7th International Workshop on Models and Data for Plasma-Material Interactions in Fusion Devices (MoD-PMI)

Dynamics of vacancies and self-interstitial atoms in beryllium and its implications on hydrogen retention

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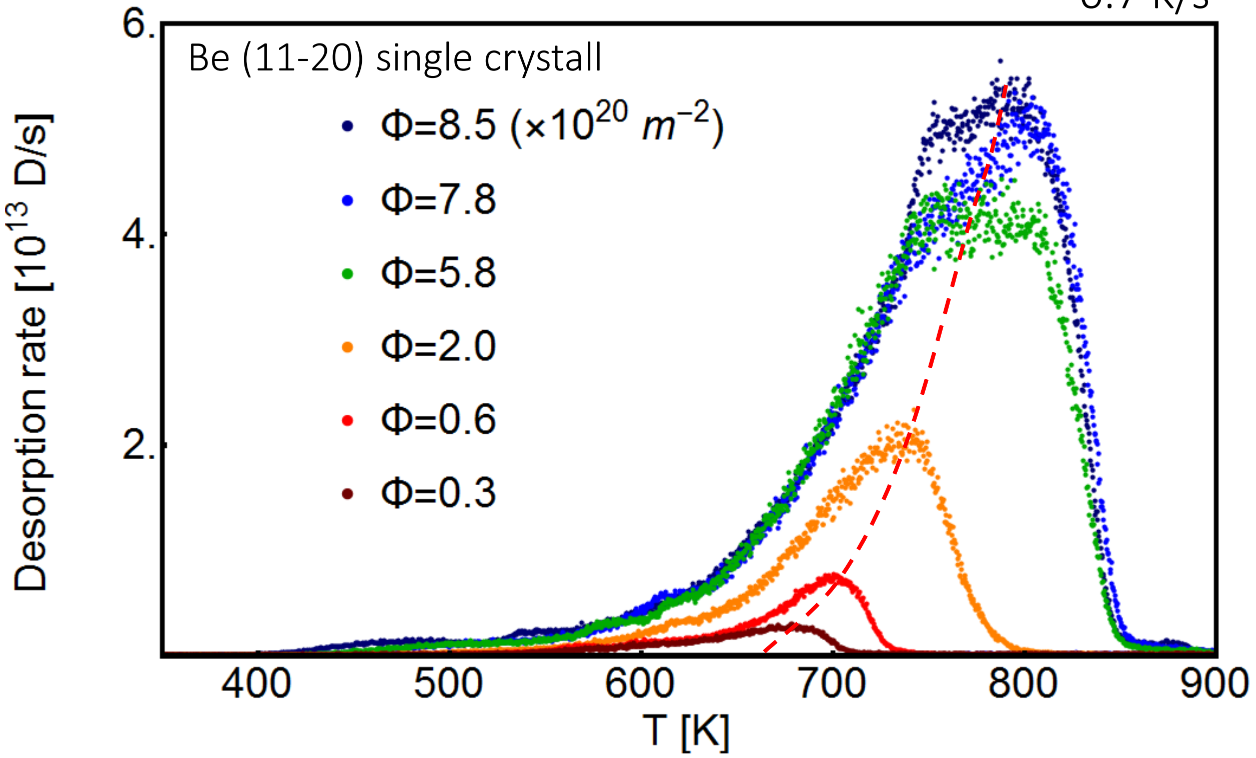
Experimental: Earlier experiments in ARTOSS (D ion beam exposure under UHV)

Low to moderate exposure fluence [1]

- only single peak, high T desorption
- peak shifts to higher T with fluence

1 keV/D
0.7 K/s

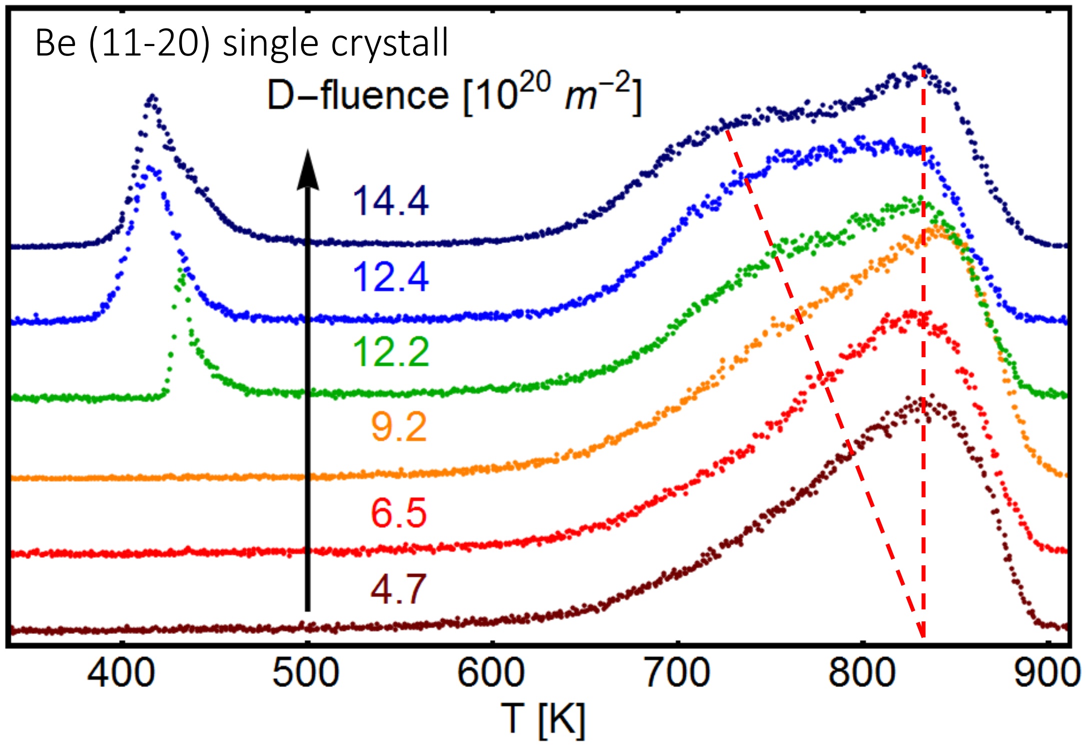


[1] M. Oberkofler, PhD thesis 2012 IPP 17/31

Moderate to high exposure fluence [2]

- high T peak left shoulder forms
- appearance of low T peak

1 keV/D
0.7 K/s



[2] M. Reinelt, NJP 11 (2009) 043023

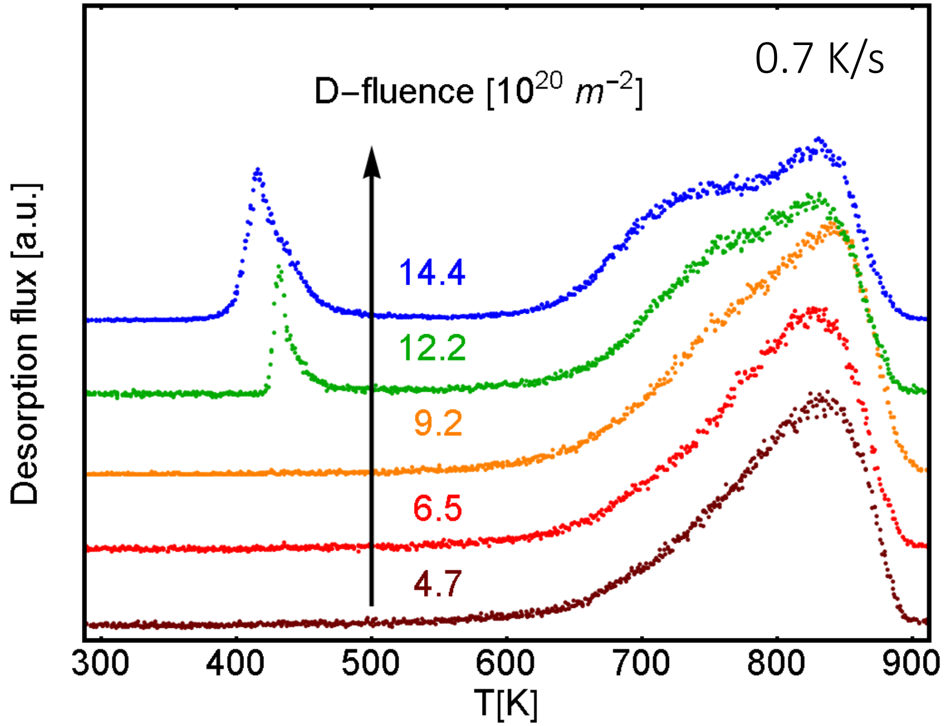
Fluence dependence of D retention in ion-beam implanted sc Be

<u>Low to moderate fluence</u>: number of V increases linearly with fluence → re-trapping leads to peak shift

