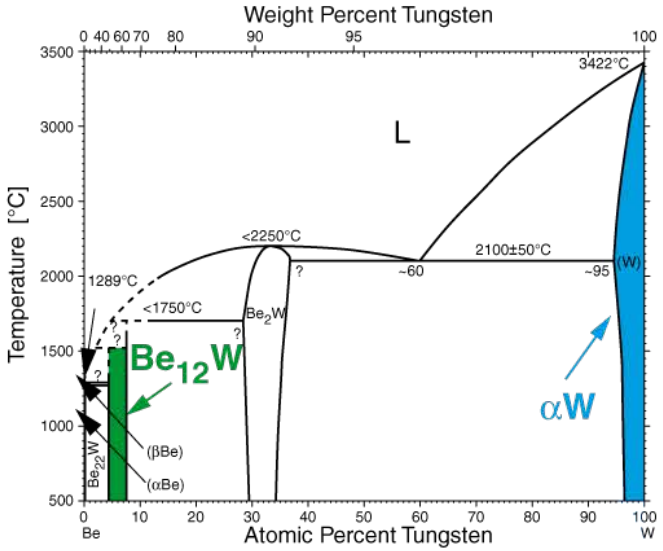
W / Be: depth profile, kinetics



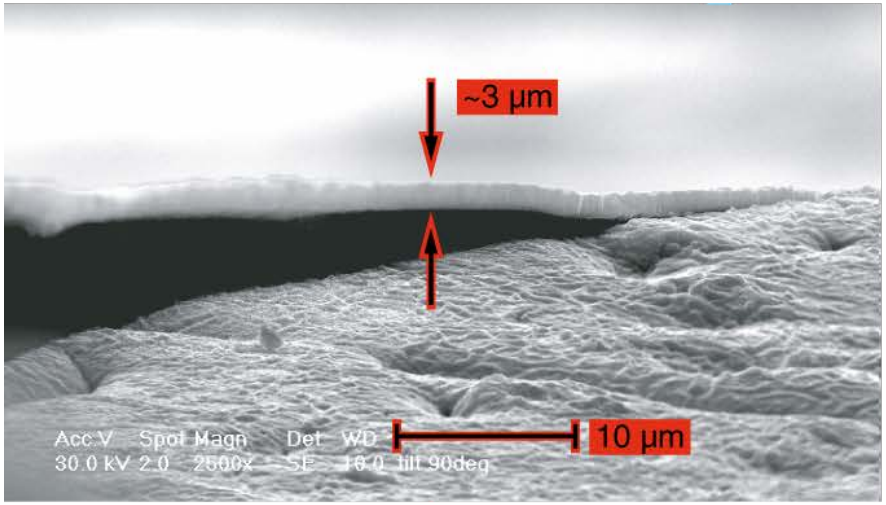


- Be$_{12}$W final phase with T_m = <2020 K
- Be diffusion through W and Be-W alloy
- interaction is diffusion-controlled

W / Be: $Be_{12}W$ phase

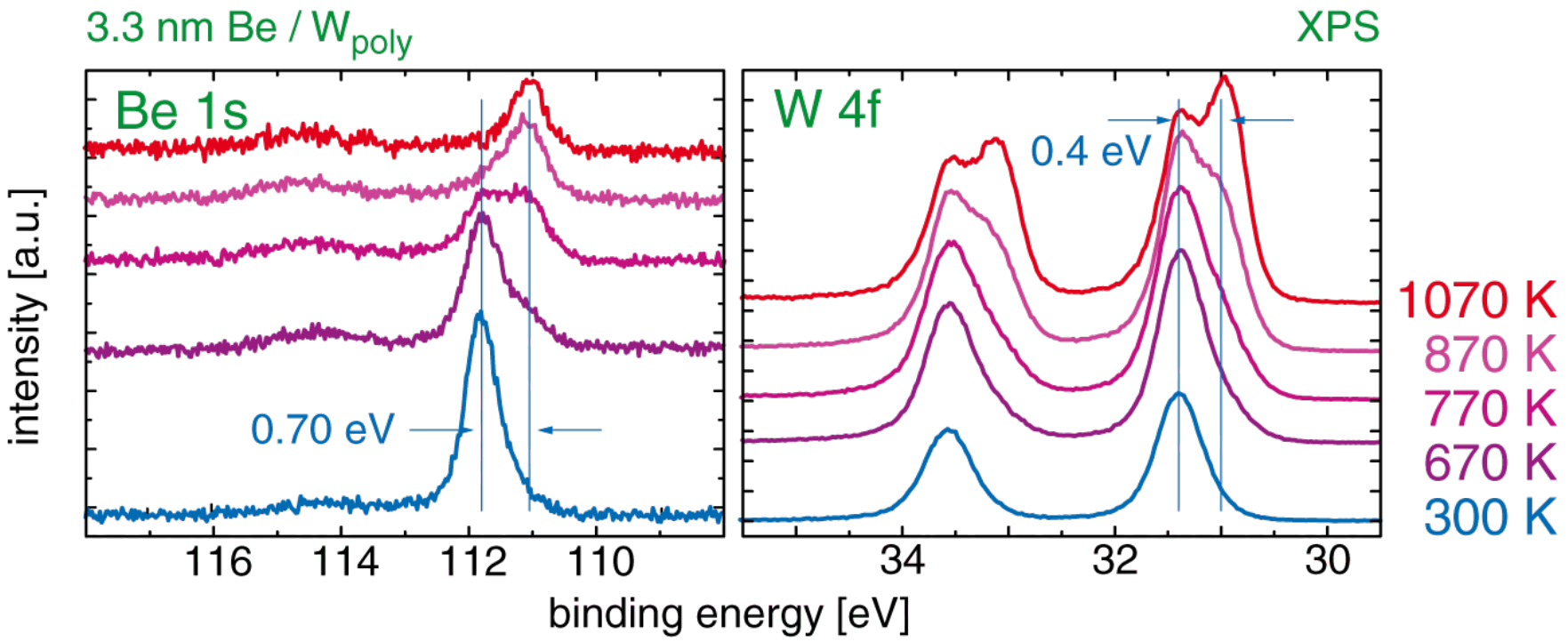


- formation of stable $Be_{12}W$ alloy phase above 1000 K
- W layer not dissolved in Be bulk
- $Be_{12}W$ melting point <2000 K



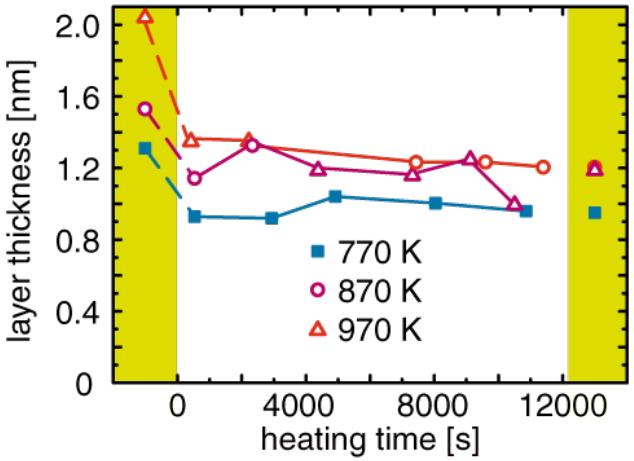
- at 1170 K a ~3 µm $Be_{12}W$ layer detaches from bulk Be
- risk of large impurity influx!

Be / W: Be_2W phase formation

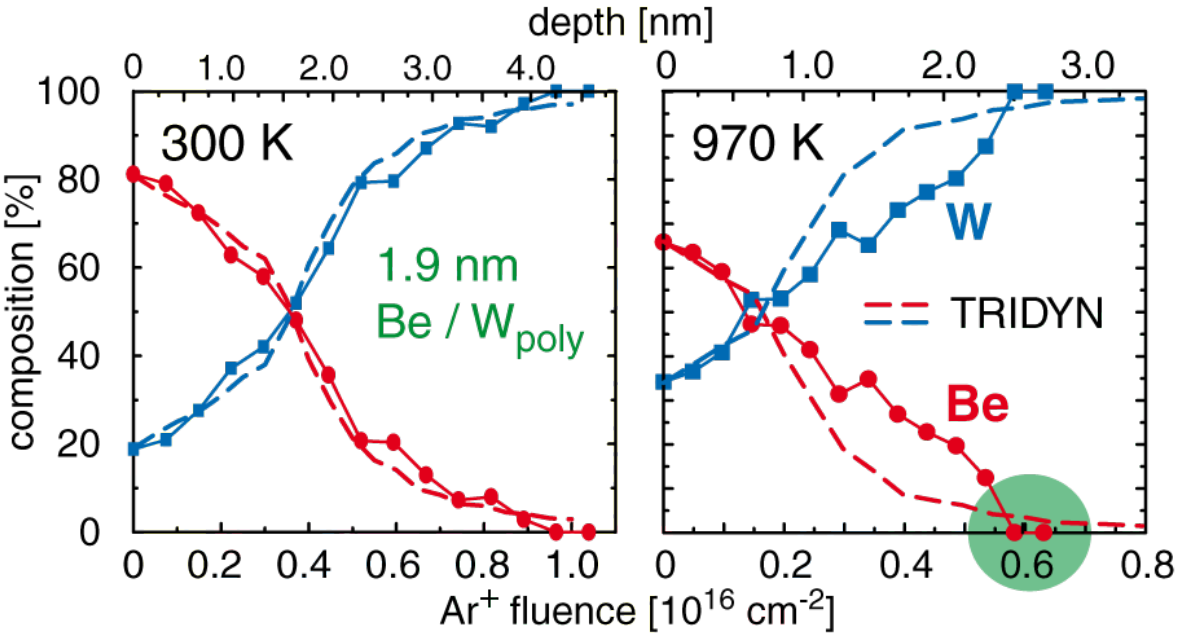


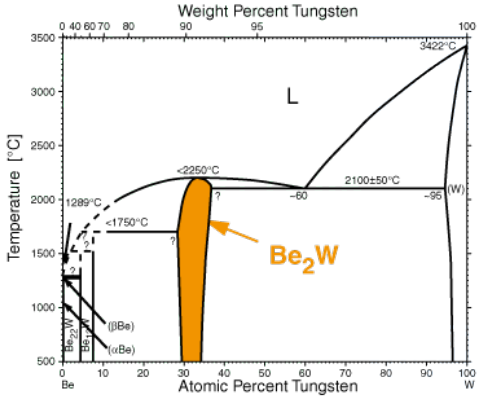
- above 770 K: alloy dominates
- alloy peaks in core levels (Be 1s, W 4f) and valence band
- above 970 K: Be_2W stoichiometry
- Be intensity loss > 570 K

Be / W: Be loss



- alloy limited to 1-2 nm (independent of initial Be thickness)
- excess Be: NO dissolution in bulk, evaporation
- sublimation faster than diffusion

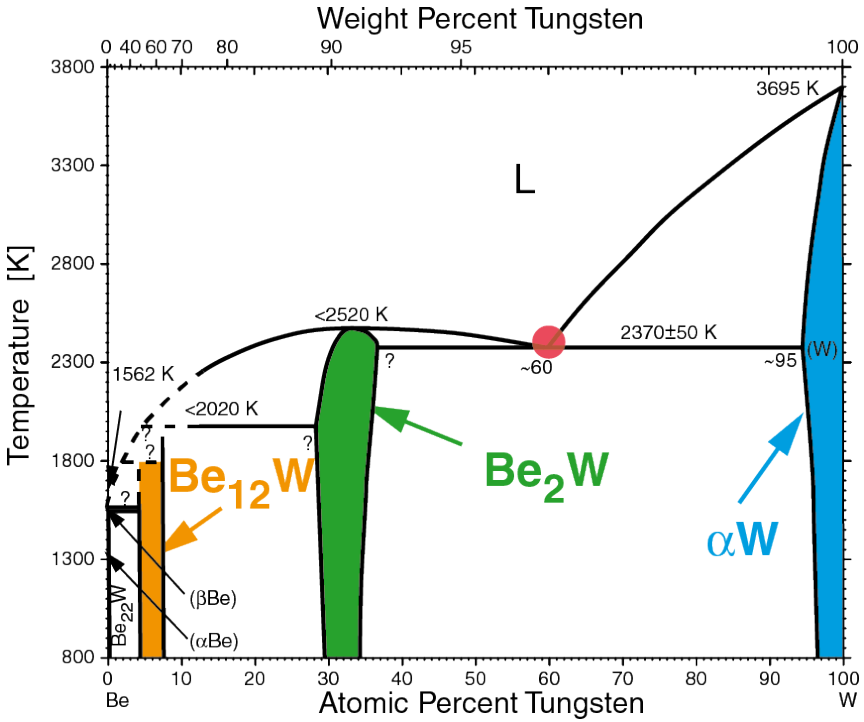




Summary: Be—W alloy formation

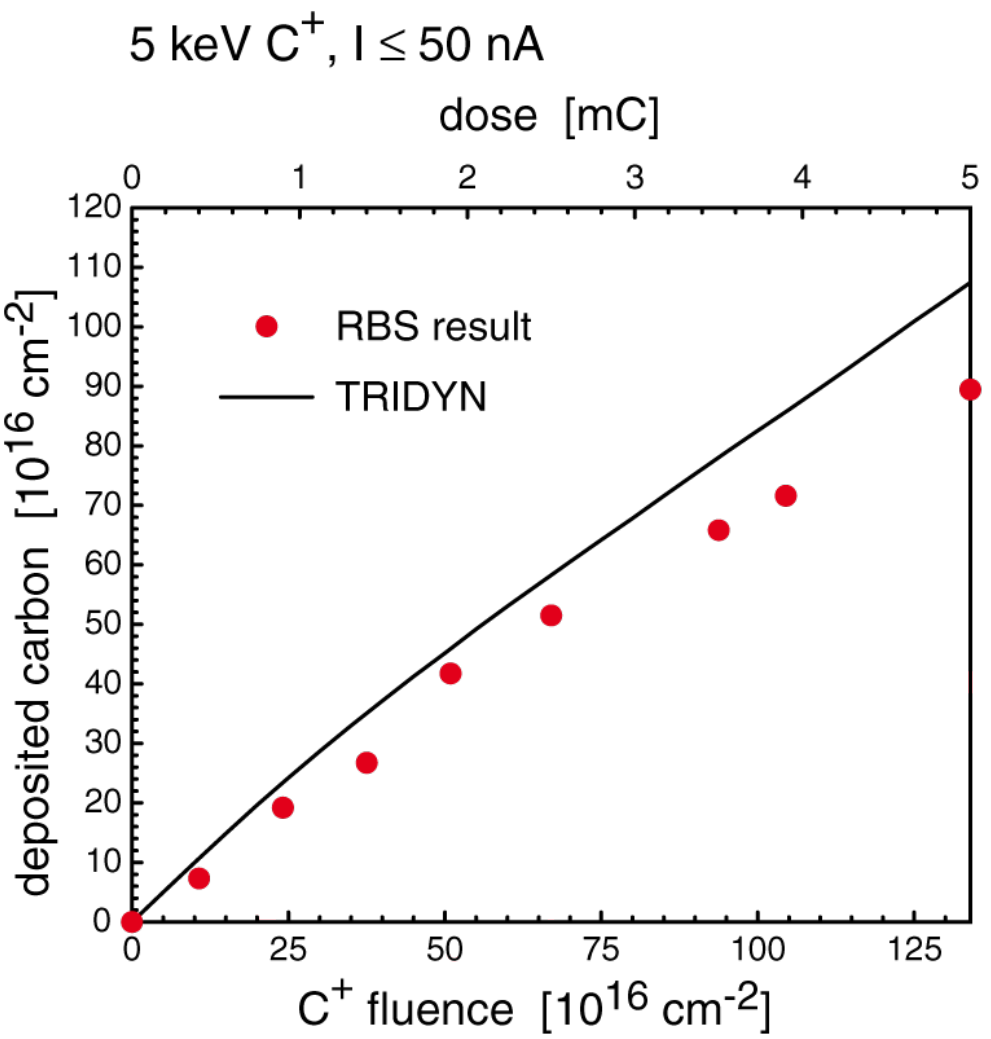
Alloy formation depends on:

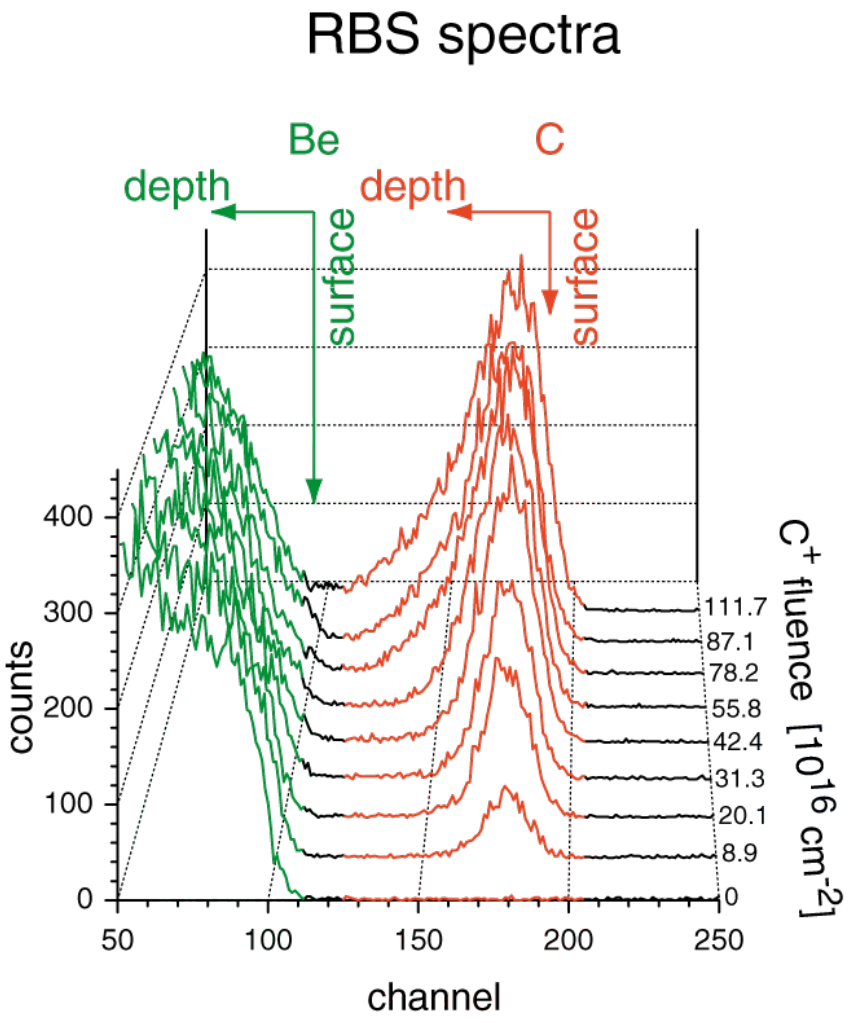
- Temperature
- Deposited amounts and sequence
- Flux balance: deposition, sublimation, erosion fluxes



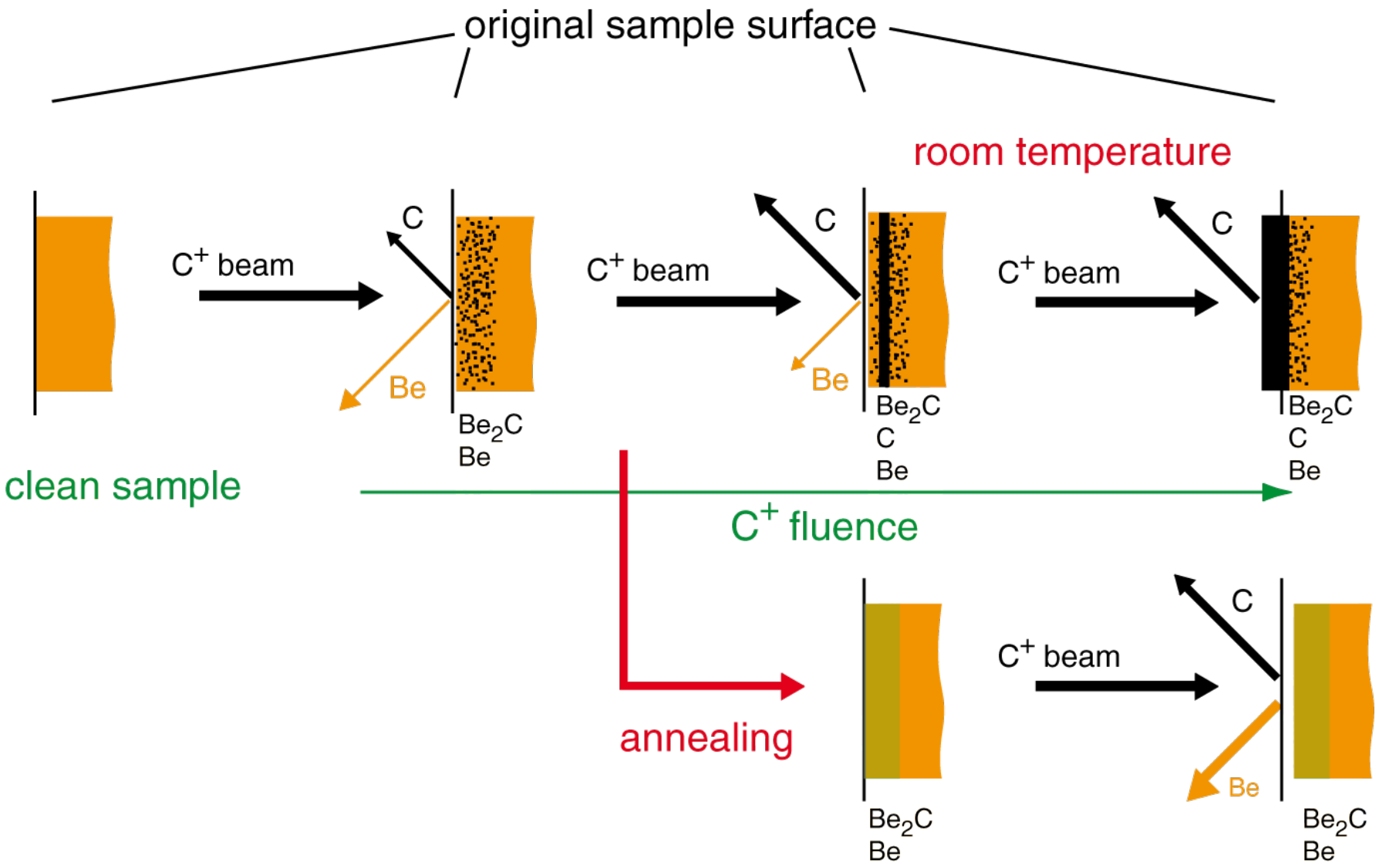
$C^+ \rightarrow Be$, $CO^+ \rightarrow Be$ ion-induced processes