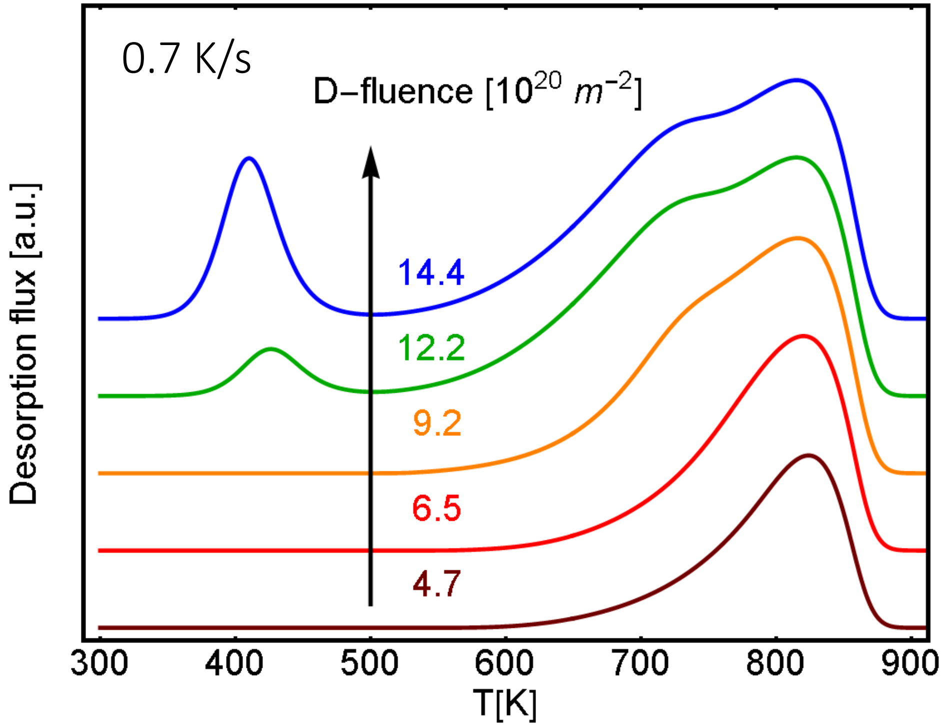
<u>Moderate to high fluence</u>: V production saturates (?) → D/V ratio increases with fluence up to D/V = 5 (DFT)

→ excess D goes to surfaces (extended surface area as an approximation for open surface porosity)