$C^+ \rightarrow$ Be: layer formation

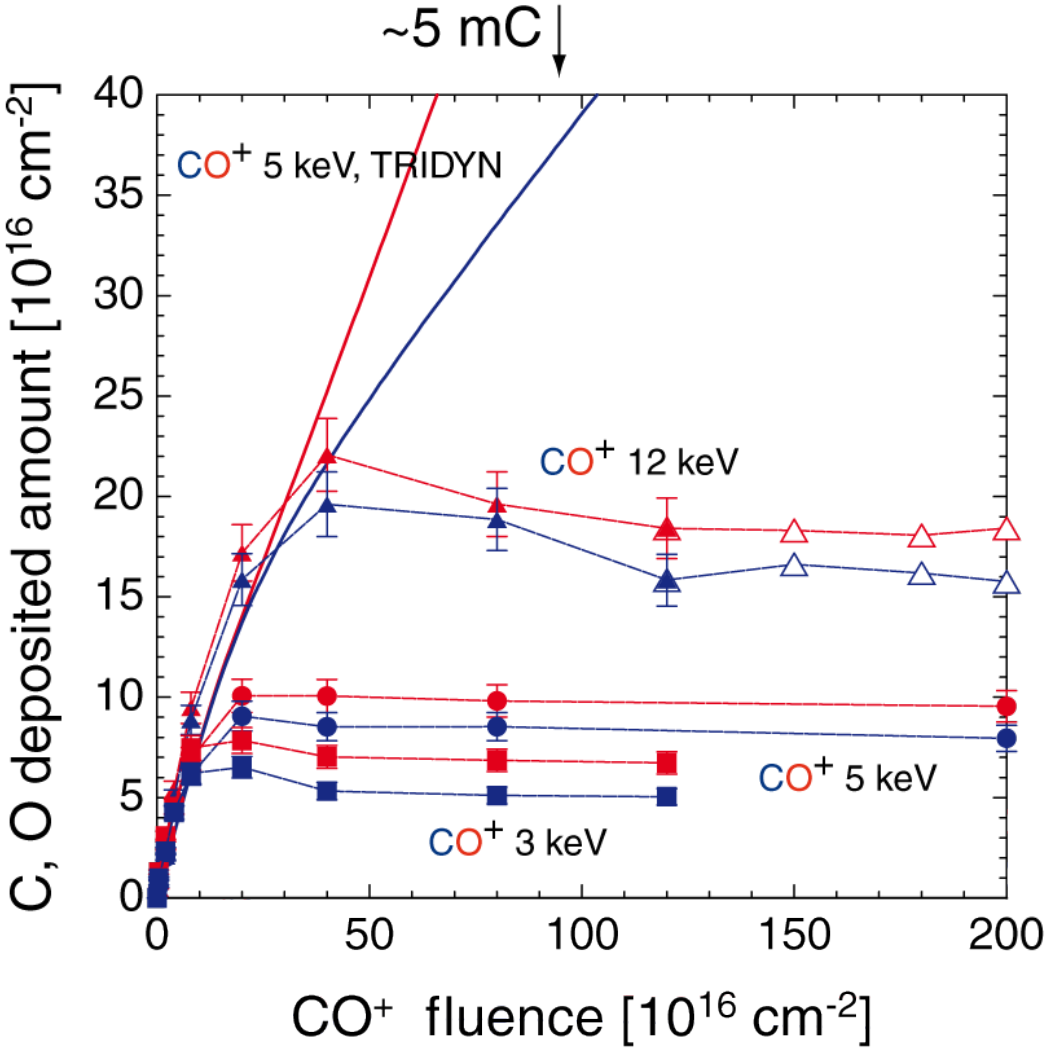


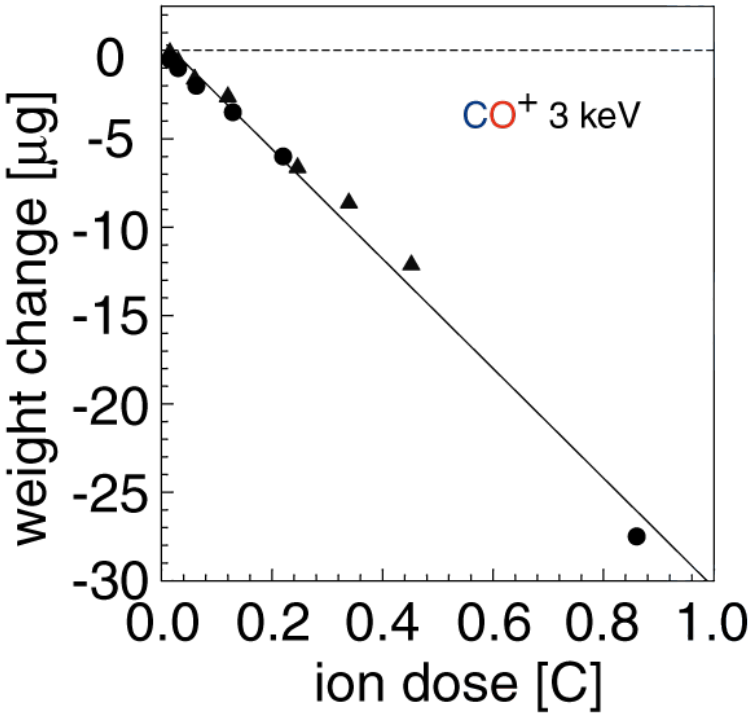


$C^+ \rightarrow$ Be: model



$CO^+ \rightarrow$ Be: deposition / erosion

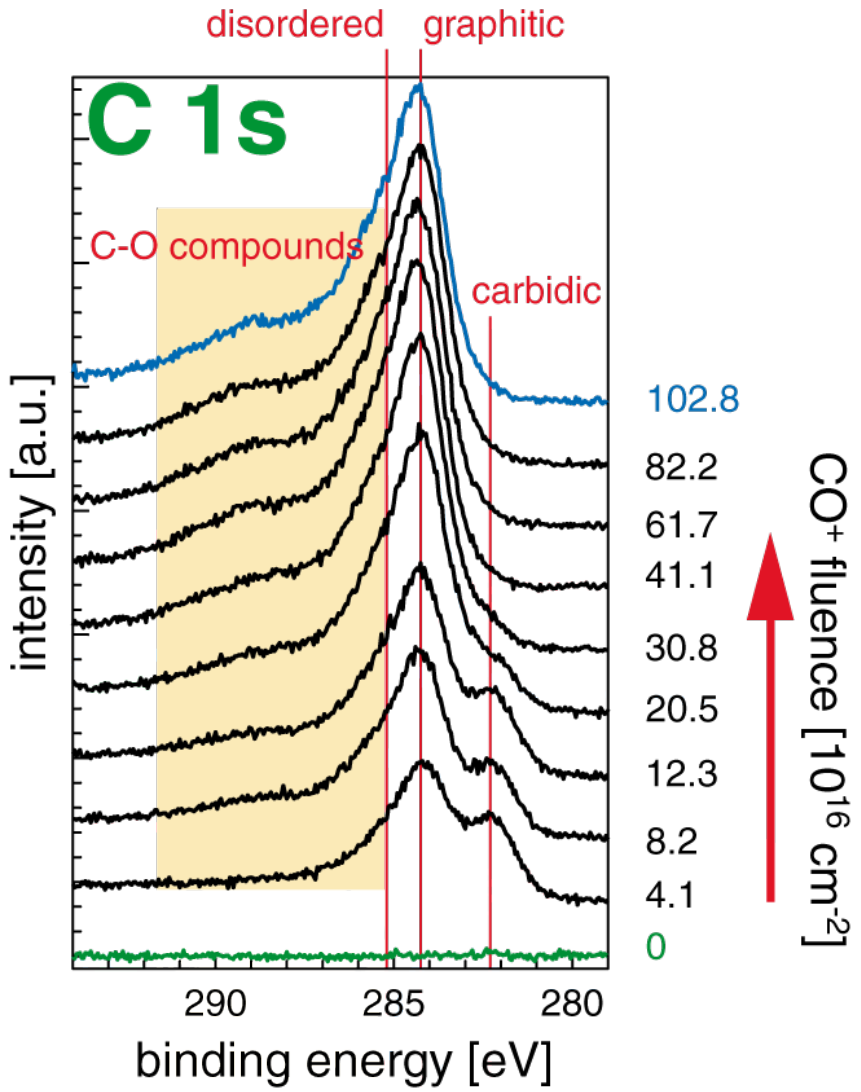


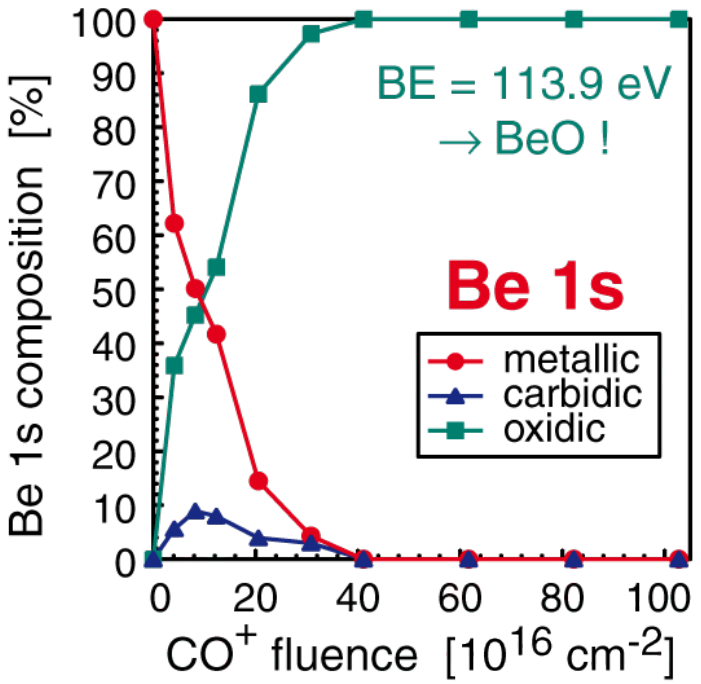


$Y_{Be} = 0.33$

continuous erosion

$CO^+ \rightarrow$ Be: chemical species

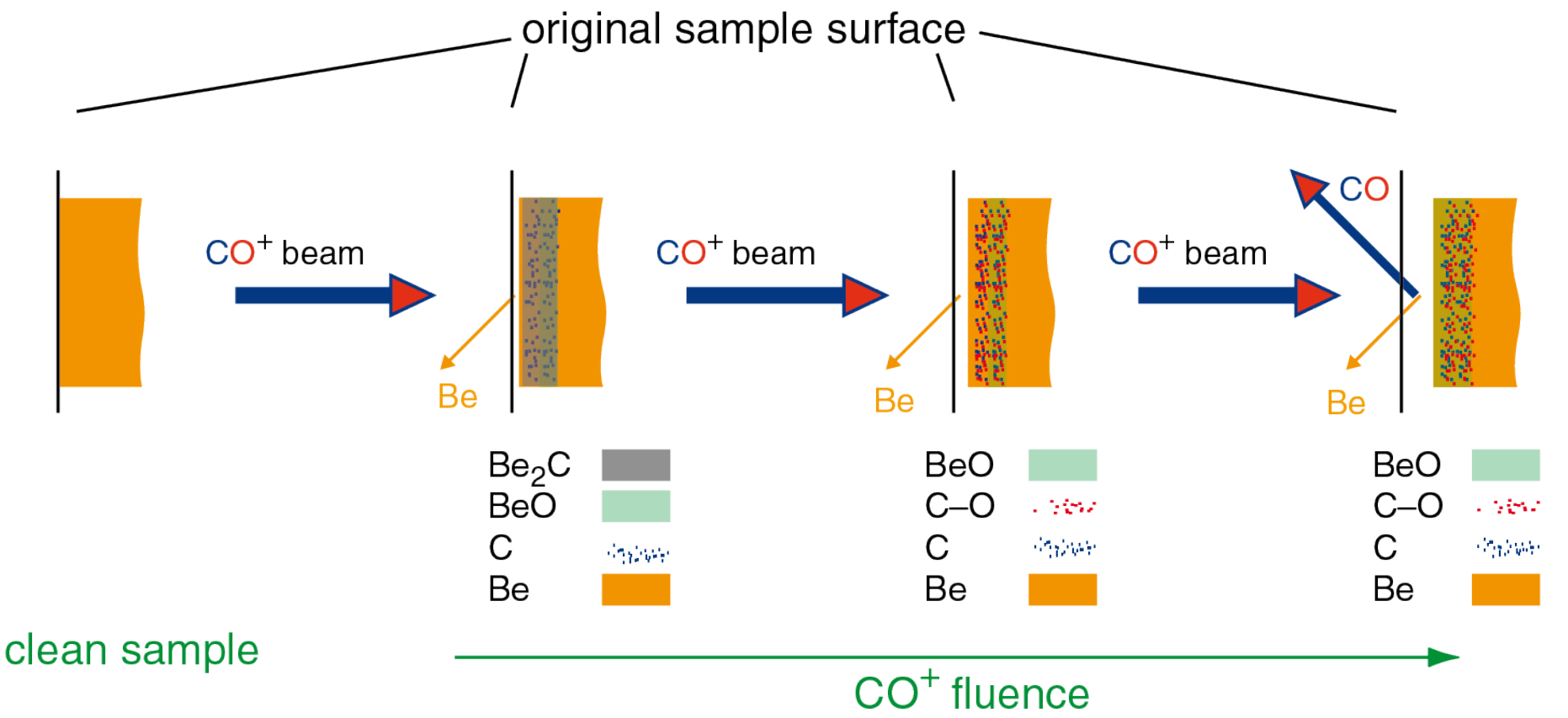




$\Delta G_f^0(Be_2C) = -115$ kJ/mol

$\Delta G_f^0(BeO) = -579$ kJ/mol

$CO^+ \rightarrow$ Be: model



	Be	C	O
$Y_{exp.}$	0.33	1.00	1.00
Y_{TRIDYN}	0.36	0.24	0.29

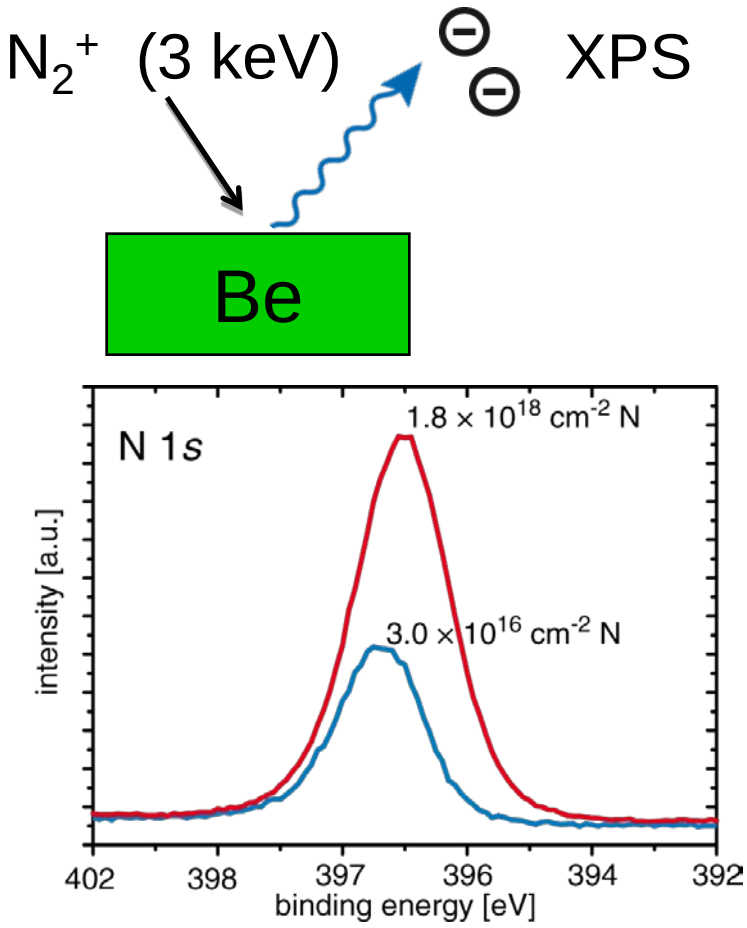
Summary: C ion implantation in Be

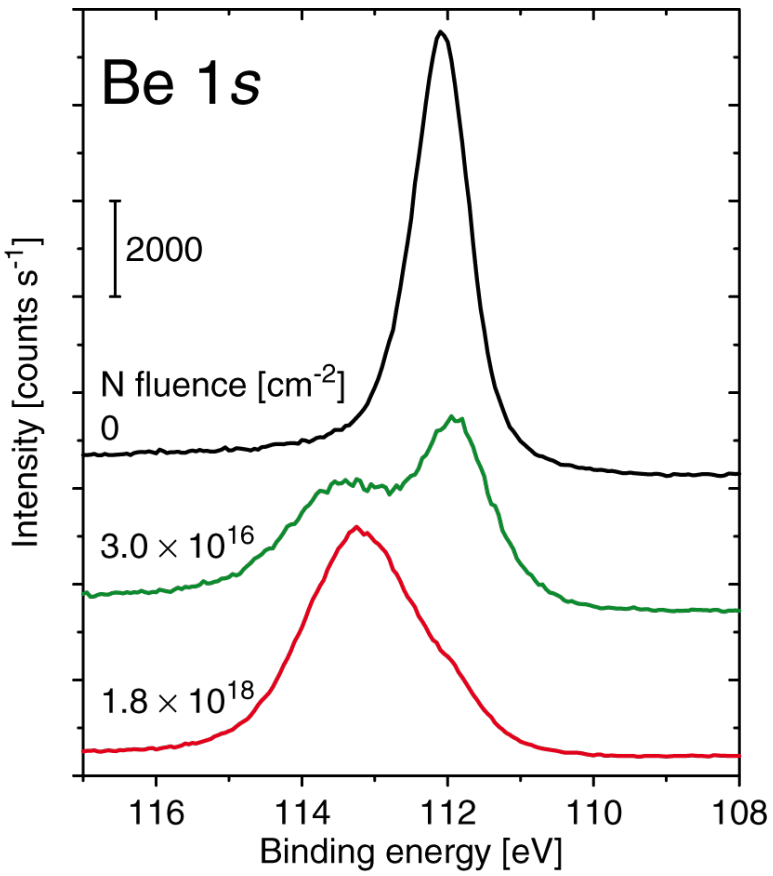
Ternary system opens new reaction pathways

- Binary system: purely kinematic process at 300 K
- Ternary system: chemical reaction path dominates
- Ion energy triggers compounds formation at 300 K
- Deposition-dominated situation can turn into erosion-dominated process

$N^+ \rightarrow Be$

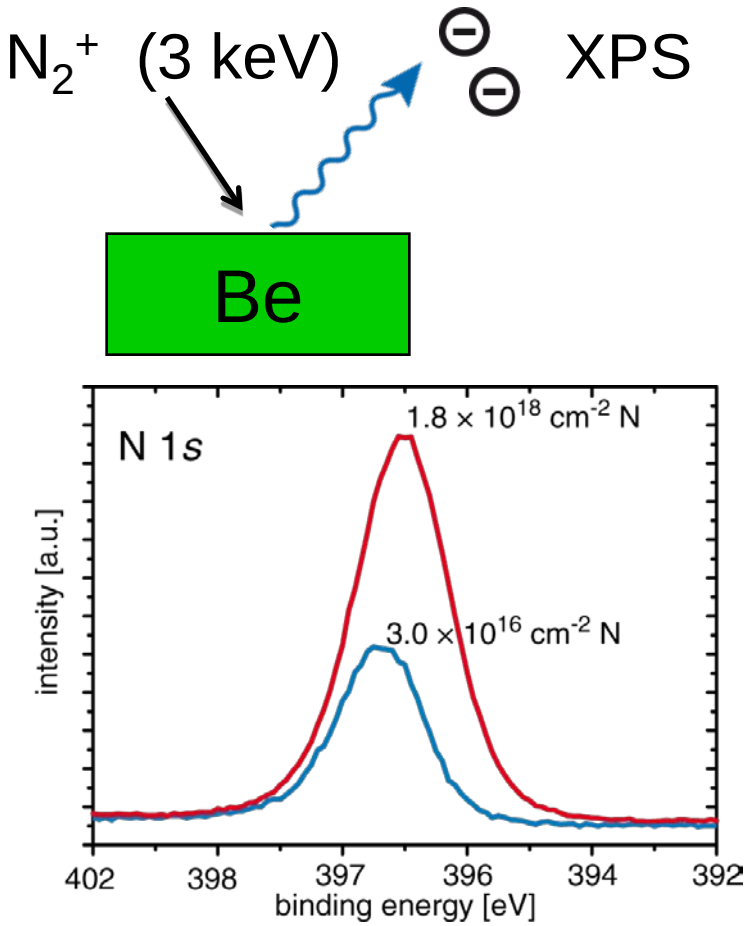
Be—N phase formation

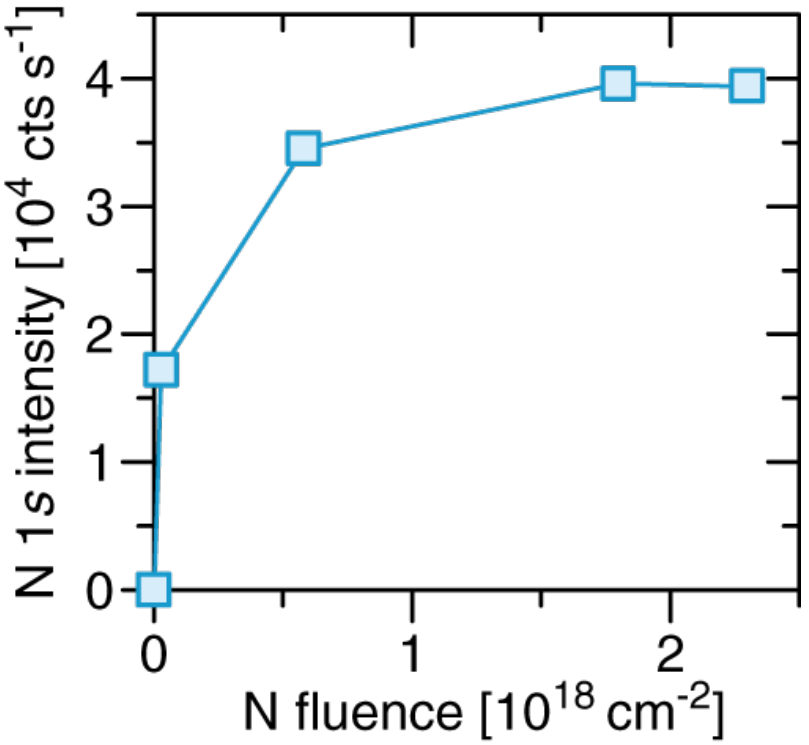




- nitride formation during N ion implantation
- shift of both Be 1*s* and N 1*s* peaks

Be—N phase formation and saturation

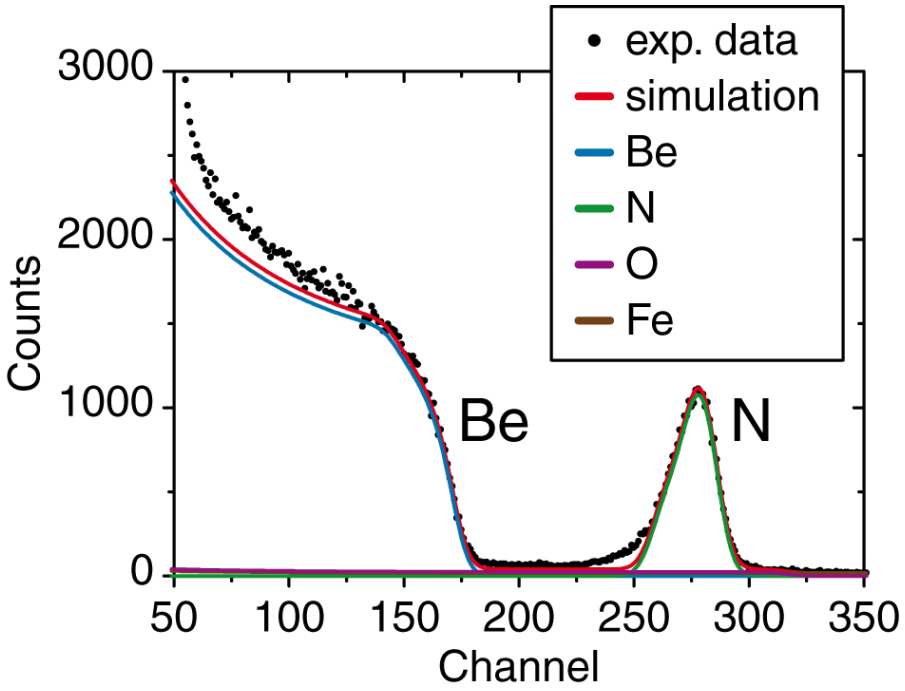


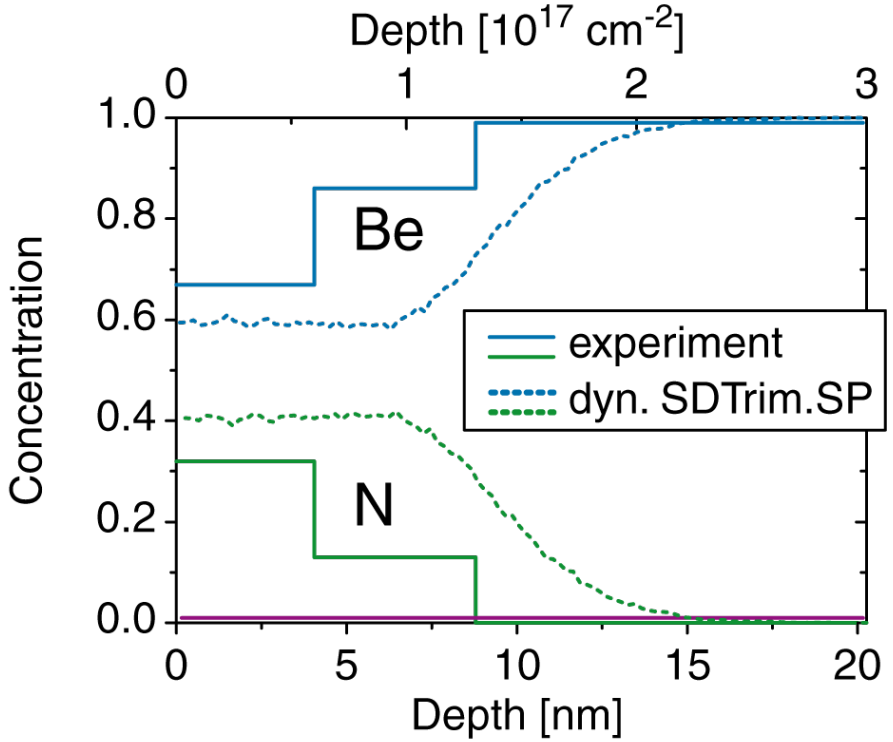


- nitride formation during N ion implantation
- shift of both Be 1*s* and N 1*s* peaks
- N saturates within implantation range (XPS and RBS)

N depth distribution

RBS 800 keV ^{4}He, θ=105°

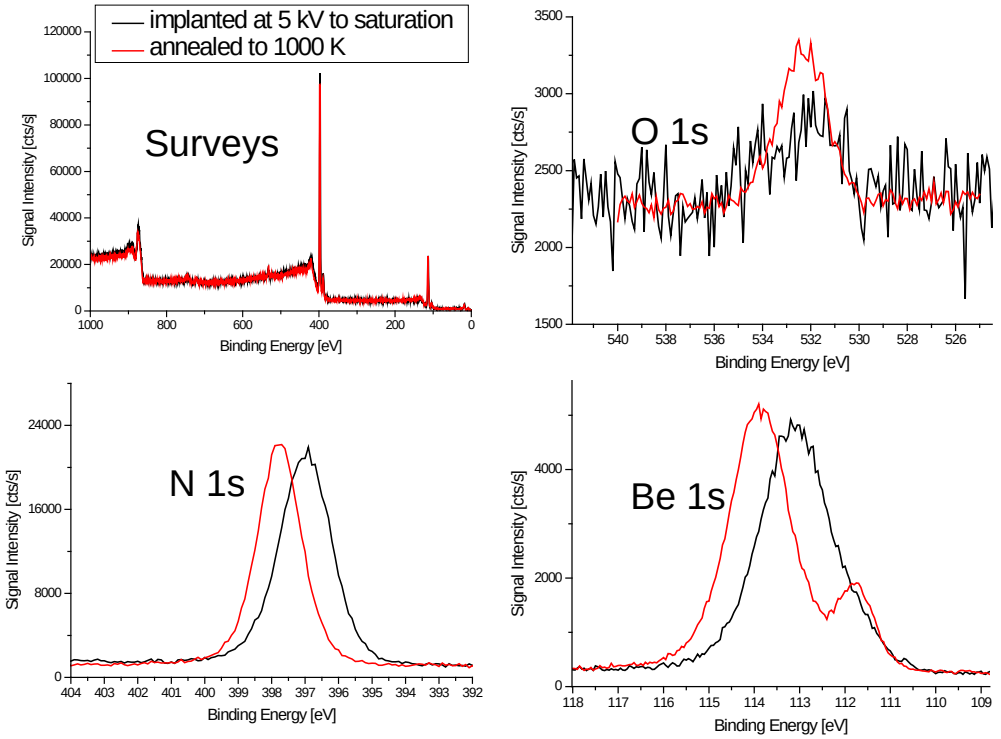




- N_2^+ assumed for simulation → reasonable agreement
- Be_3N_2 layer: 9 nm (> 1% N), density 3x10^{22} cm^{-3} from literature
- implantation range ∝ energy → JET (300 eV ions) < 1 nm nitride
  → no degradation in electrical conductivity (cmp. to BeO)

Thermal stability of Be—N phases

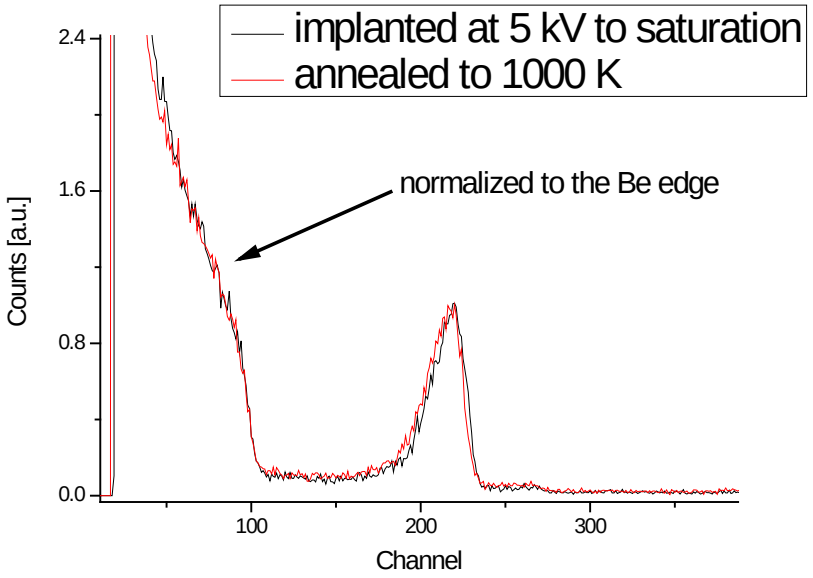
XPS



- annealing to 1000 K causes chemical shifts
- no significant reduction in the N content

  Literature: Be_3N_2 very stable, solid β phase >1700 K, melting point 2500 K

RBS



- N amount and depth profile after implantation and after annealing to 1000 K identical
- no decomposition of nitride
- no diffusion into the bulk

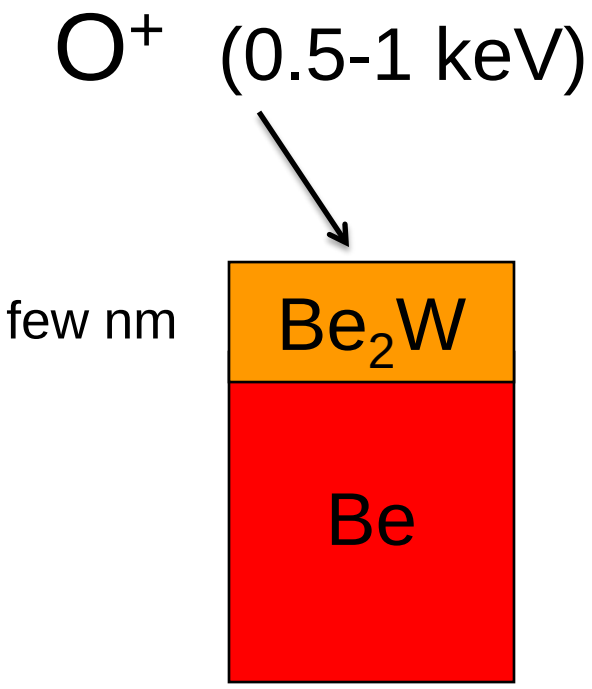
Summary: N ion implantation in Be

Consequences of N_2 seeding in ITER

- Nitride formation within ion range
- No chemical erosion
- No volatile species, sudden gas release
- No increased hydrogen retention

$O^+ \rightarrow Be_2W/W$ chemically resolved depth profiling

O^+ implantation into Be_2W

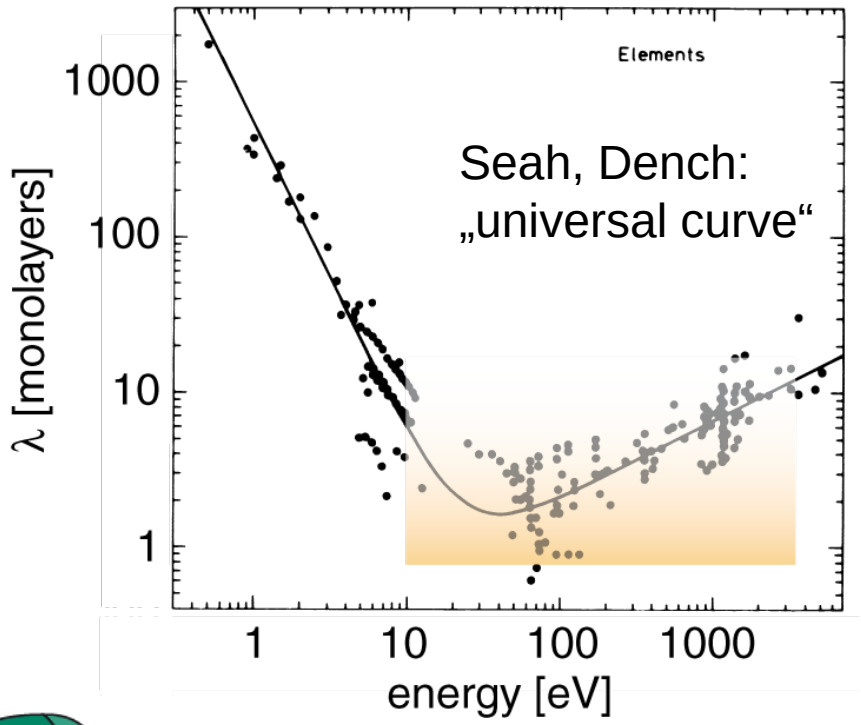


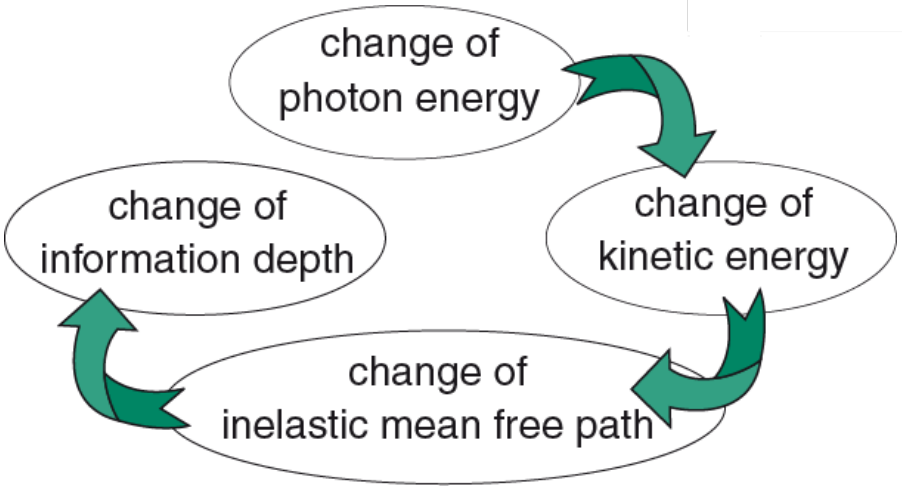
1. Be_2W preparation (W deposition on Be, 900 K annealing)
2. Implantation of O ions at 1 kV
3. Annealing at 600 K
4. O ion implantation at 500 V

XPS analysis at BESSY II (6 depths, Be 1*s*, W 4*f*, O 1*s*, Au 4*f*)

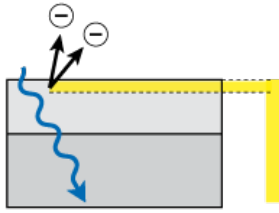
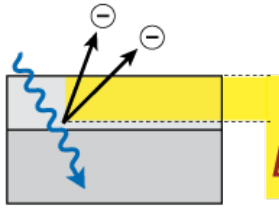
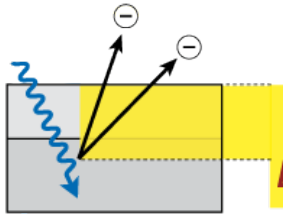
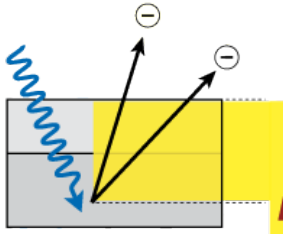
Depth-resolved XPS chemical analysis

$$E_{kin} = h\nu - E_B + \phi$$

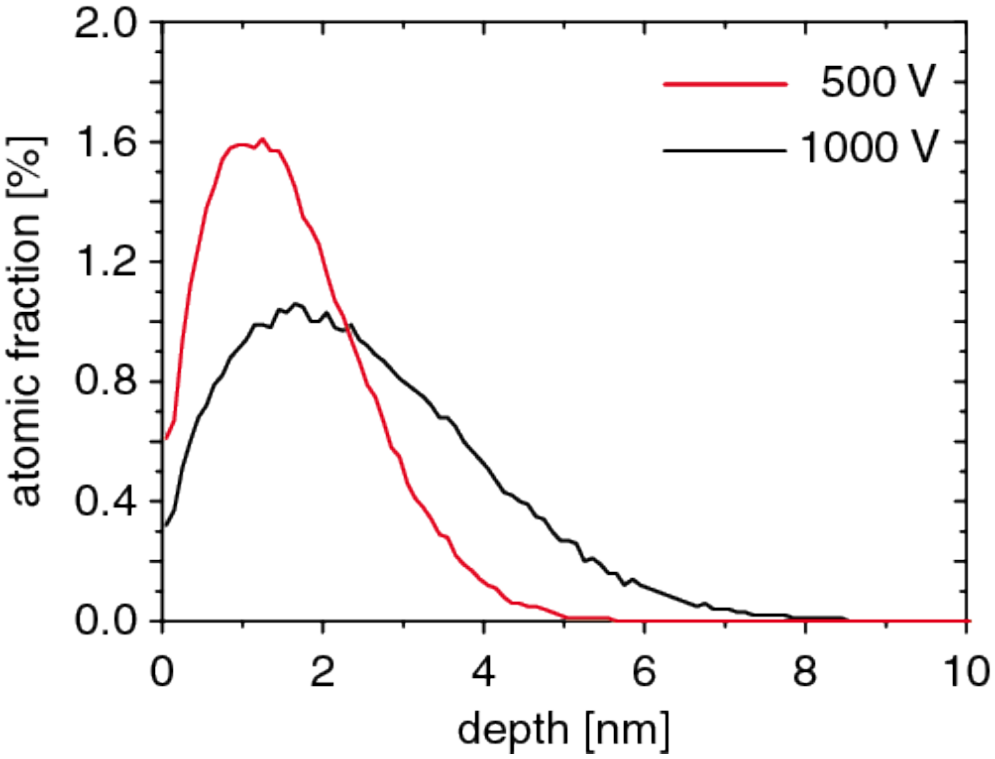




Depth-resolved XPS

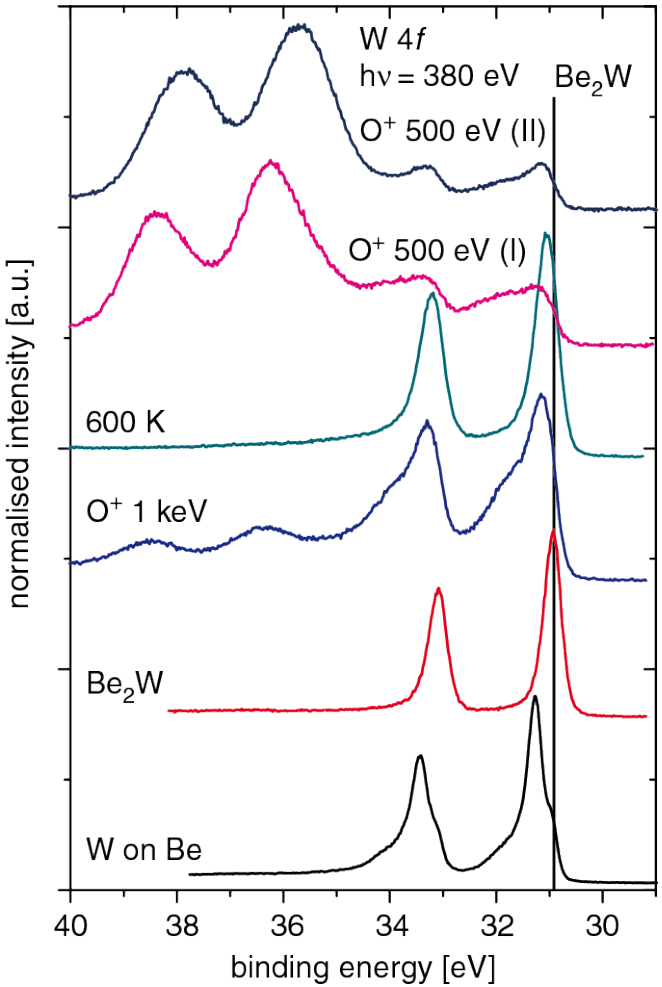
excitation energy				kinetic energy	mean free path
W 4*f*	Be 1*s*	C 1*s*		depth *d1* E_{kin} = 60 eV	$\lambda \approx 0.31$ nm
$h\nu$ = 90 eV	$h\nu$ = 170 eV	$h\nu$ = 340 eV			
$h\nu$ = 330 eV	$h\nu$ = 410 eV	$h\nu$ = 580 eV		depth *d2* E_{kin} = 300 eV	$\lambda \approx 0.64$ nm
$h\nu$ = 510 eV	$h\nu$ = 590 eV	$h\nu$ = 760 eV		depth *d3* E_{kin} = 480 eV	$\lambda \approx 0.80$ nm
$h\nu$ = 730 eV	$h\nu$ = 810 eV	$h\nu$ = 980 eV		depth *d4* E_{kin} = 700 eV	$\lambda \approx 0.97$ nm

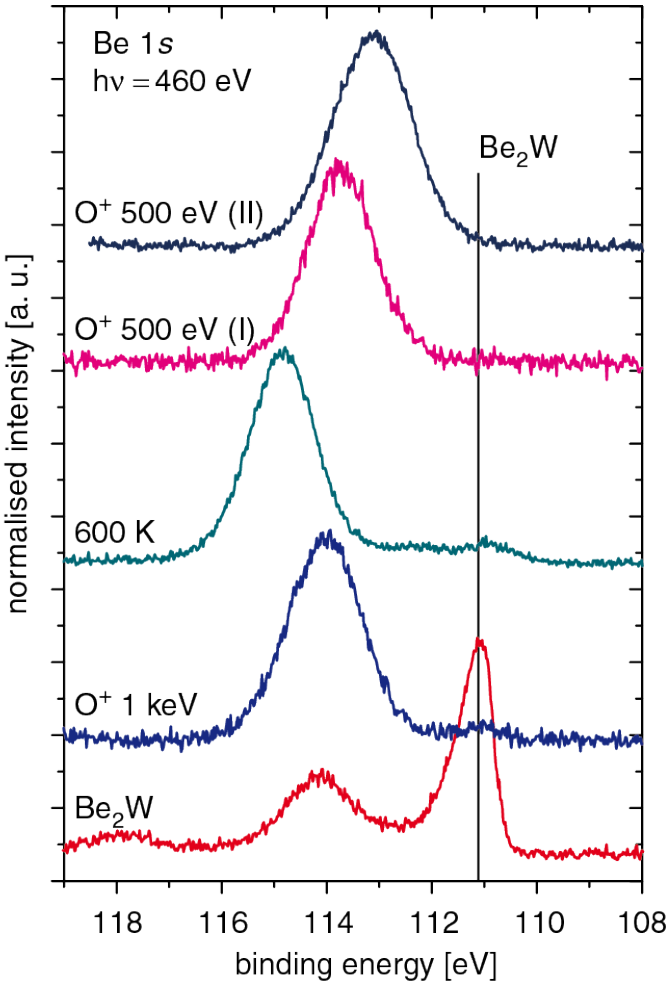
SDTrim.SP: O ion implantation profiles in Be_2W