Experiment (sc Be) *Reinelt et al. NJP 2009*



Modelling *Matveev et al. NIMB 2018*

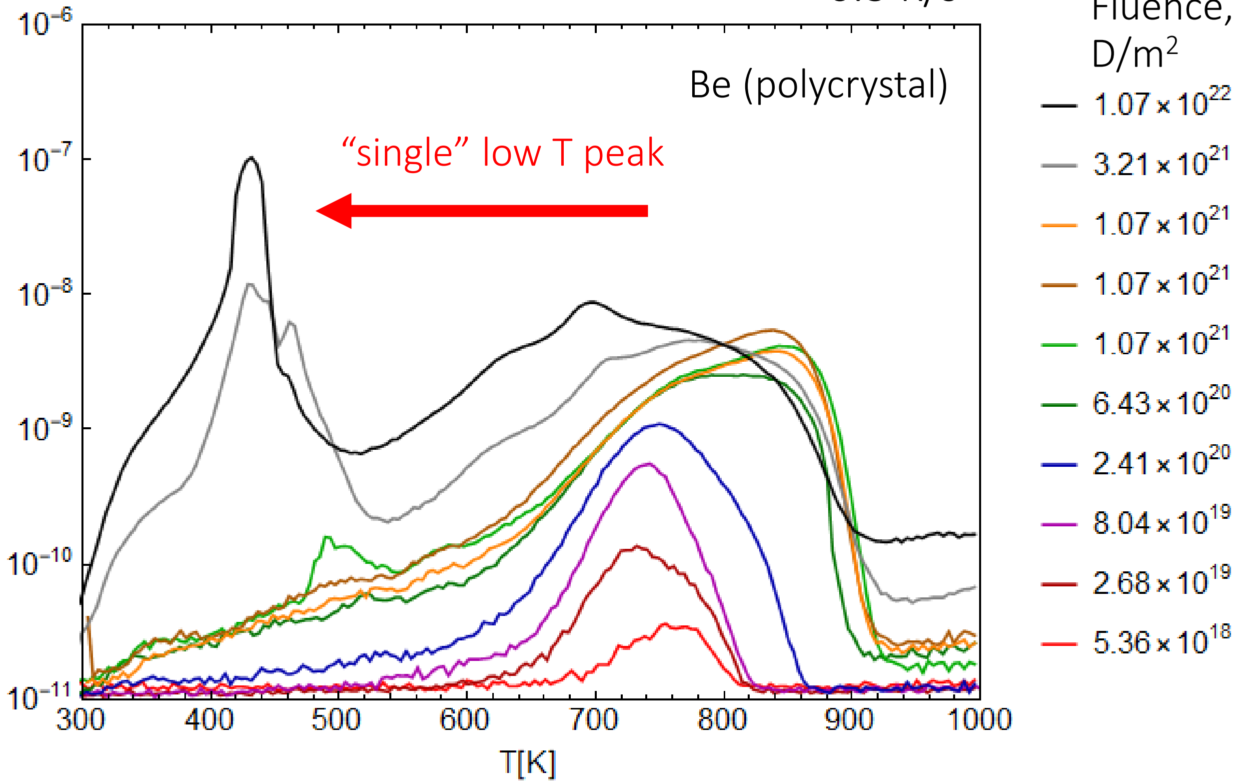


Experimental: More recent experiments in ARTOSS

Retention and release at different fluences ranging over ~3 orders of magnitude

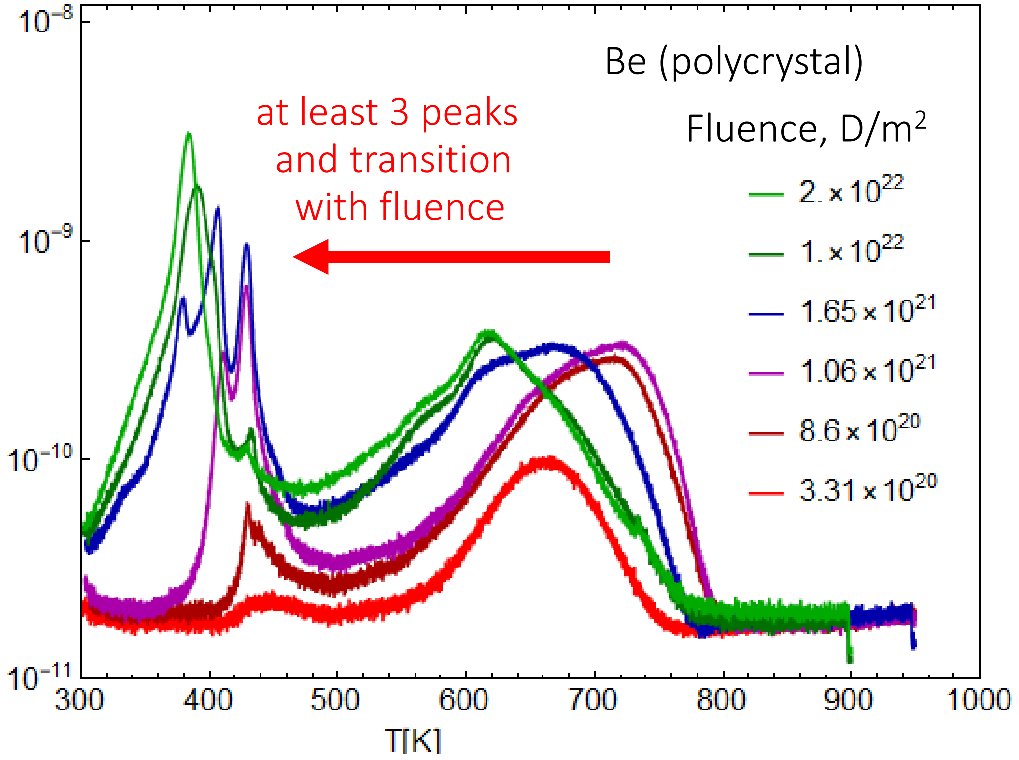
“fast” TDS

1 keV/D
0.3 K/s



“slow” TDS

1 keV/D
0.01 K/s

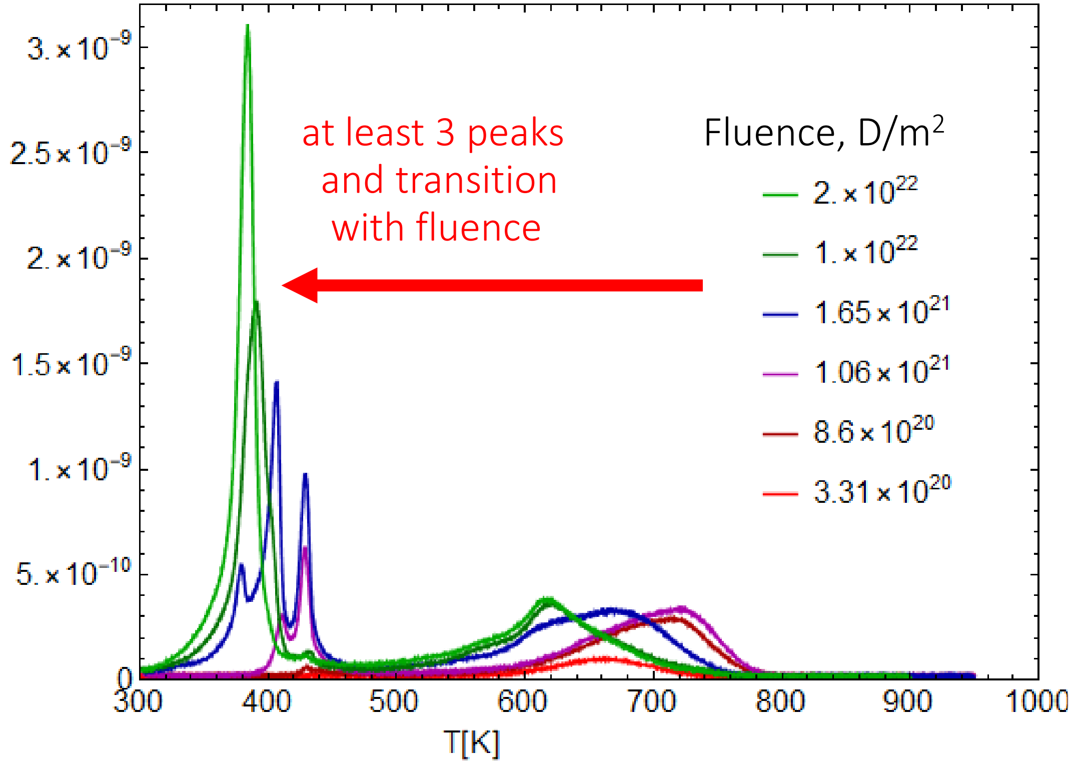


M. Eichler, JNM 19 (2019) 440–444

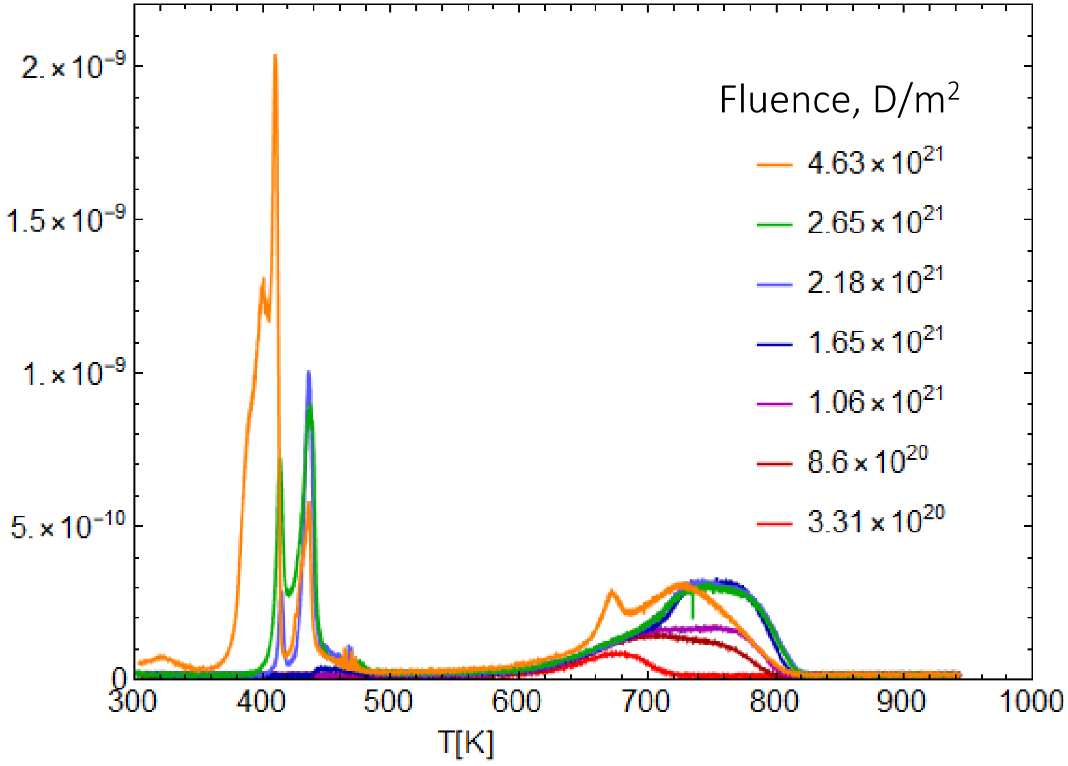
Experimental: More recent experiments in ARTOSS

Retention and release at different fluences ranging over ~3 orders of magnitude

Be (polycrystal) — 1 keV/D, 0.01 K/s



Be (single crystal) — 1 keV/D, 0.01 K/s



M. Eichler, JNM 19 (2019) 440–444

Experimental: Retention in Be:D co-deposited layers (lab vs JET)

Similarity to co-deposited layers with high D content -> very sharp low temperature peak