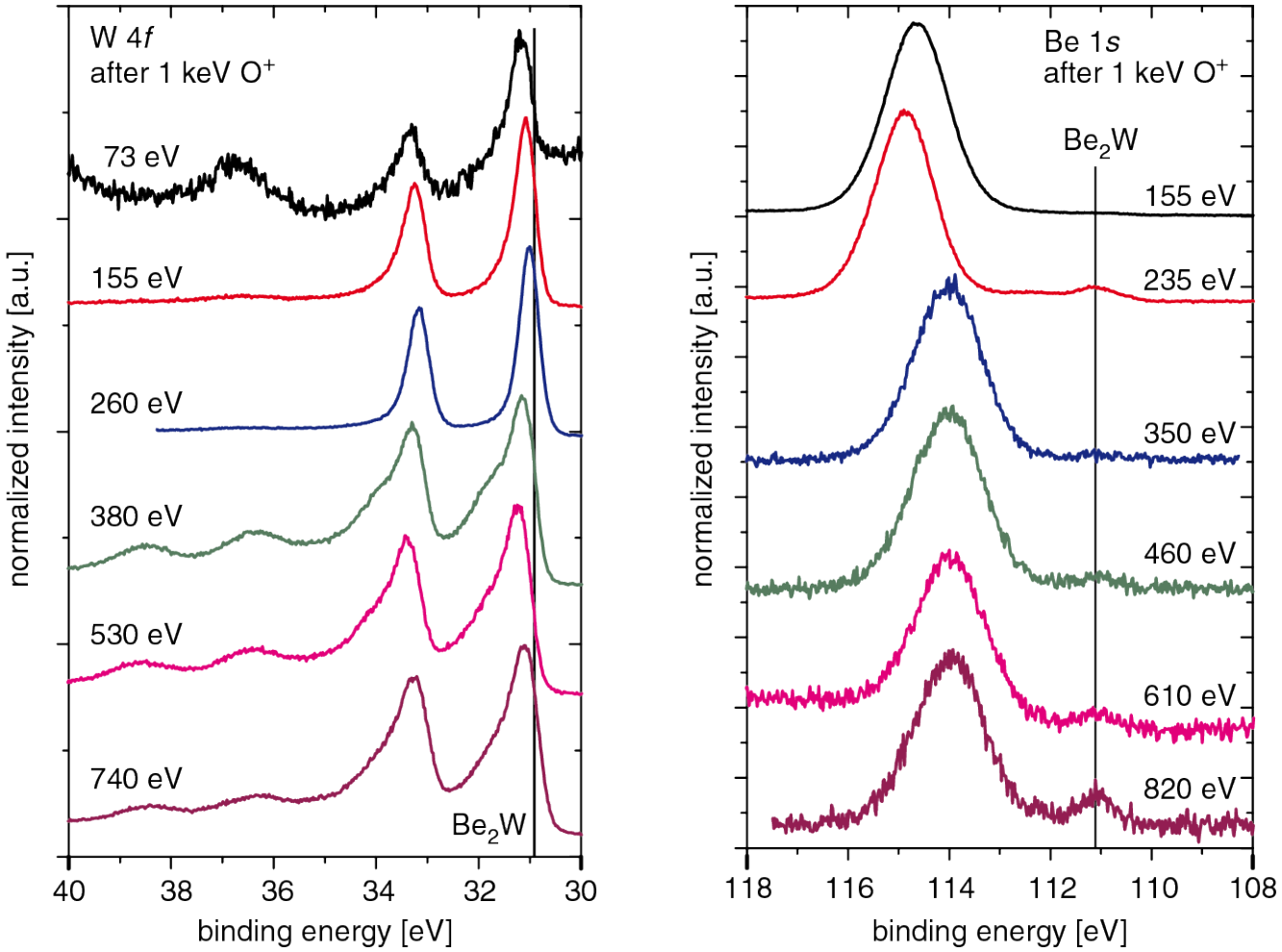
- Assumption: 82% O_2^+ and 18% O^+
- Fluence: 5 x 10^{14} cm^{-2}
- Implantation maxima around 1 and 2 nm

Overview: chemical changes during implantation / annealing

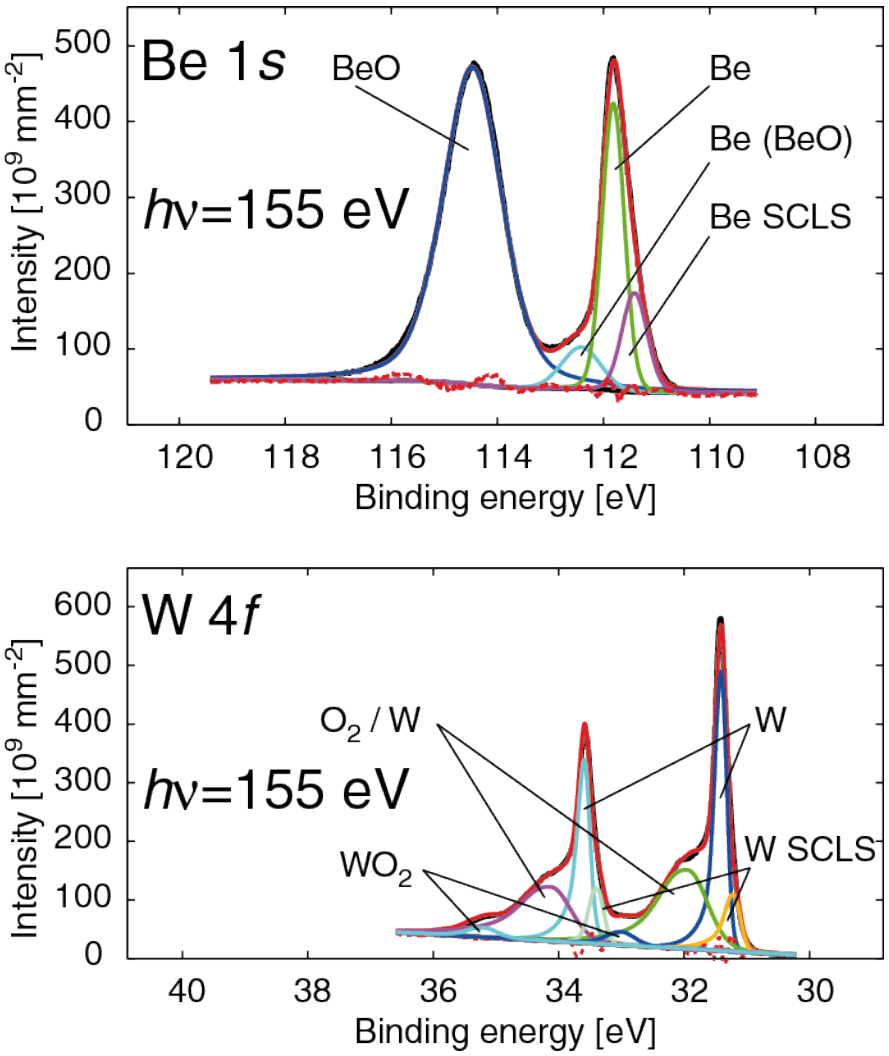




Depth-resolved chemical analysis



Chemical species: Peak fitting



Real situation: elements distributed over analysis depth

$$I_{x,hv}^{norm} = \sum_{i=1}^{n} \rho_{x,i} \lambda_{i,E_{kin}} \cos\alpha \left(1 - \exp\left[-\frac{d}{\lambda_{i,E_{kin}} \cos\alpha}\right]\right) \exp\left[\sum_{j=1}^{n-1} -\frac{d}{\lambda_{j,E_{kin}} \cos\alpha}\right]$$

$I_{x,hv}^{norm}$: norm. intensity

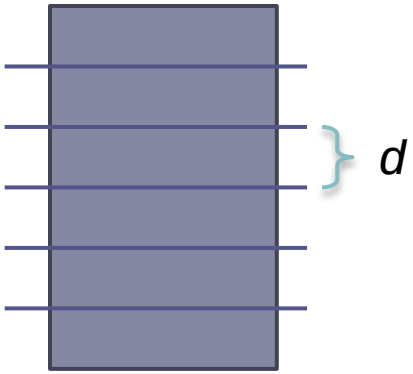
$\rho_{x,z}$: density

z: depth

$\lambda_{k,E_{kin}}$: IMFPs: Gries (1996): mixtures and compounds

α: exit angle

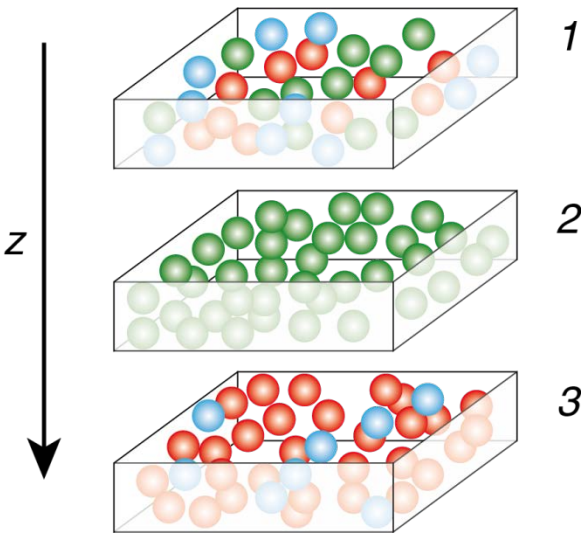
d: layer thickness



- Element distribution $\rho_{x,i}$ is the result we are looking for!
- But: $\rho_{x,i}$ necessary to calculate the IMFPs → nonlinear problem!

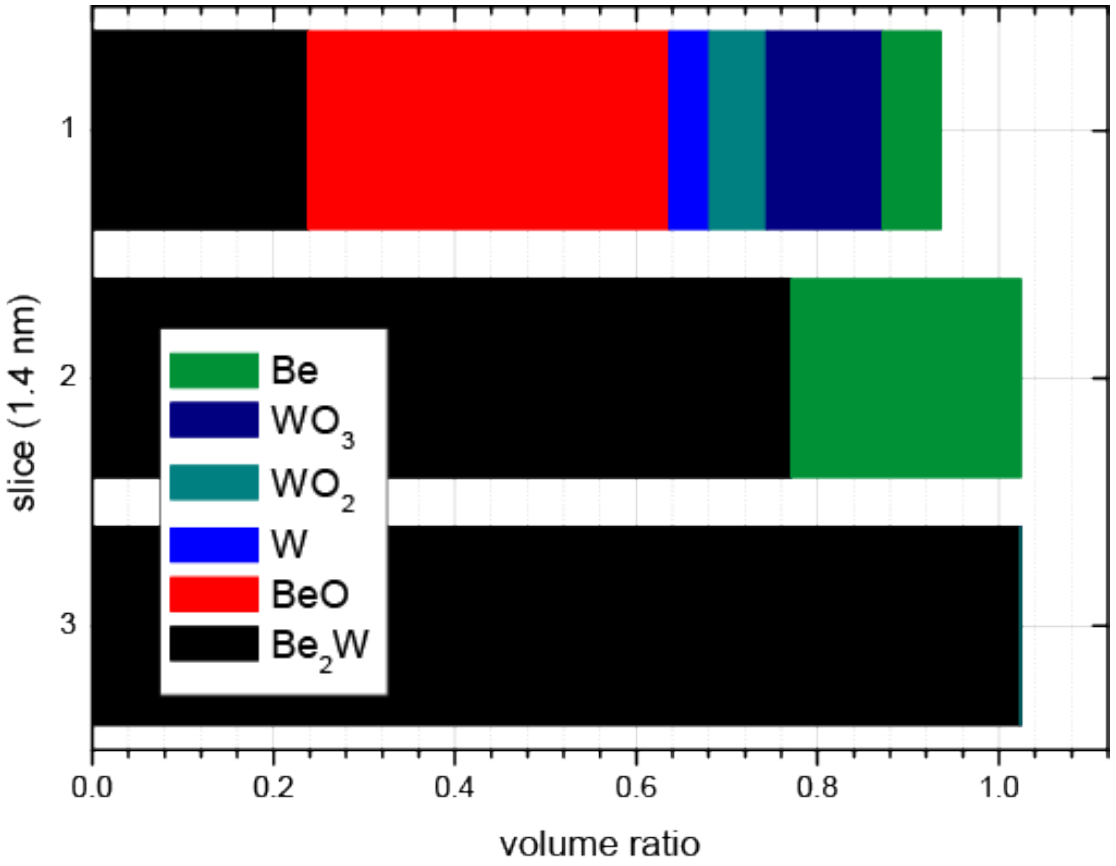
→ Set of equations can only be solved numerically
(Mathematica, interior point method)

Fit procedure



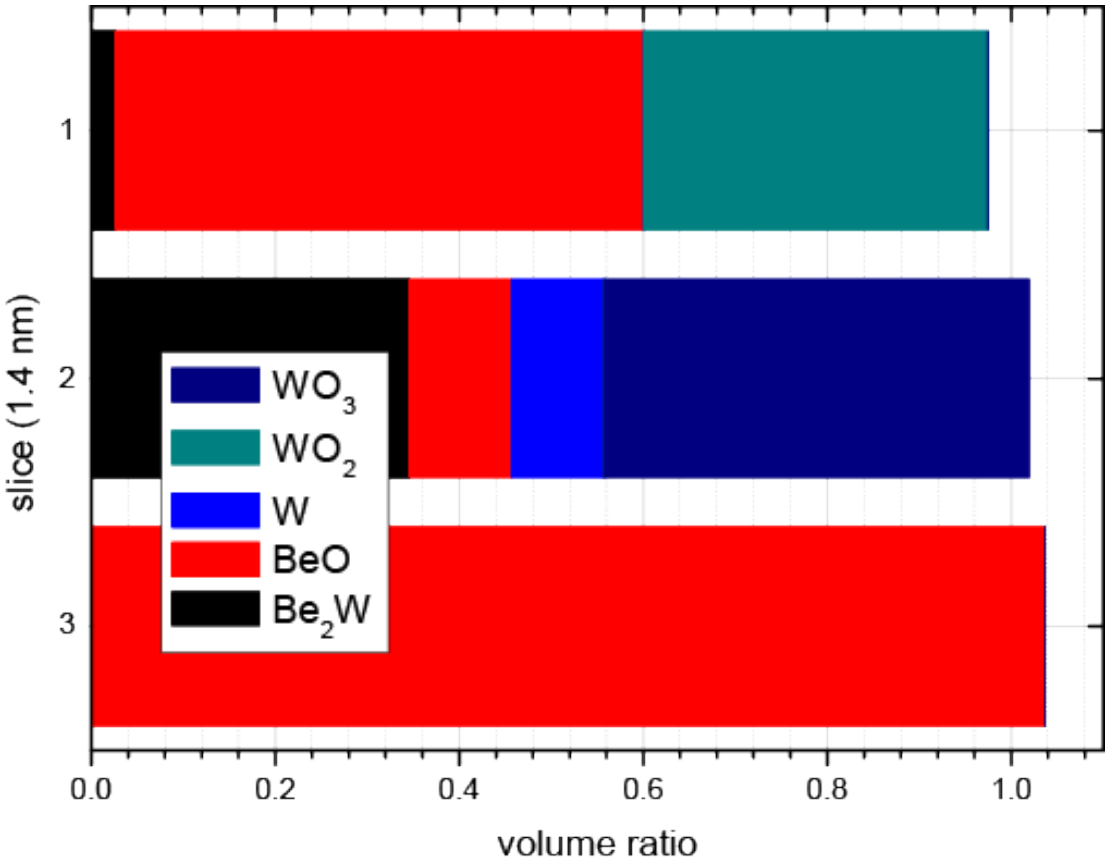
- Fill slices with elements and compounds detected by XPS
- Respect boundary conditions:
  - realistic volume density of each layer
  - fixed stoichiometries for compounds
- Calculate XPS intensities according to element distribution, attenuation by overlayers
- Fit particle densities to reproduce experimental intensities for all photon energies

Profile: Be_2W formation



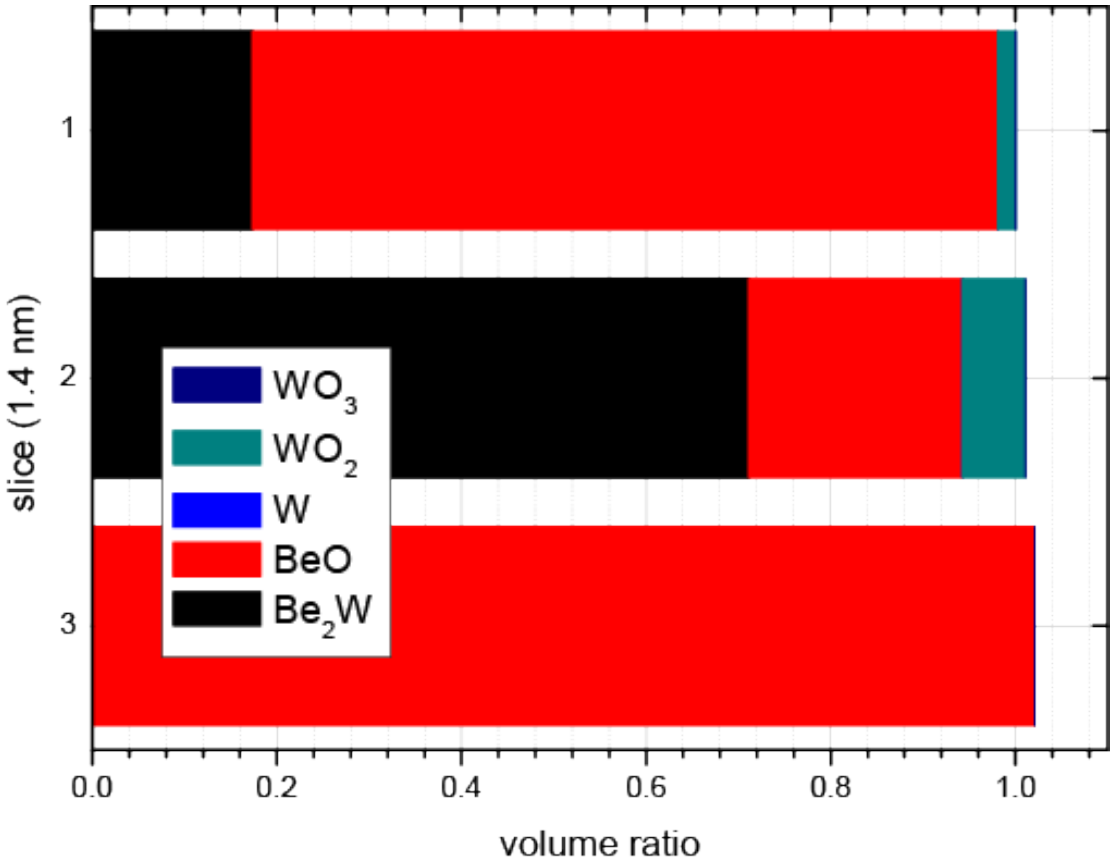
- Be_2W dominates
- surface oxidation (residual gas)