Samples of different origin

UCSD

[1] A. Založnik NF 59 (2019) 126027

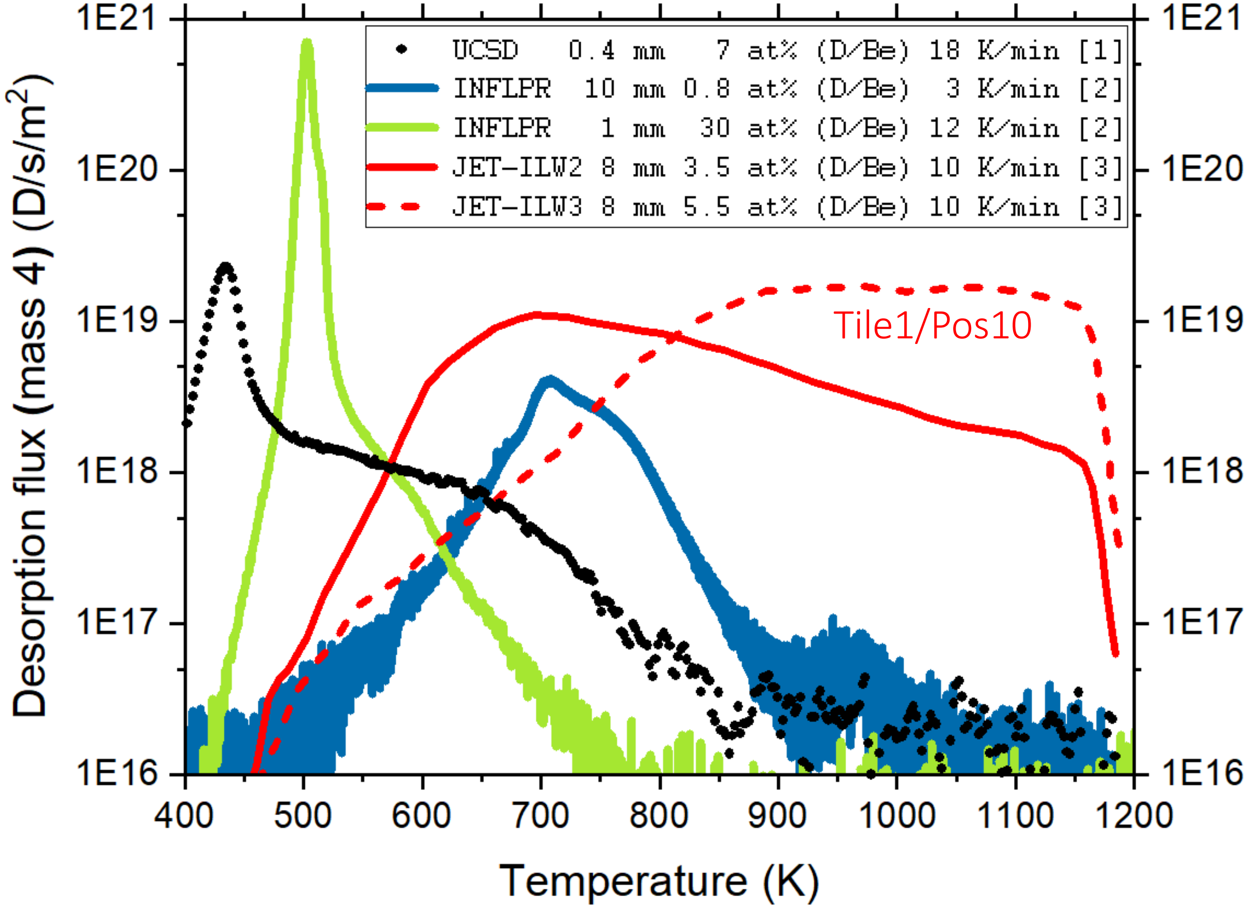
INFLPR, Bucharest

[2] M. Zlobinski NME 19 (2019) 503

JET

[3] J. Likonen NME 19 (2019) 166

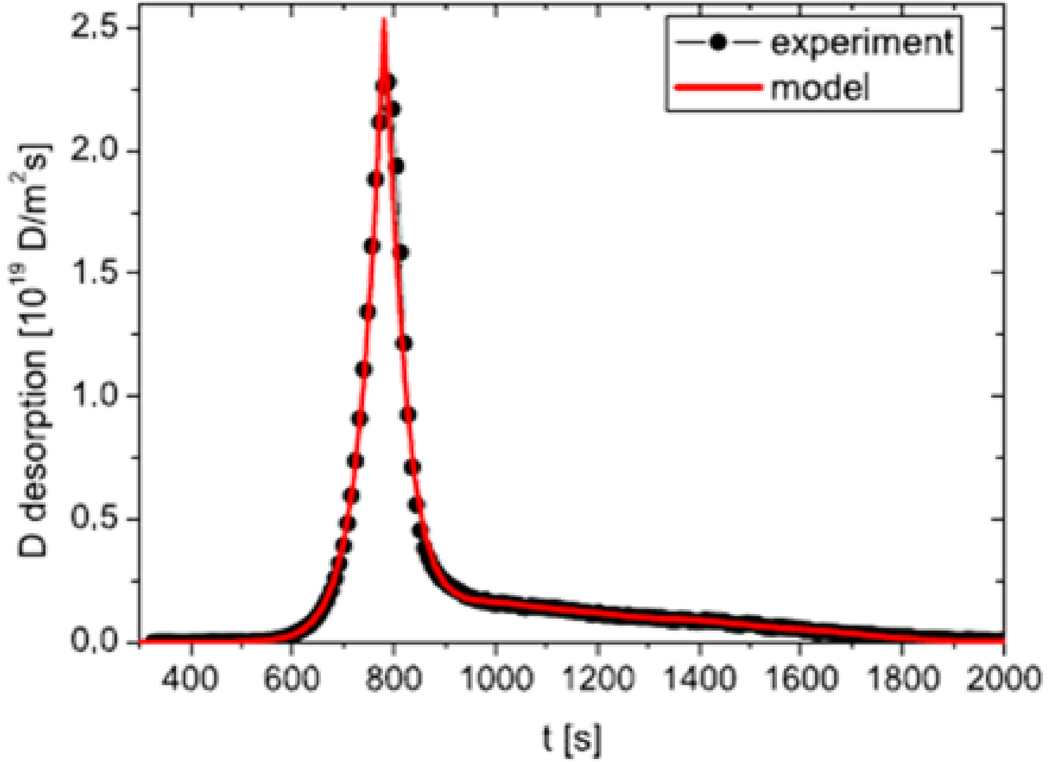
D. Matveev Phys. Scr. (2020) 014053

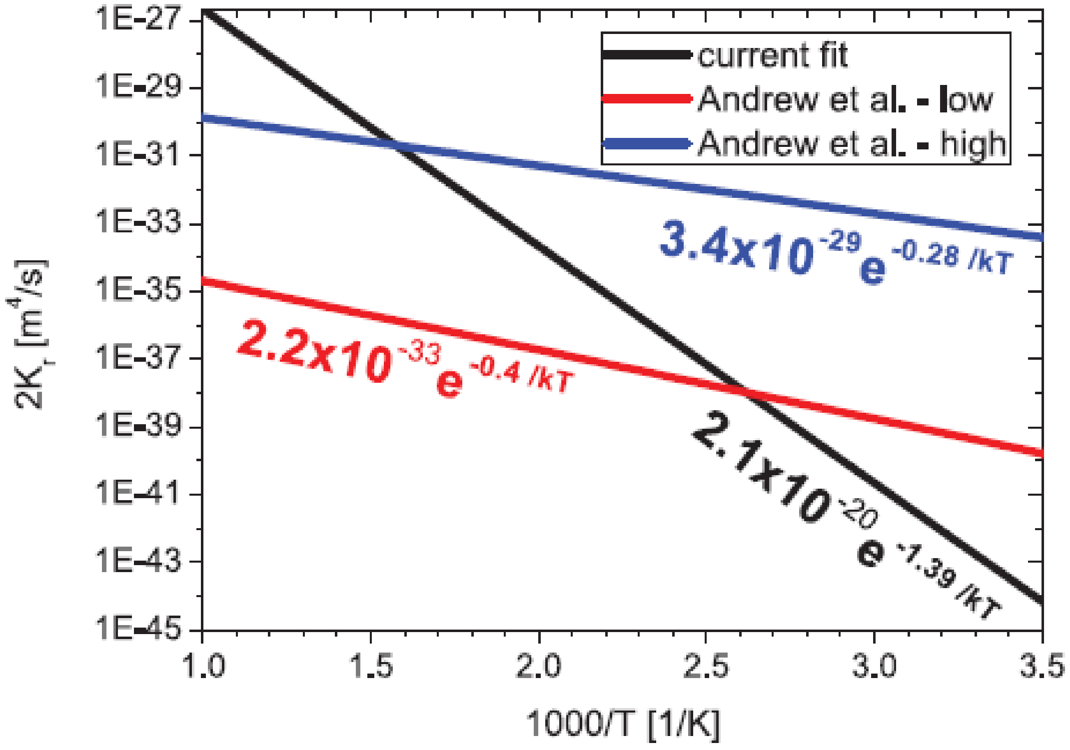


Models for the sharp low temperature desorption

1) Decomposition of BeD_2 with fitted recombination

A. Založnik NF 59 (2019) 126027

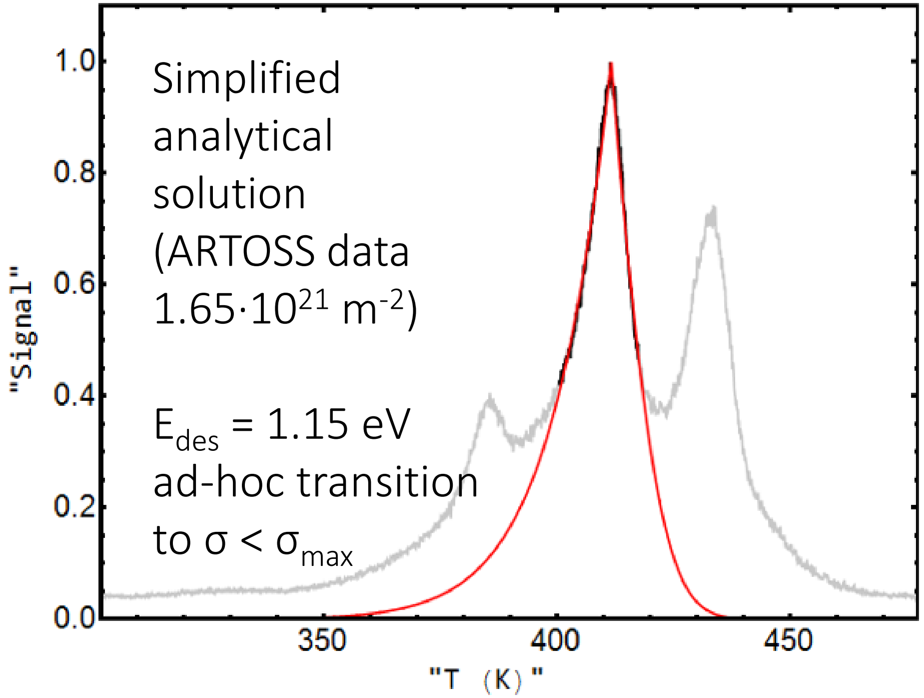


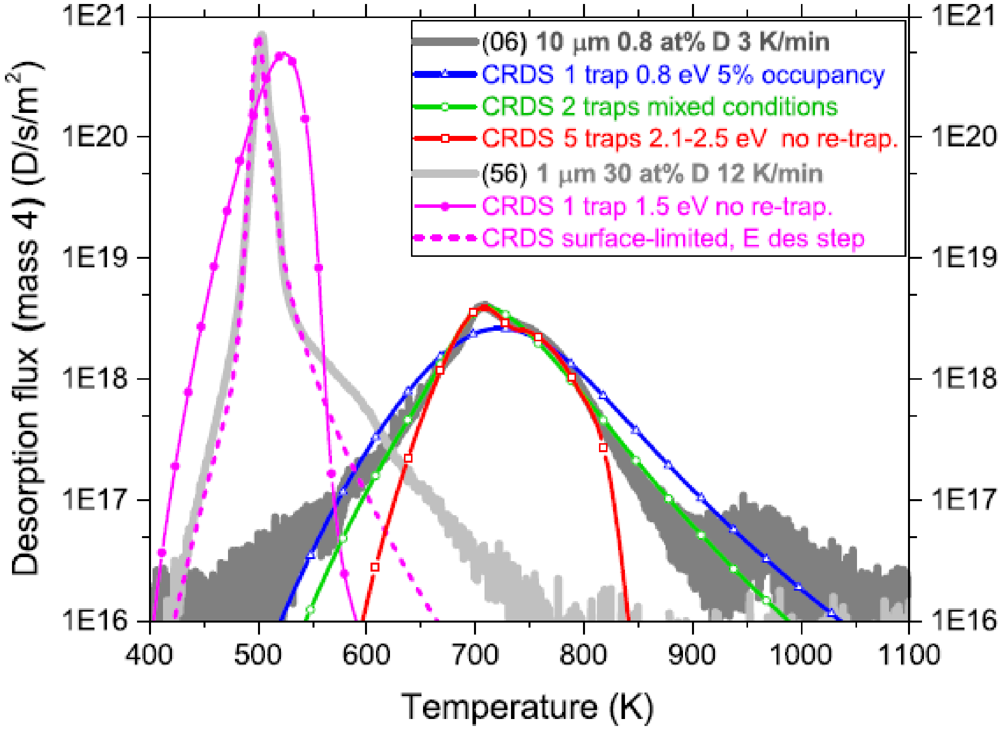


Models for the sharp low temperature desorption

2) Desorption-limited outgassing with saturated surface

D. Matveev Phys. Scr. (2020) 014053