1 keV O^+



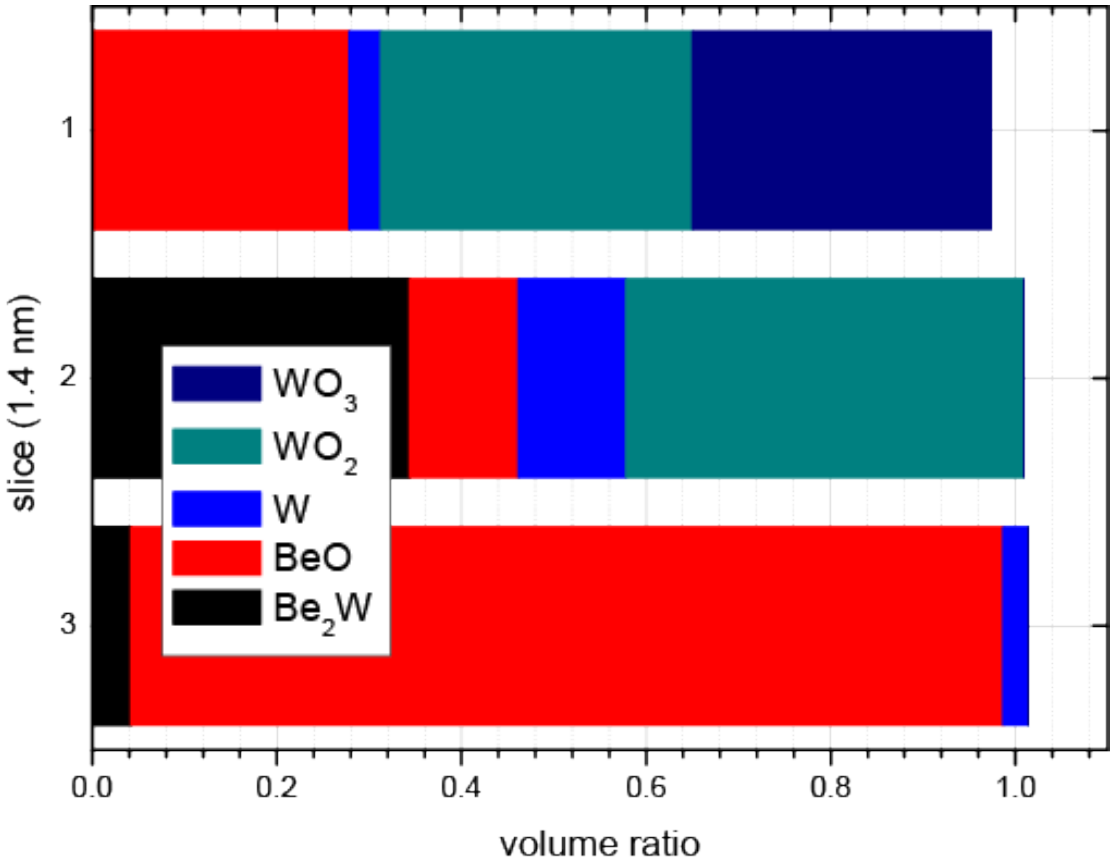
- O^+ implantation profile: maximum ~2 nm
- Be_2W is oxidized in slice 3
- available W (from Be_2W) oxidized

1 keV O^+, 600 K annealing



- BeO most stable compound: all O bound to Be
- available W (from WO_x) forms Be_2W

500 eV O^+



- WO_x formed: strong volume increase (large specific volume)
- remaining BeO in deeper layers not within analysis range
- surface BeO sputtered?

Summary: Ternary phase analysis: $O^+ \rightarrow Be_2W/Be$

Depth-resolved chemical analysis

- Synchrotron XPS allows access to identical depth intervals for different elements
- Careful data normalization required
- Qualitative analysis identifies depth-resolved reaction zones

Quantitative analysis

- Sample discretized in homogeneous slices
- Numerical (non-linear) fit procedure required (multi-parameter fit)
- Reactions during implantation and annealing compatible with implantation profile

Challenges

- Elaborate measurements at synchotron required
- More efforts needed to assess statistical confidence

Modeling of surface reactions

Wall processes modeling: Conceptual approach

Aim: Integration of **surface evolution** in **global modeling** of PWI processes

Surface composition determines:

- erosion (phys., chem.)
- hydrogen inventory
- thermomech. properties (melting, sublimation, …)

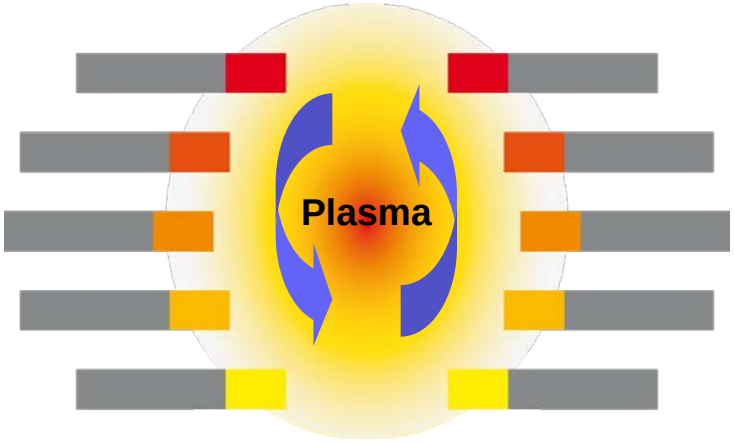
Full description of material processes:

- diffusion of *i* components in *j* materials (*D(c, T)*)
- all reaction rates
- collision-induced reactions

→ much too complicated for integration in **analytical model**!

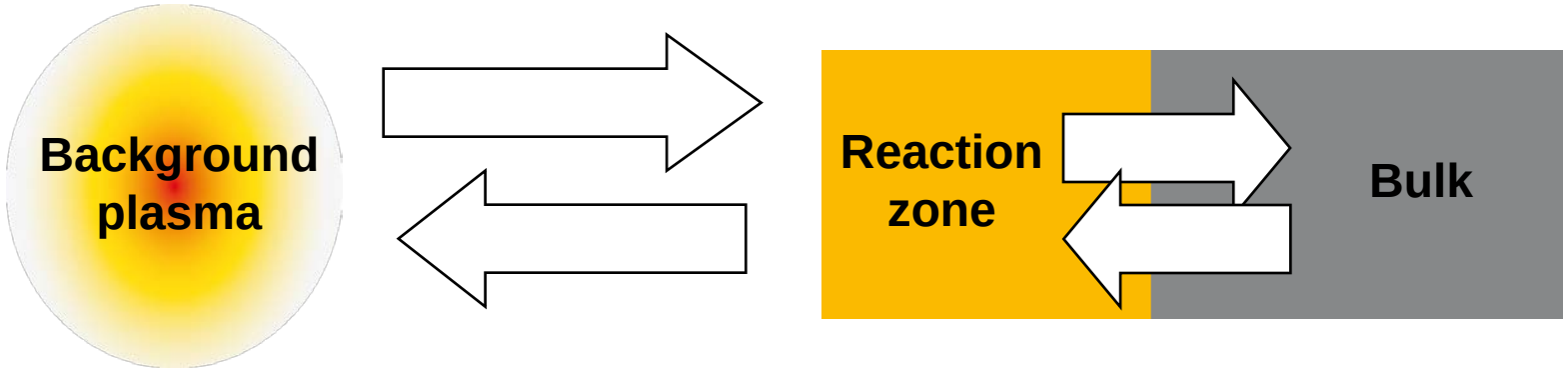
Analytical PWI model

Treat complex **plasma-wall interactions** and **material evolution** in a simplified way



Analytical model:

- first wall: *n* tiles, different loads
- background plasma (B2 + EIRENE …)
- redistribution matrix (DIVIMP)
- SDTrim sputter yields
- parametrized surface materials evolution



Surface reaction modeling

Full description of material processes:

- diffusion of *i* components in *j* materials (*D(c, T)*)
- all reaction rates
- collision-induced reactions

Parametrized material evolution

1st approximation: **homogeneous layer**

- one reactive layer
- homogeneous distribution of elements
- rate equation system

2nd approximation: **reaction front system**

- layered reaction zone
- reaction fronts
- rate equation system

Modeling approach: Description of chemistry

1. Define all substances

Be
W
C
Be_2C
W_2C
WC
Be_2W
$Be_{12}W$
Be_{gas}
BeO
O_{ads}
WO_3
$WO_{3,gas}$

+ Initial areal densities [#/m²]

2. Elementary reactions

$2\,Be + C \rightarrow Be_2C$
$Be_2C \rightarrow 2\,Be + C$
$W + C \rightarrow WC$
$WC \rightarrow W + C$
$2\,W + C \rightarrow W_2C$
$W_2C \rightarrow 2\,W + C$
$W + 2\,Be \rightarrow Be_2W$
$Be_2W \rightarrow W + 2\,Be$
$W_2C \rightarrow WC + W$
$WC + W \rightarrow W_2C$
$Be + O \rightarrow BeO$
$BeO \rightarrow Be + O$
$W + 3\,O \rightarrow WO_3$
$WO_3 \rightarrow W + 3\,O$

Sublimation:
$Be \rightarrow Be_{gas}$
$WO_3 \rightarrow WO_{3,gas}$

O-Adsorption:
$O_{2,gas} \rightarrow O_{ads}$
$O_{ads} \rightarrow O_{2,gas}$

3. Define equations for reaction fluxes

$$\Gamma_1\left[\tfrac{1}{m^2 s}\right] = [Be]^2[C]k_1 \exp\frac{-\Delta E_1}{kT} \quad \text{with} \quad k_1\left[\tfrac{m^4}{s}\right]$$

$$\Gamma_2\left[\tfrac{1}{m^2 s}\right] = [Be_2C]k_2 \exp\frac{-\Delta E_2}{kT} \quad \text{with} \quad k_2\left[\tfrac{1}{s}\right]$$

4. Define balances

Change of areal density of substance =
+ all formation reaction fluxes
– all destruction reaction fluxes
± all "non-chemical" fluxes

$$\frac{d[Be]}{dt} = -2\Gamma_1 + 2\Gamma_2 + \ldots \qquad \frac{d[Be_2C]}{dt} = +\Gamma_1 - \Gamma_2 + \ldots$$

→ Set of ordinary differential equations

$$y'(t) = f(t, y(t)), \quad \text{with initial value} \quad y(t_0) = y_0$$

Modeling: Where to get input data?

- **Standard literature:** vapor pressures, enthalpies of formation

- **XPS measurements:** investigation of thin layers
  (lab, synchrotron)
  → chemical phase information
  → determination of reaction enthalpies
  → ions: relevant depth information
  (binary systems: Be-C, Be-W, W-C, W-O, Be-O,
  ternary systems: Be-C-O, Be-W-O, Be-W-C …)

- **RBS measurements:** e.g. diffusion data

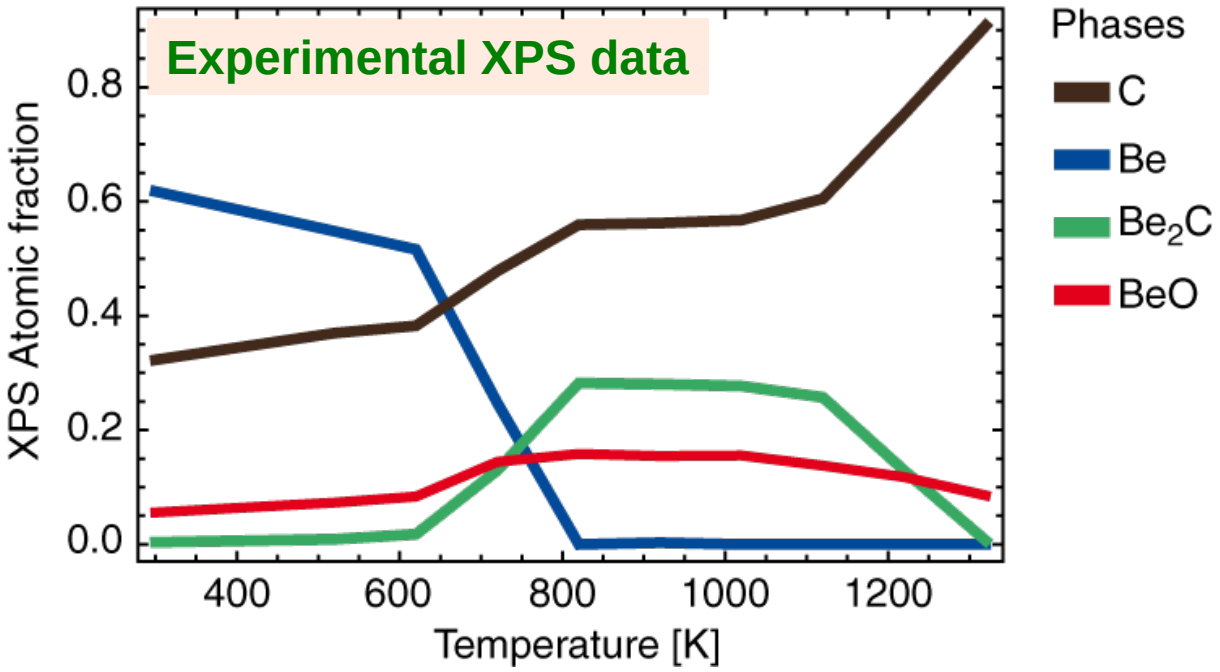
Binary Be-C system

- Be / C
- homogeneous layer model

Benchmarking: Be/C

System

- substrate: pyrol. graphite
- 1.6 nm Be surface layer
- ~10^{-10} mbar O_2
- homogeneous reaction layer



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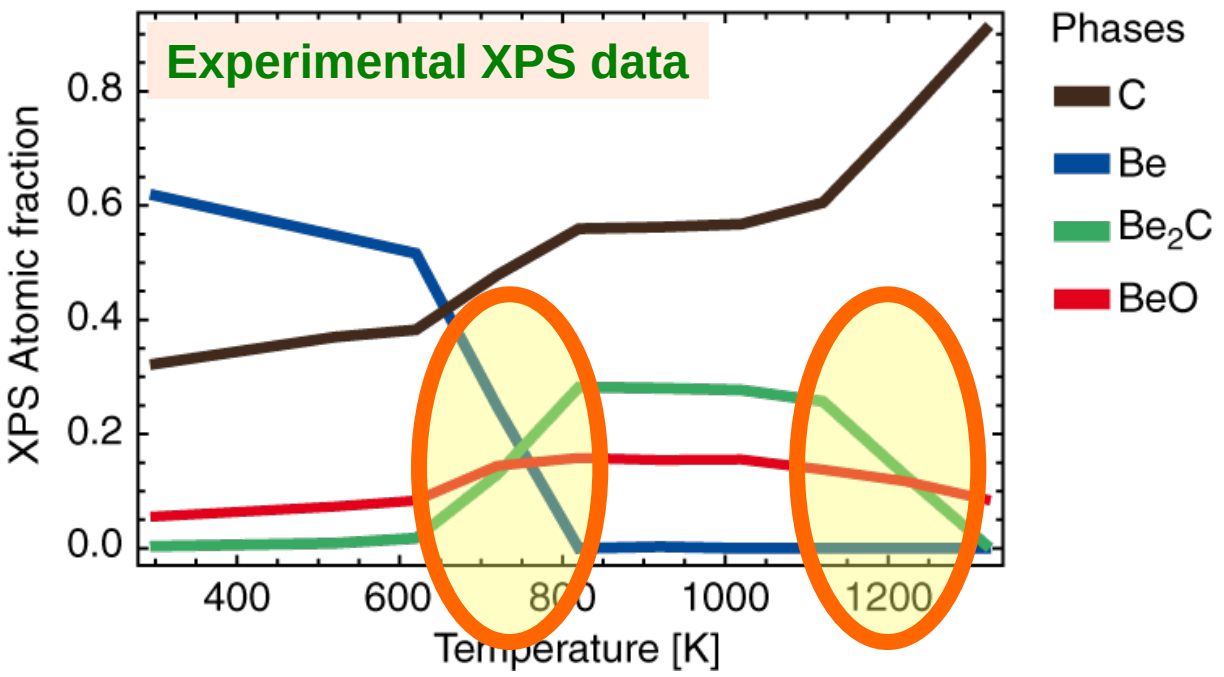