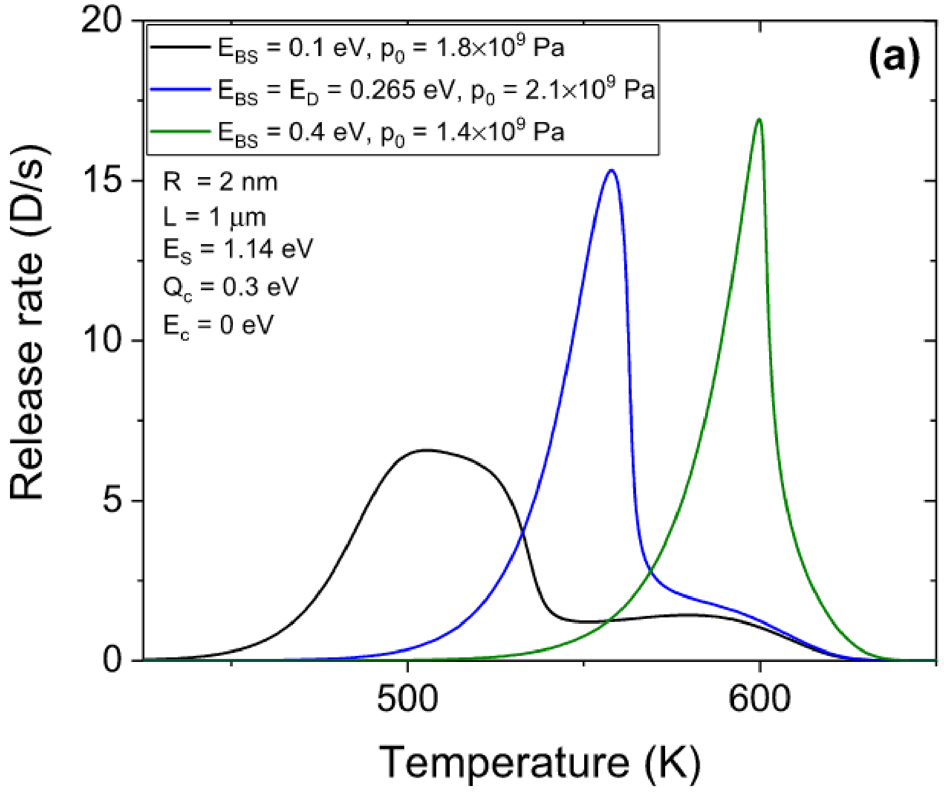


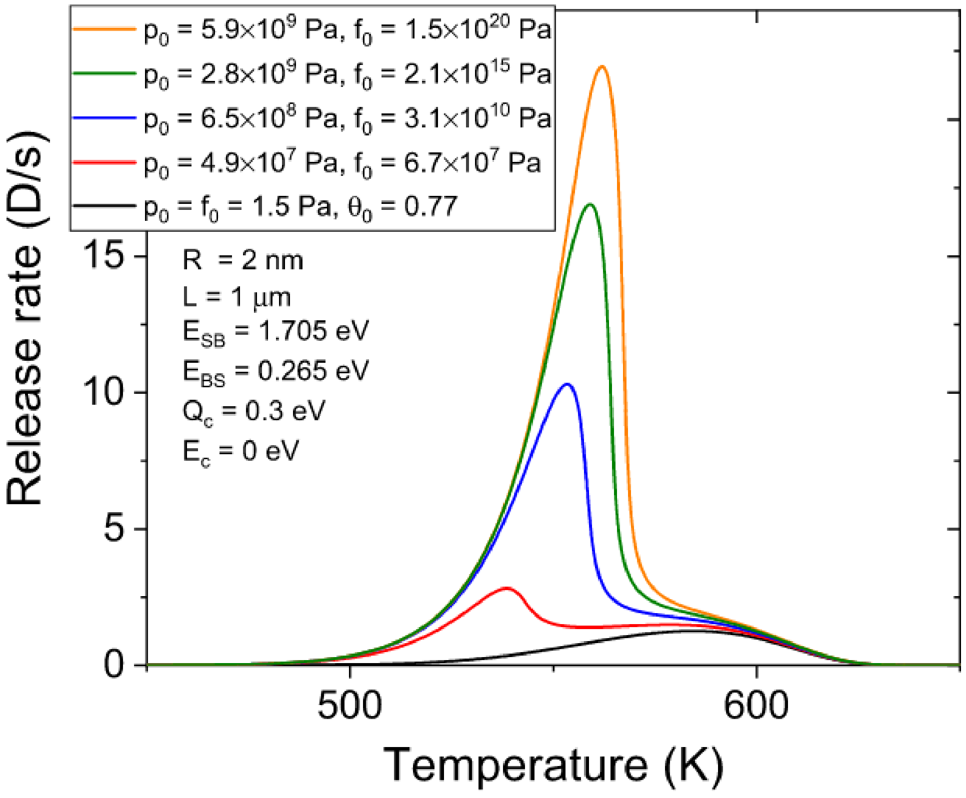
Desorption is limited by the surface and de-trapping and diffusion are assumed to be fast Surface is saturated up to the maximum capacity σ_{max}. Desorption follows the temperature dependence of the recombination coefficient until D influx from the bulk cannot keep $\sigma = \sigma_{max}$

Models for the sharp low temperature desorption

3) Release from gas-filled cavities (spherical voids)

M. Zibrov and K. Schmid, NME 30 (2022) 101121
NME 32 (2022) 101219



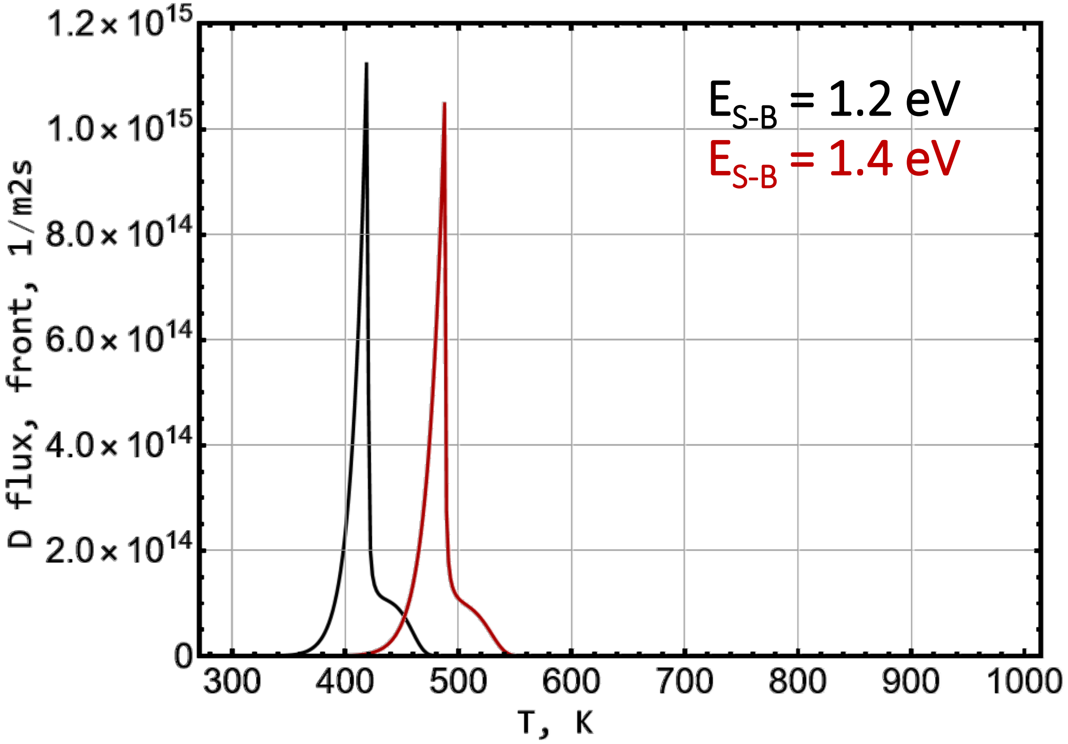


EOS for D_2 in the cavity at high pressure ($p \leq 10^{11}$ Pa): *J.-M. Joubert, Acta Mater. 59 (2011) 1680*

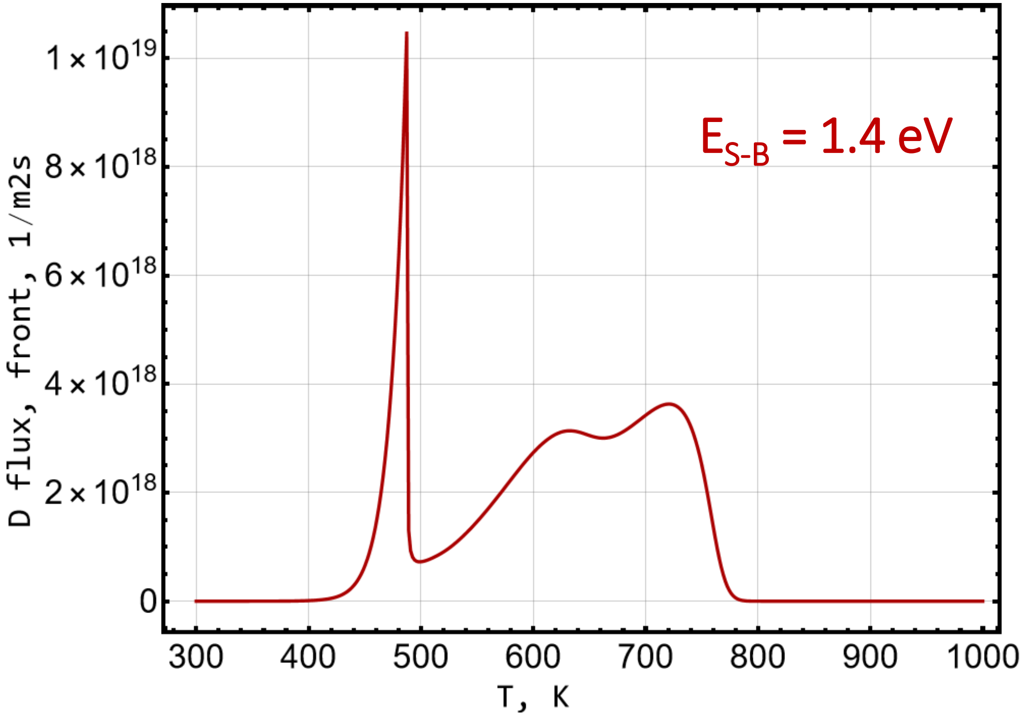
Models for the sharp low temperature desorption

Release from gas-filled cavities (spherical voids)

voids only 0.7 K/s

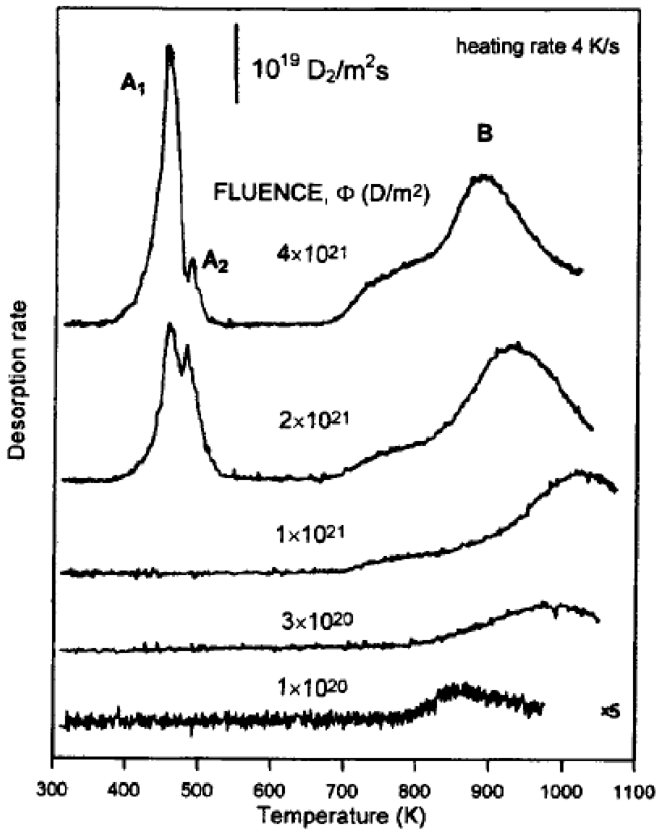


voids + vacancies 0.7 K/s

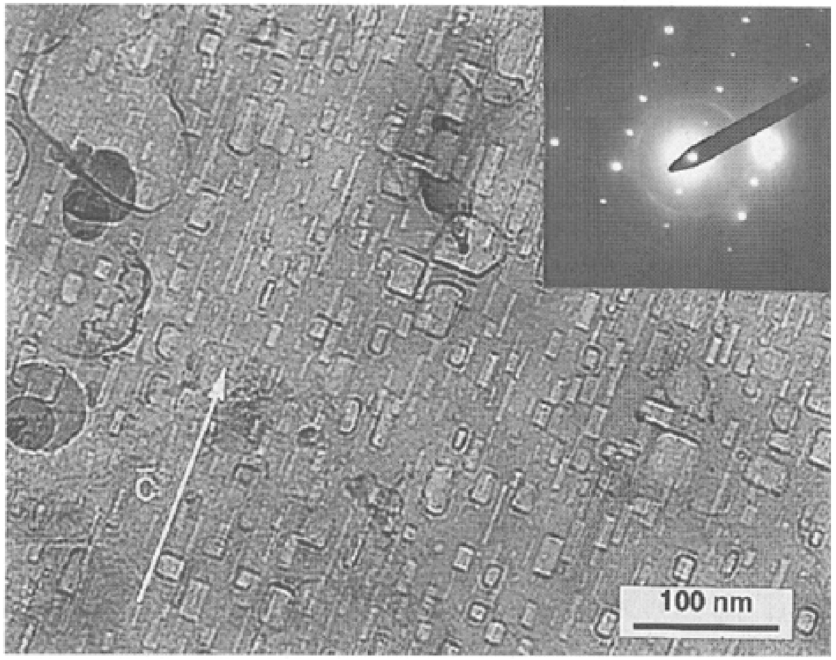


Models for the sharp low temperature desorption

Release from gas-filled cavities (spherical voids)