$2\,Be + C \rightarrow Be_2C$

$Be + O \rightarrow BeO$

$Be_2C \rightarrow 2\,Be + C$

$Be \rightarrow Be\,(g)$

$Be + O \rightarrow BeO$

Benchmarking: Be/C

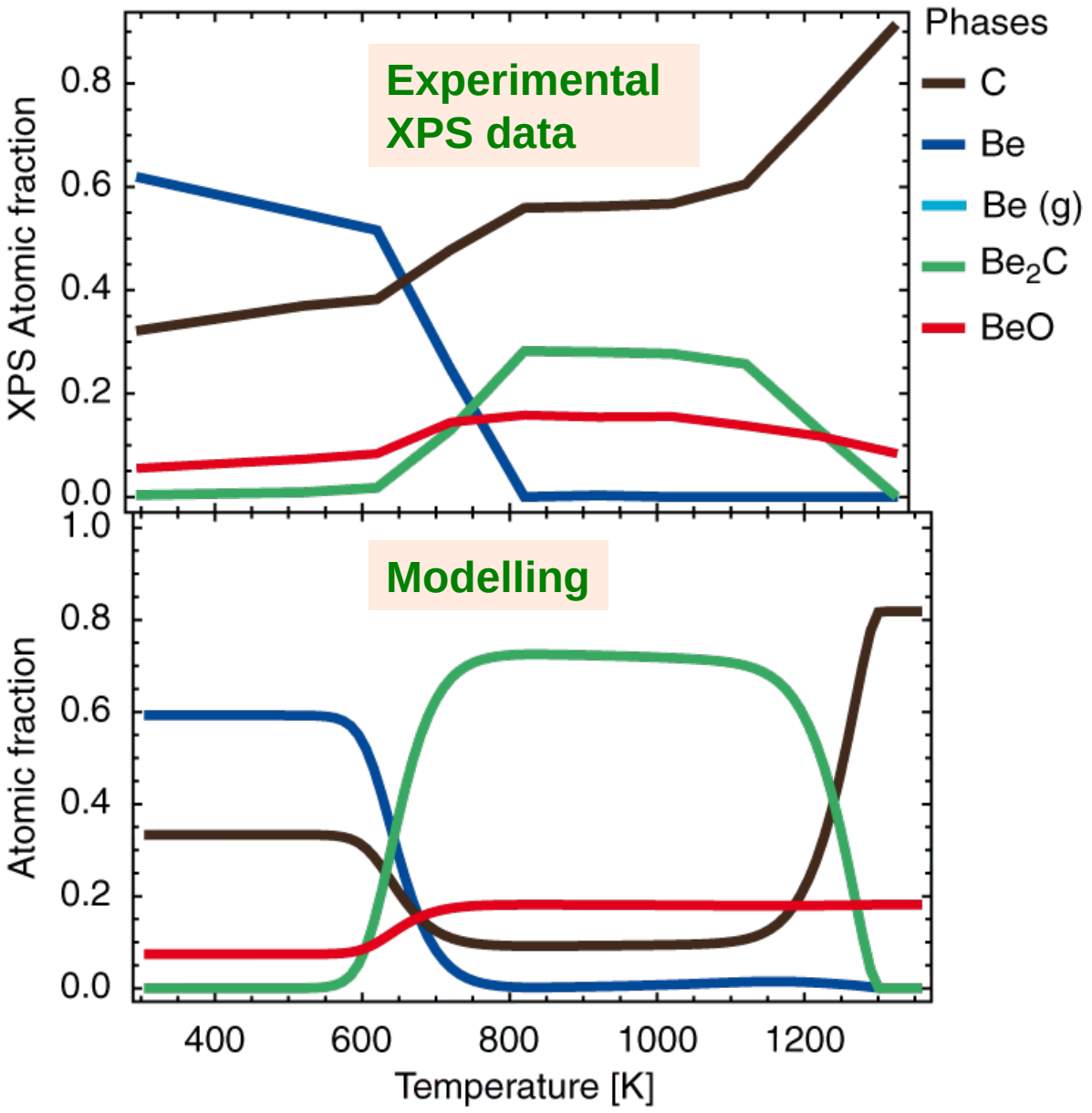
System

- substrate: pyrol. graphite
- 1.6 nm Be surface layer
- ~10^{-10} mbar O_2
- homogeneous reaction layer

Fully coupled rate equation system

Be_2C formation:
ΔE=1.8 eV (exp.), $k_0 = 10^{-29}$ m^4/s

Be_2C dissociation:
ΔE=3.0 eV (from ΔH_f), $k_0 = 10^{13}$ s^{-1}



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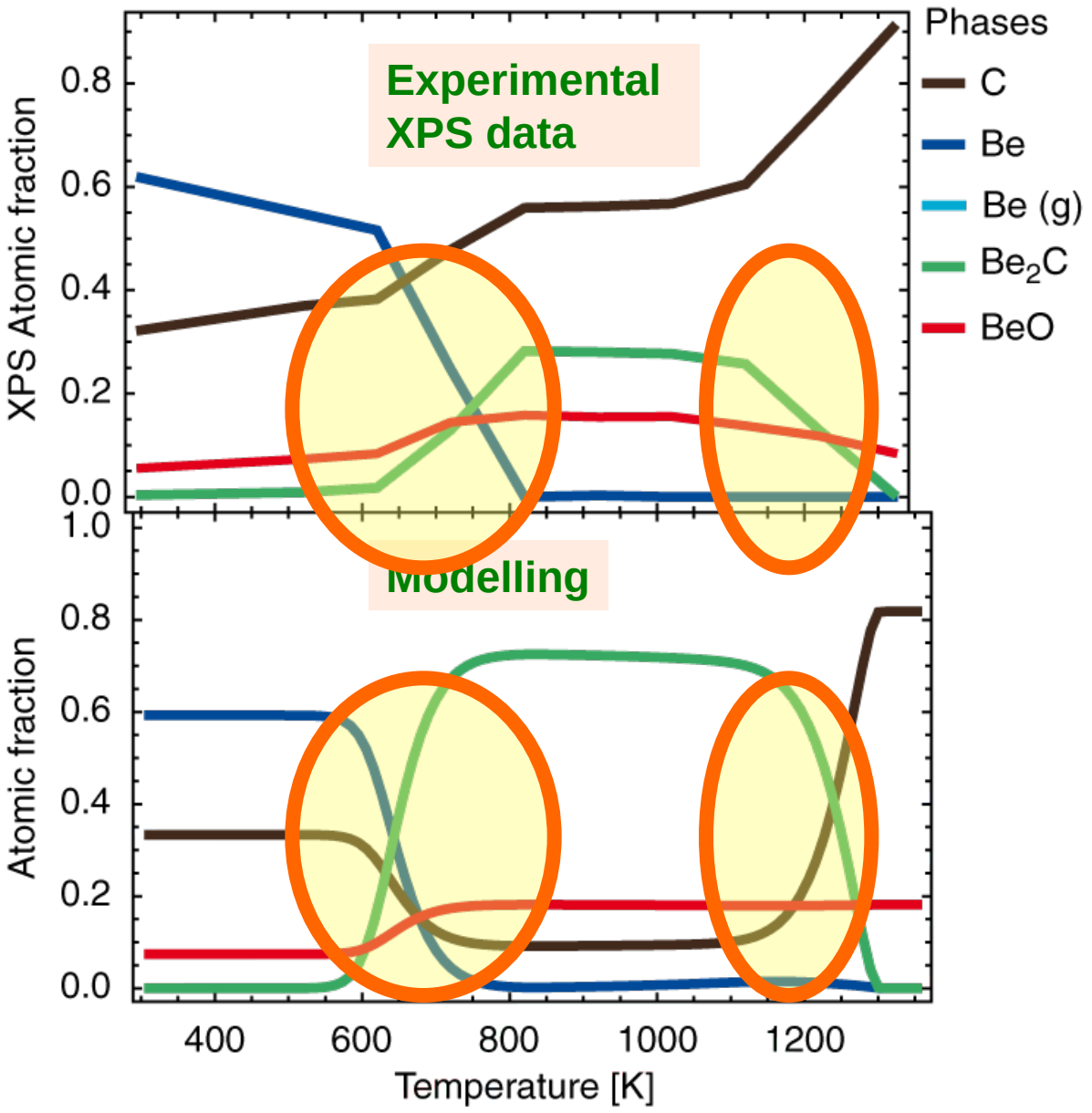


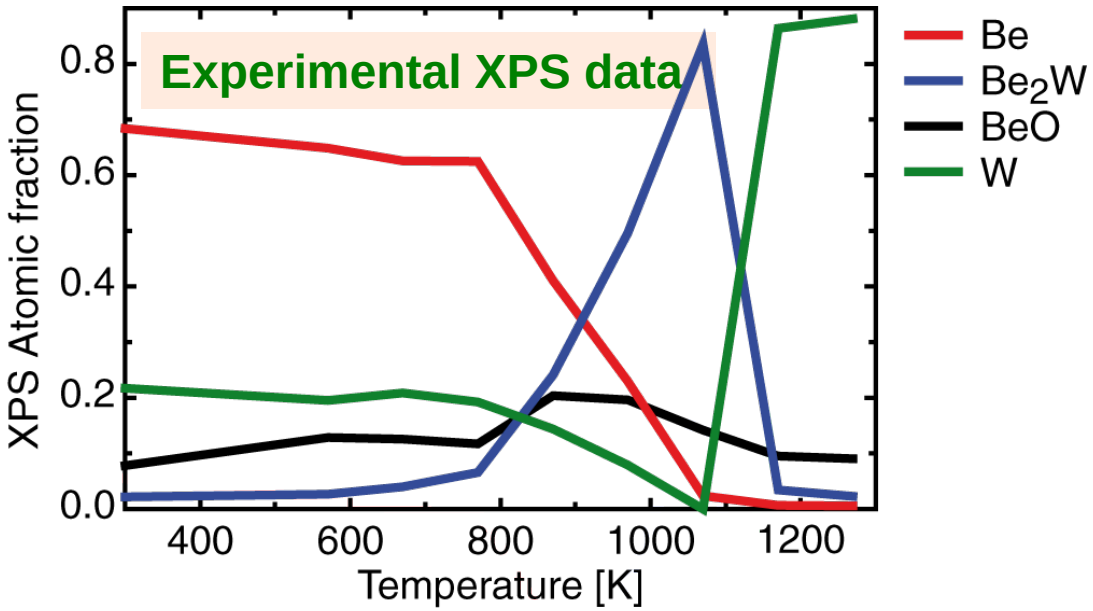
Binary Be-W system

- Be / W
- reaction front model

Benchmarking: Be/W

System

- substrate: W
- 2.1 nm Be surface layer
- layered system with reaction fronts



Benchmarking: Be/W

System

- substrate: W
- 2.1 nm Be surface layer
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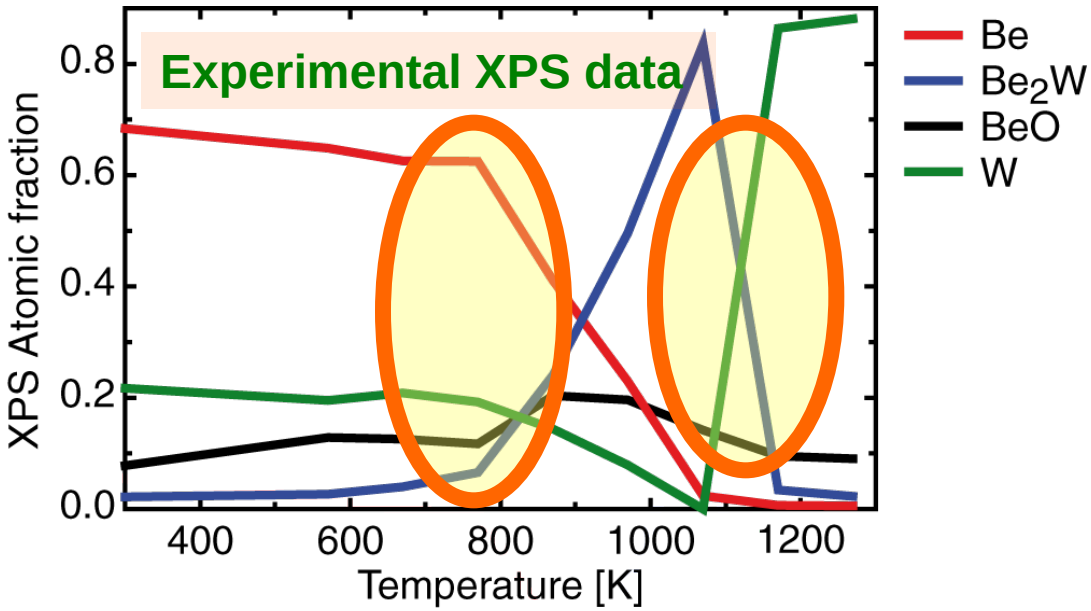


Be diffusion in Be_2W	Be_2W dissociation
Be diffusion in BeO	BeO dissociation
	Be sublimation

Benchmarking: Be/W

System

- substrate: W
- 2.1 nm Be surface layer
- layered system with reaction fronts

Fully coupled rate equation system

Diffusion:

$E_D(Be\ in\ alloy) = 1.5$ eV, $D_0 = 10^{-12}\ m^2\ s^{-1}$

$E_D(Be\ in\ BeO) = 1.6$ eV, $D_0 = 10^{-6}\ m^2\ s^{-1}$

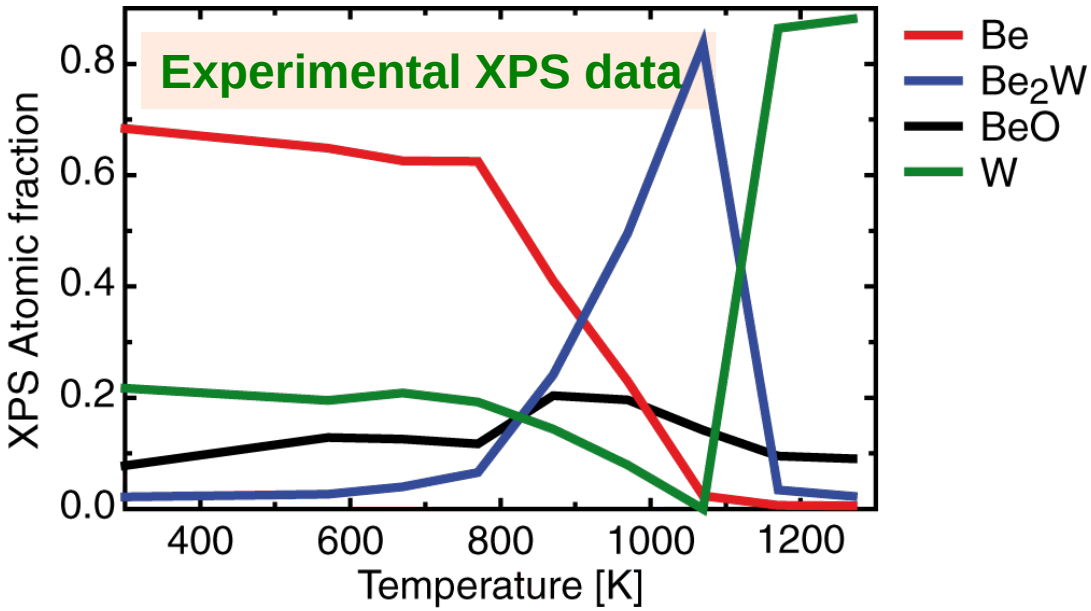
Dissociation:

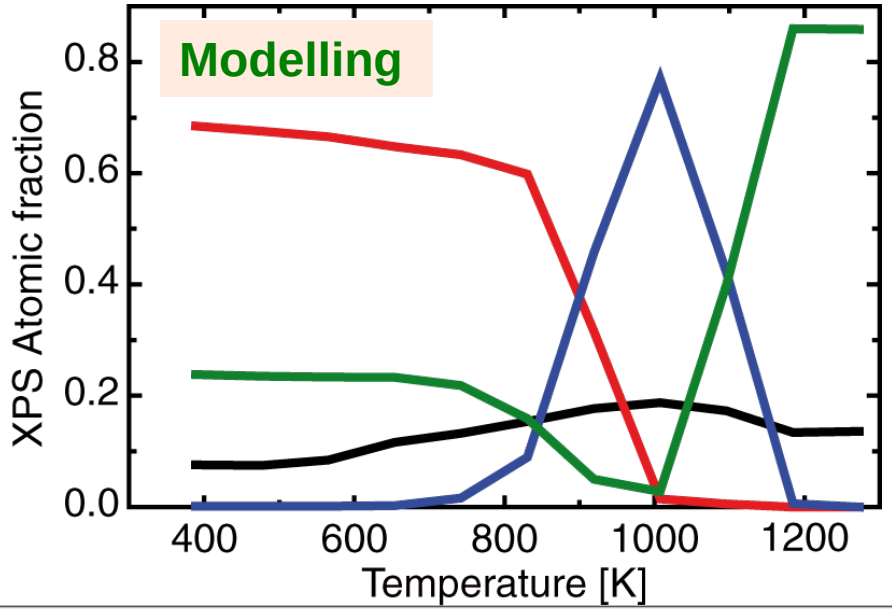
$E_A(Be_2W) =$ 3.1 eV, $k_0 = 10^{13}\ s^{-1}$

$E_A(BeO) =$ 6.0 eV, $k_0 = 10^{13}\ s^{-1}$

Sublimation:

$E_S(Be) =$ 3.2 eV, $k_0 = 4.3 \times 10^{34}\ s^{-1}$





Benchmarking: Be/W

System

- substrate: W
- 2.1 nm Be surface layer
- layered system with reaction fronts

Fully coupled rate equation system

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$E_D(Be\ in\ alloy) = 1.5$ eV, $D_0 = 10^{-12}\ m^2\ s^{-1}$

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$E_A(Be_2W) =$ 3.1 eV, $k_0 = 10^{13}\ s^{-1}$