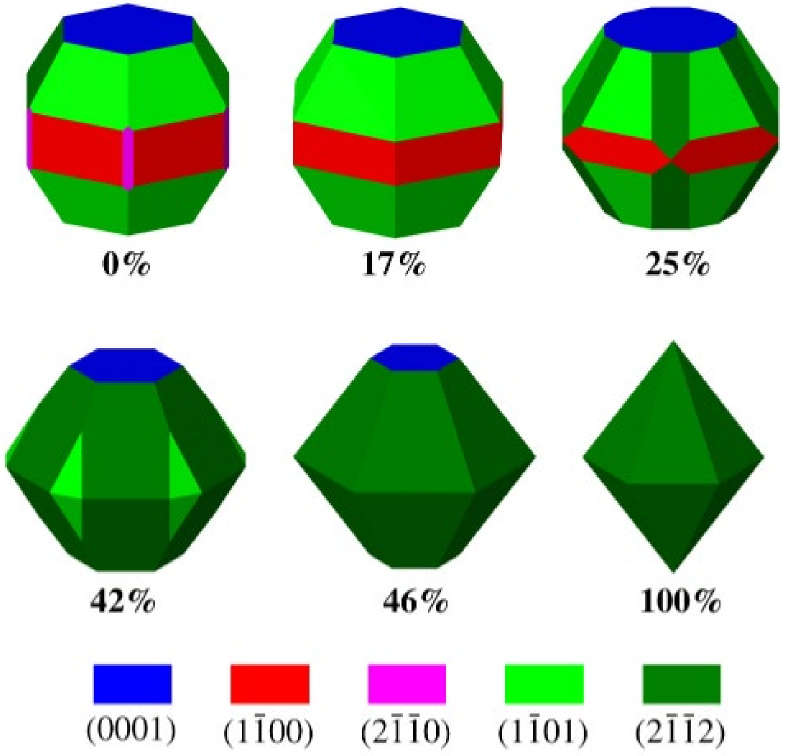
5 keV/D @ 300K | 4 K/s



10 keV/D @ 500K | $4x10^{21}$ D/m^2

Chernikov / Markin JNM 233-237 (1996) 860 / 865

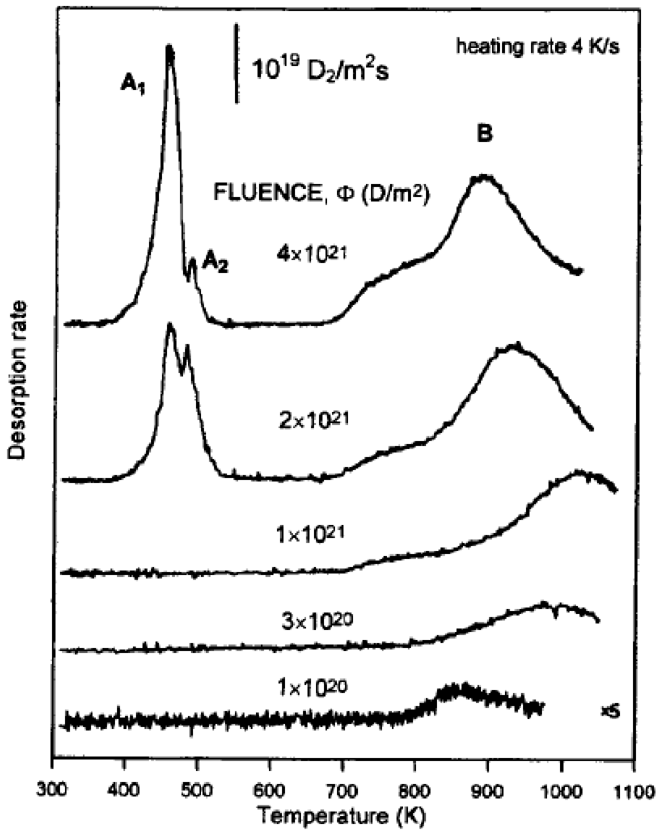
Equilibrium shape of void vs H coverage



Bachurin FED 109-111 (2016) 1432

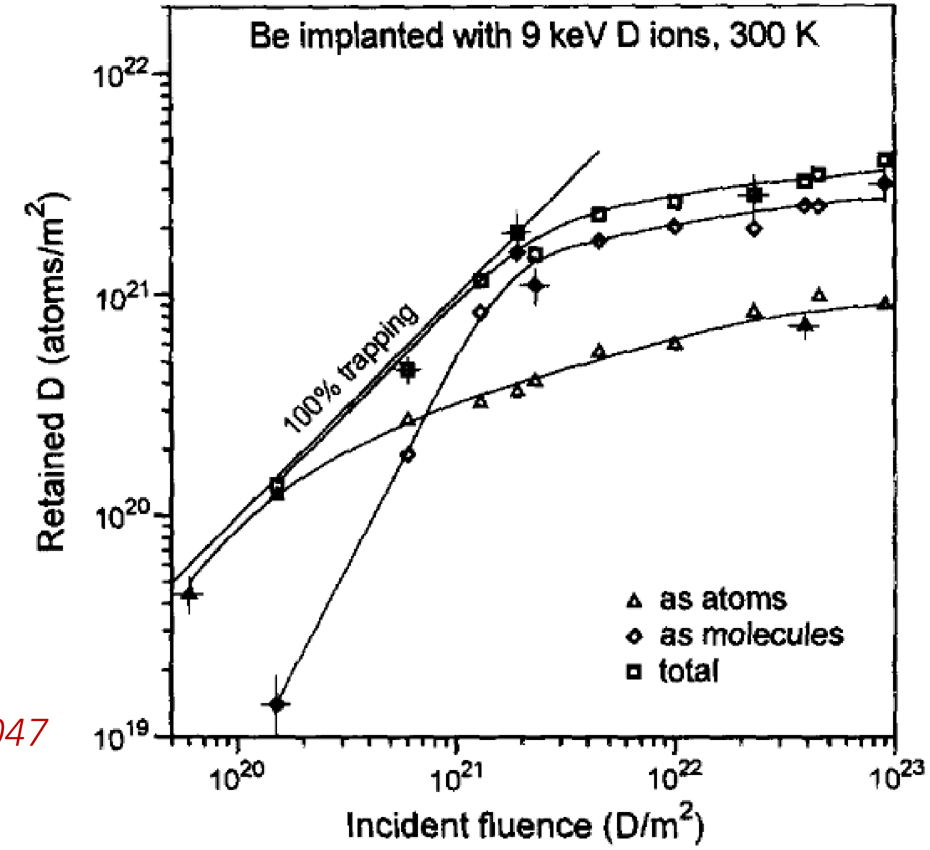
Models for the sharp low temperature desorption

Release from gas-filled cavities (spherical voids)



5 keV/D @ 300K | 4 K/s

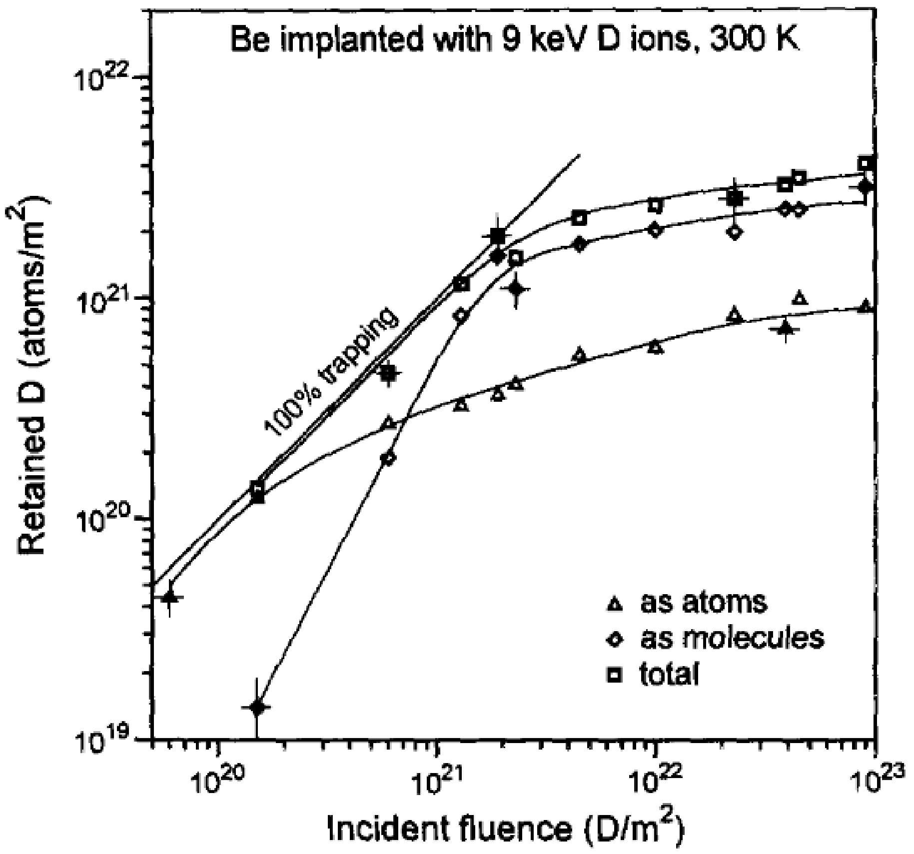
Markin JNM 233-237 (1996) 865



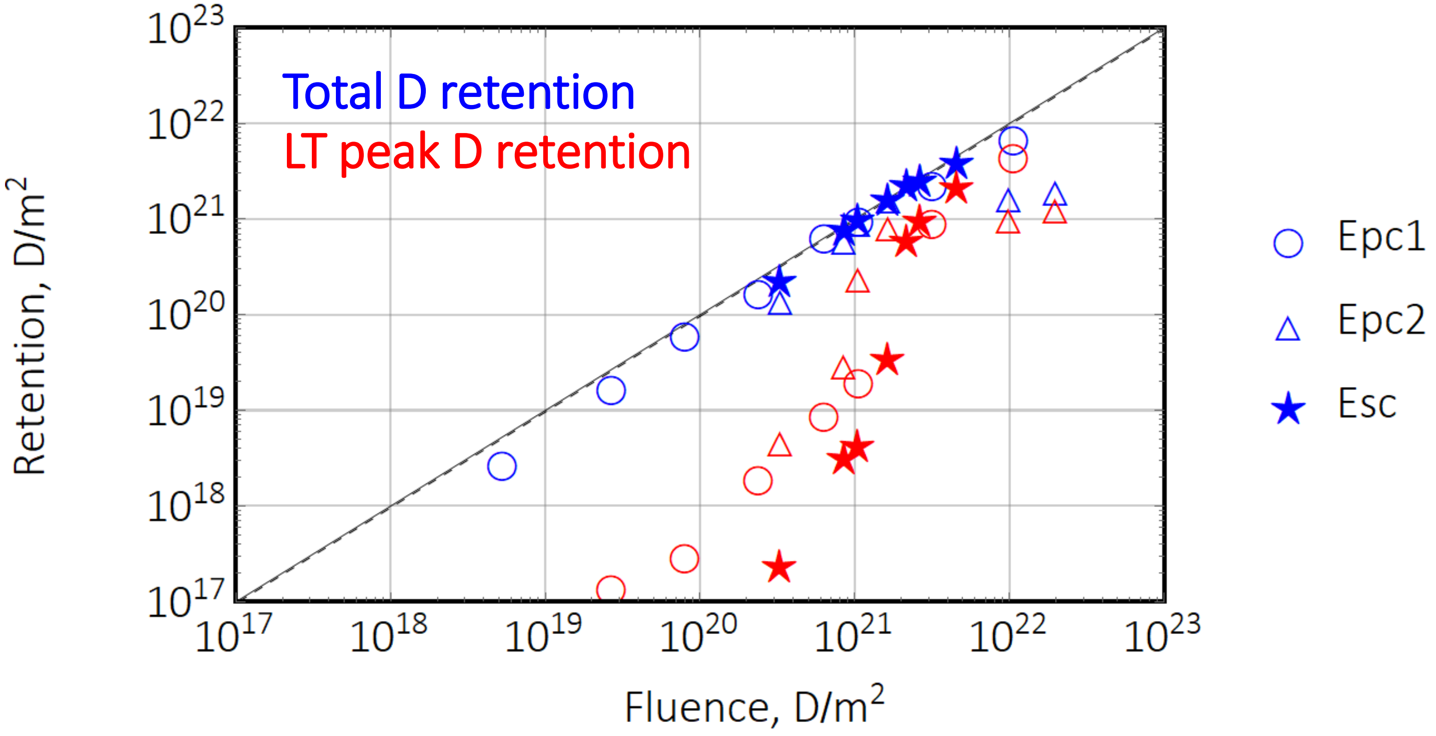
Alimov JNM 241-243 (1997) 1047

Experimental: Recent experiments in ARTOSS

Retention and release at different fluences ranging over ~3 orders of magnitude



Alimov JNM 241-243 (1997) 1047



M. Eichler, JNM 19 (2019) 440–444

Modelling: TDS phase

(CRDS – Coupled Reaction Diffusion Systems)