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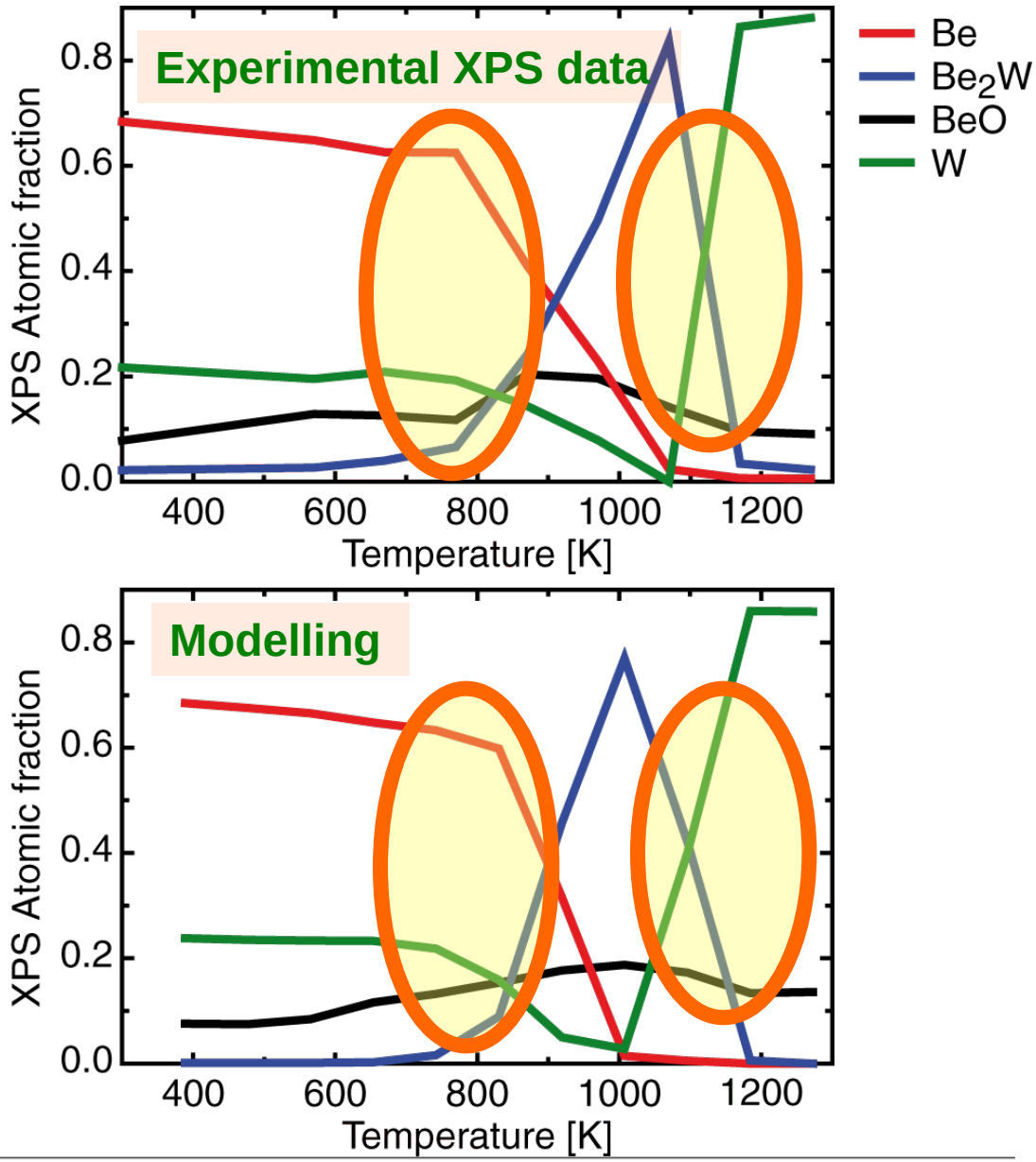
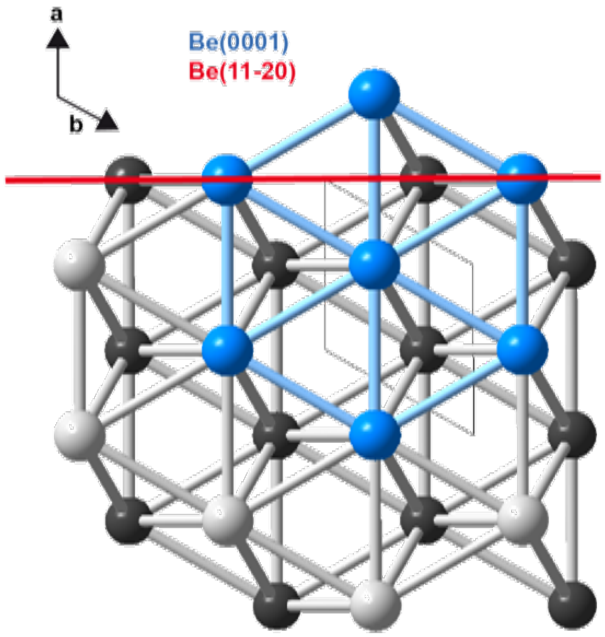


Summary: Modeling of surface reactions

- Fundamental reaction parameters from well-defined experiments
- XPS yields chemical data (qualitative and quantitative), complemented with other techniques
- Integration of surface chemistry into a modeling approach for PWI: predictive power for different locations with different loads
- Further identified reactions and processes can easily be integrated in modeling approach
- Tool for wall material compatibility testing: knowledge of material evolution due to PWI allows modification of local parameters (temperature, fluxes, composition)

Hydrogen isotope retention

D diffusion in beryllium



Be crystal lattice

Be(0001) plane ∥ to surface

Be(11-20) plane ⊥ to surface

- Beryllium has **not an "ideal" hcp** structure. Be-Be distances are closer in <0001> than perpendicular to it (e.g. <11-20>)
- DFT (Density Functional Theory) calculations show anisotropy in transport processes with respect to Be basal planes

Modeling: 2D coupled rate equations

Strategy

- Solve a coupled reaction diffusion system (CRDS) consisting of an arbitrary number of diffusing species *i=A,B,C…* in 1, 2 or 3 dimensions
- Solve system of partial differential equations for the time dependent 2D depth profile $\rho(x,z,t)$ [m^{-3}]

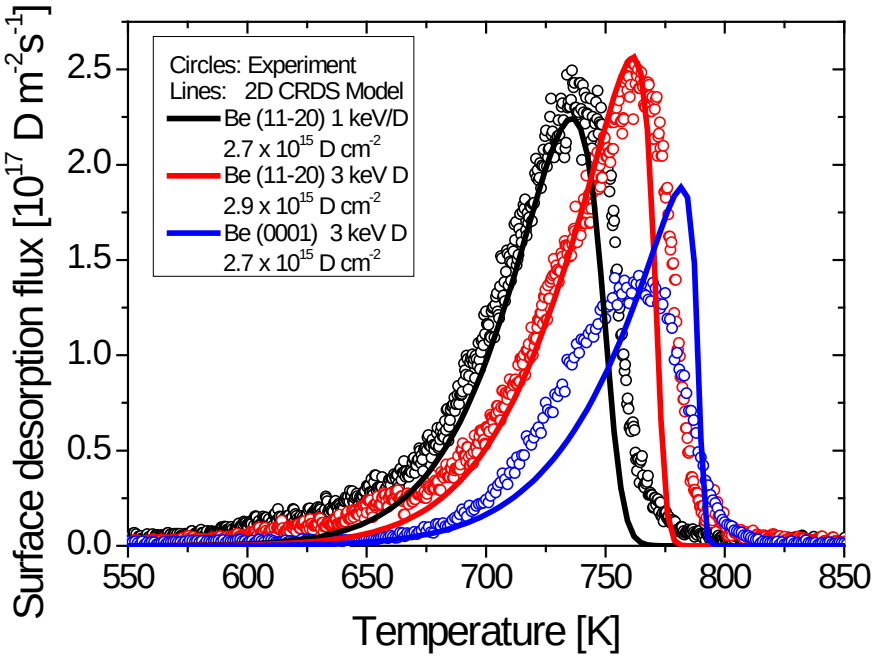
$$\frac{\partial \rho_A(x,z,t)}{\partial t} = \frac{\partial}{\partial x}\left(D_x(T(t)) \frac{\partial \rho_A(x,z,t)}{\partial x} \right) + \frac{\partial}{\partial z}\left(D_z(T(t)) \frac{\partial \rho_A(x,z,t)}{\partial z} \right) +$$

$$+ \sum \Gamma_i^{Form}(\rho_{A,B,C\ldots}) - \sum \Gamma_i^{Annihilation}(\rho_{A,B,C\ldots}) + \Gamma_i^{Source}(x,z,t)$$

$$A + B \rightarrow C \qquad\qquad C \rightarrow A + B$$

$$\Gamma_1(\rho_A,\rho_B,t) = k_1 \rho_A \rho_B \exp\left(-\frac{\Delta E_1}{k_B T(t)}\right) \qquad \Gamma_2(\rho_C,t) = k_1 \rho_C \exp\left(-\frac{\Delta E_2}{k_B T(t)}\right)$$

TPD of D implanted in Be single crystals



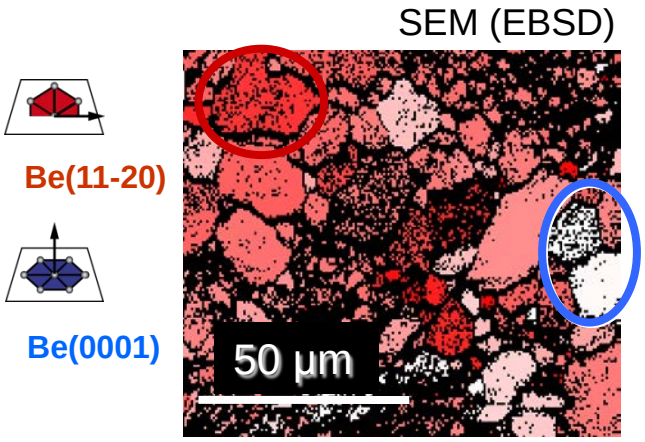
TPD spectra and 2D-CRDS simulations after implantation of D at 1 keV/D and 3 keV/D in Be(0001) and Be(11-20)

1. Desorption temperature shift for different implantation energies
2. Desorption temperature shift for Be(0001) and Be(11-20)
3. Less D retention in Be(0001) than in Be(11-20)

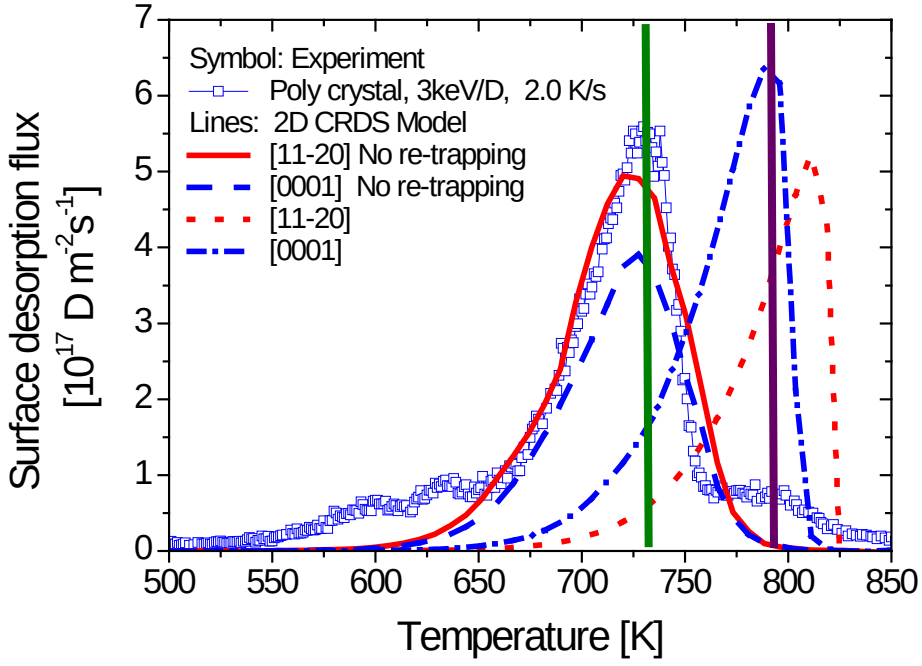
1. Deeper implantation → longer diffusion path to the surface → higher TPD peak temperature
2. Anisotropy of Be lattice → 2D anisotropic modelling required to implement results from DFT calculations
3. Dynamics during D implantation (MV+SI annihilation and trapping in MV) determines retention

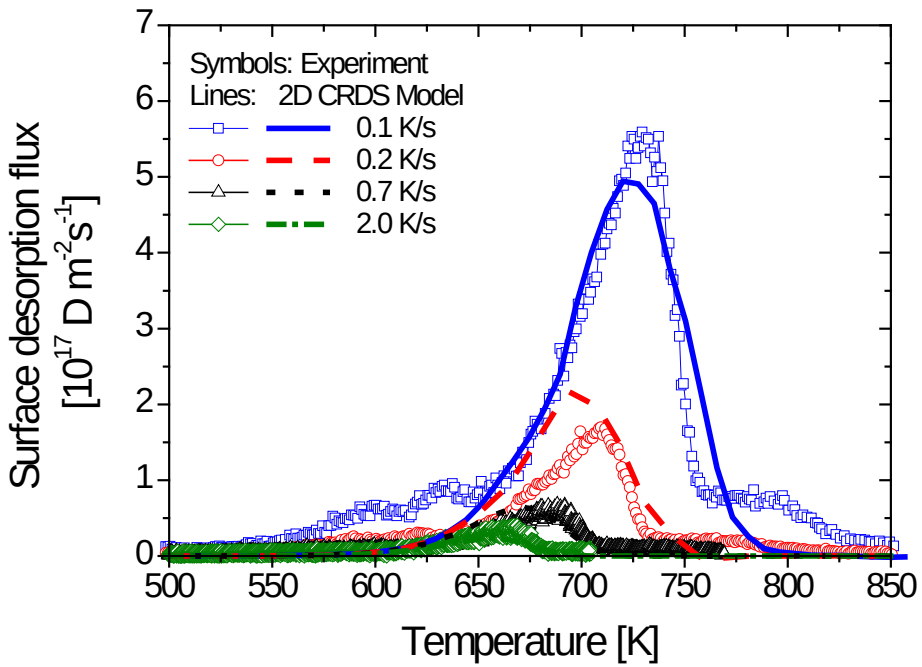
TPD from Be polycrystal

Identical parameters also applied for polycrystalline Be



- Shift for Bepoly reproduced with no retrapping: fast grain boundary diffusion
- heating ramp variation reproduced: no (self)trapping during heating





Parameters for D release and diffusion

Experimentally and DFT determined parameters for full description

		ν	ΔE_{act} [eV]	ΔE_{act} [eV]
		CRDS	CRDS	DFT 1 [1]
Diffusivity ∥ Basal Plane	*Mobile Hydrogen H_{mob}*	3.11E-06	<0.4*	0.2
	Mono vacancy MV	3.11E-06	0.7	0.7
	Self interstitial SI	3.11E-06	0.4	0.4
	Trapped Hydrogen H_{trap}	-	-	
Diffusivity ⊥ Basal Plane	H_{mob}	7.68E-06	<0.4*	0.4
	MV	7.68E-06	0.7	0.7
	SI	7.68E-06	0.004	0.004
	H_{trap}	-	-	
Trapping	$H_{mob} + MV \rightarrow H_{trap}$	1.00E+13	0.4	0.4
Detrapping	$H_{trap} \rightarrow H_{mob} + MV$	1.00E+11*	1.75	1.75
Annihilation	$MV + SI \rightarrow -$	1.00E+13	0.004	0.004
Self trapping	$H_{mob} + 1\ H_{trap} \rightarrow 2\ H_{trap} + SI$	1.00E+13	0.4	0.4

Anisotropy in diffusion of self-interstitials crucial for modeling!

Summary: Hydrogen retention modeling

- Fundamental reaction parameters from well-defined experiments
- XPS yields chemical data (qualitative and quantitative), complemented with other techniques
- Integration of surface chemistry into a modeling approach for PWI: predictive power for different locations with different loads
- Further identified reactions and processes can easily be integrated in modeling approach
- Tool for wall material compatibility testing: knowledge of material evolution due to PWI allows modification of local parameters (temperature, fluxes, composition)

Investigated systems

1. Binary Be-based systems

- C/Be, Be/C — lab., DFT
- $C^+ \rightarrow$ Be — lab.
- Be/W, W/Be — lab., DFT
- $N^+ \rightarrow$ Be — lab., DFT
- O_{at}, $O_2 \rightarrow$ Be — lab.

3. Ternary Be-based systems

- $CO^+ \rightarrow$ Be — lab.
- $O^+ \rightarrow Be_2W$/W — synchr.
- C/BeO/W — synchr.
- Be/C/W, C or Be excess — lab.
- C/Be/W, C or Be excess — lab.
- Be/WO_2, Be/WO_3 — lab.
- C/W/Be — synchr.
- WO_x/Be — synchr.

2. Hydrogen isotope retention and release

- $D^+ \rightarrow Be_{poly}$, Be(0001), Be(1 1 -2 0) — lab., DFT
- $D^+ \rightarrow$ O/Be, BeO — lab., DFT

Outlook: Reaction and erosion studies

Open issues and work plan

- Interactions of nitrogen with Be—W alloys, together with presence of other impurities (O, C)
  Here, a large set of DFT calculations, incl. the interaction of hydrogen with N-containing compounds, is available (A. Allouche). These results require experimental verification.
- Erosion studies of Be and Be compounds by N ions
  Experiments are planned in an IPP-TU Wien collaboration, starting this November at IPP (quantitative erosion measurements using quartz crystals microbalances).
- Full exploitation of available depth-resolved XPS measurements of ternary Be compounds (new measurements where required)
  Data from BESSY measurements available, analysis tool available.
- Investigate sutable DFT-determined parameters as input for SDTRIM.SP calculations for compounds
  Replace surface binding energies by DFT-based energies in TRIM calculations. Collaboration IPP—U Aix-Marseille.

Outlook: Hydrogen retention and release mechanisms

Open issues and work plan

- Investigate influence of intrinsic and ion-induced defects in D retention
  Compare TPD studies from D^+-implanted Be with atomic D (defects: intrinsic or ion-induced).
- Investigate retention and release mechanisms for Be compounds and compound layers on Be
  Extend studies on metallic Be to compounds and layers.
- Interpretation of H isotope retention by CRDS (coupled reaction diffusion system) modeling
  Extend available model to compounds. Include posible DFT results (Cooperation IPP—U Aix-Marseille).

Application of fundamental data on Be and Be compounds to simulations for JET and ITER

- Extend and apply existing models (WallDyn) by integrating the determined parameters for various wall processes