Matveev et al. NIMB 2018

$$\frac{\partial c}{\partial t}\bigg|_{\text{H}} = \text{Diffusion}\big|_{\text{H}} - \sum \text{Trapping}\big|_{\text{H}} + \sum \text{De-trapping}\big|_{\text{H}}$$

$$\frac{\partial c}{\partial t}\bigg|_{\text{V(0)}} = \text{Diffusion}\big|_{\text{V(0)}} - \text{Trapping}\big|_{\text{H(1)}} + \text{De-trapping}\big|_{\text{H(1)}}$$

$$\frac{\partial c}{\partial t}\bigg|_{\text{V(i)}} = \text{Trapping}\big|_{\text{H(i)}} - \text{De-trapping}\big|_{\text{H(i)}} - \text{Trapping}\big|_{\text{H(i+1)}} + \text{De-trapping}\big|_{\text{H(i+1)}}$$

$$\frac{\partial c}{\partial t}\bigg|_{\text{V(m)}} = \text{Trapping}\big|_{\text{H(m)}} - \text{De-trapping}\big|_{\text{H(m)}}$$

DFT data on diffusion and trapping: *L. Ferry, PhD Thesis (2017), CNRS / JNM 524 (2019) 323-329*

Modelling: implantation phase

(CRDS – Coupled Reaction Diffusion Systems)

D, V0 and SIA - Gaussian sources based on SDTrimSP

$$\frac{\partial c}{\partial t}\Big|_{\text{H}} = \text{Diffusion}\,|\,\text{H} - \sum \text{Trapping}\,|\,\text{H} + \sum \text{De-trapping}\,|\,\text{H} + \text{Source}\,|\,\text{H} + \sum \text{Annihilation}\,|\,\text{V(i)}$$

$$\frac{\partial c}{\partial t}\Big|_{\text{SIA}} = \text{Diffusion}\,|\,\text{SIA} + \text{Source}\,|\,\text{SIA} - \sum \text{Annihilation}\,|\,\text{V(i)}$$

$$\frac{\partial c}{\partial t}\Big|_{\text{V(0)}} = \text{Diffusion}\,|\,\text{V(0)} - \text{Trapping}\,|\,\text{H(1)} + \text{De-trapping}\,|\,\text{H(1)} + \text{Source}\,|\,\text{V0} - \text{Annihilation}\,|\,\text{V(0)}$$

$$\frac{\partial c}{\partial t}\Big|_{\text{V(i)}} = \text{Trapping}\,|\,\text{H(i)} - \text{De-trapping}\,|\,\text{H(i)} - \text{Trapping}\,|\,\text{H(i+1)} + \text{De-trapping}\,|\,\text{H(i+1)} - \text{Annihilation}\,|\,\text{V(i)}$$

$$\frac{\partial c}{\partial t}\Big|_{\text{V(m)}} = \text{Trapping}\,|\,\text{H(m)} - \text{De-trapping}\,|\,\text{H(m)} - \text{Annihilation}\,|\,\text{V(m)}$$

DFT data on diffusion and trapping: *L. Ferry, PhD Thesis (2017), CNRS / JNM 524 (2019) 323-329*

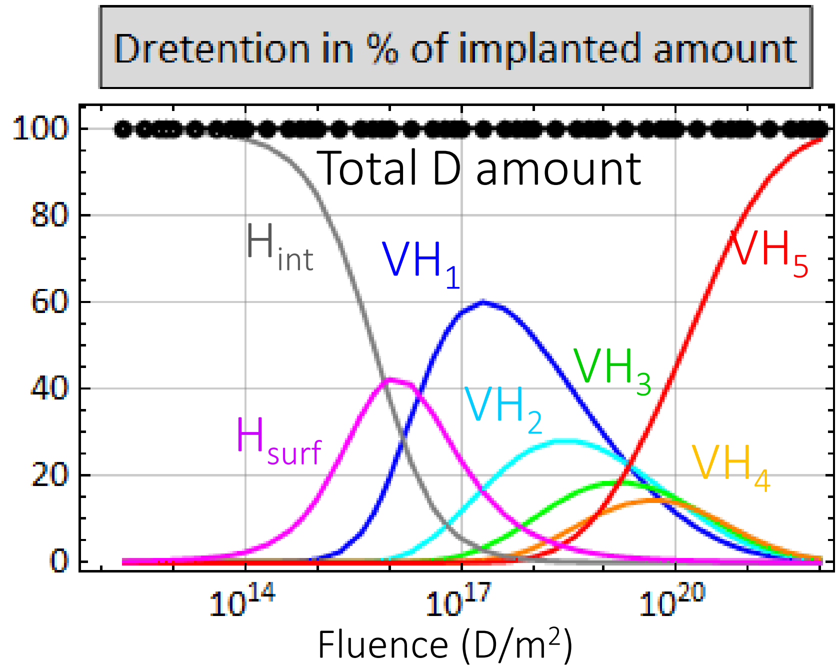
Role of V / VH_j + SIA annihilation

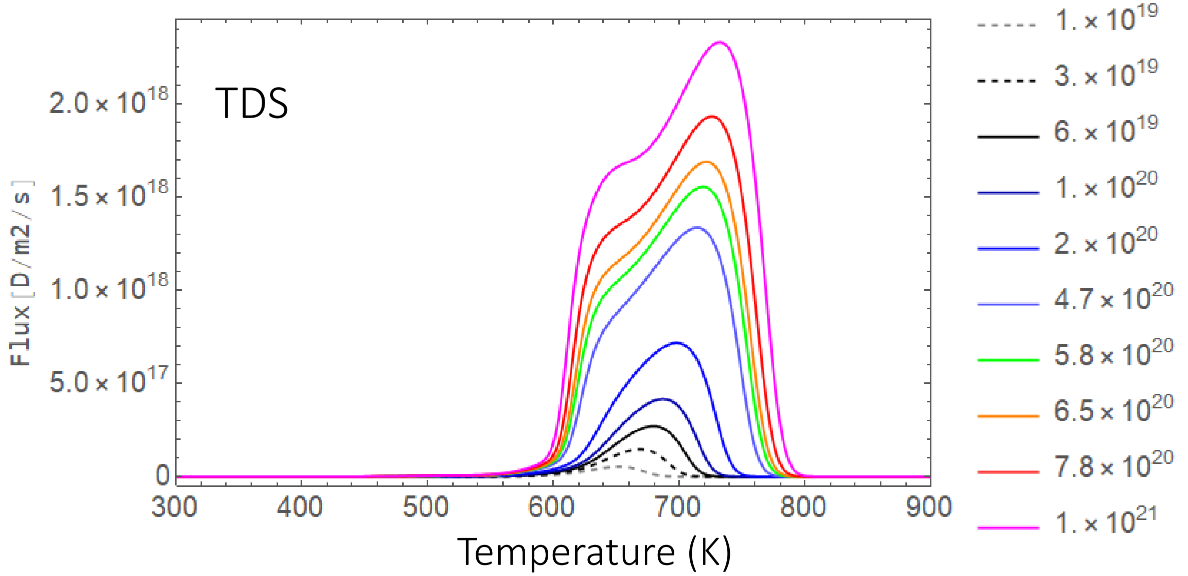
D, V and SIA - Gaussian sources based on SDTrimSP
SIA are very mobile, V are fixed (even empty V)

D is allowed to accumulate on the surface with effective surface area x100 the nominal area

With SIA + V(0) only recombination

- SIA + VH_j annihilation not permitted
- Surface remains empty – enough V to accommodate all implanted D
- V are created up to unphysical concentrations
- No saturation of high temperature TDS peak
- Contradicts experimental observations





Modelling: implantation phase

(CRDS – Coupled Reaction Diffusion Systems)

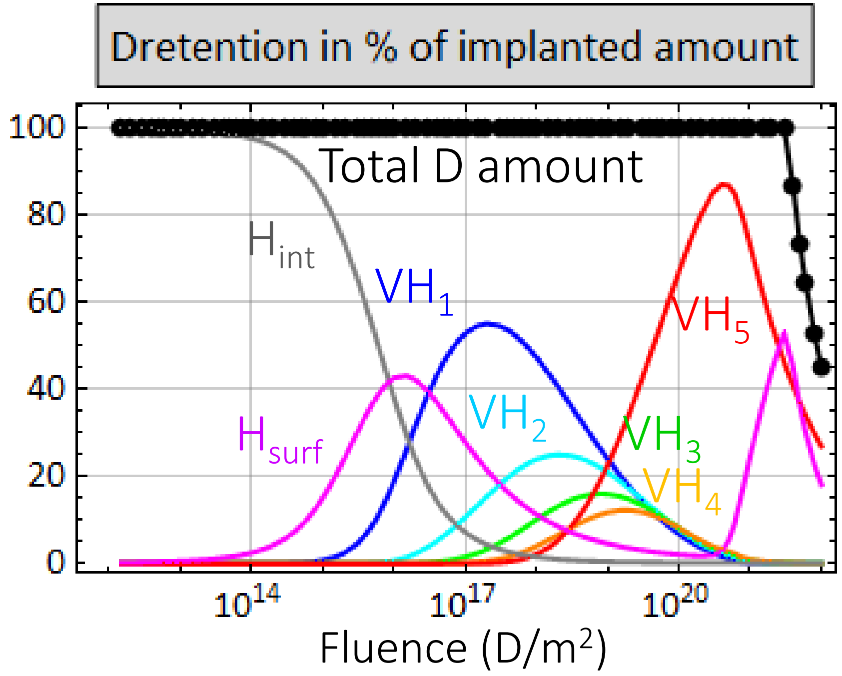
Role of V / VH_j + SIA annihilation

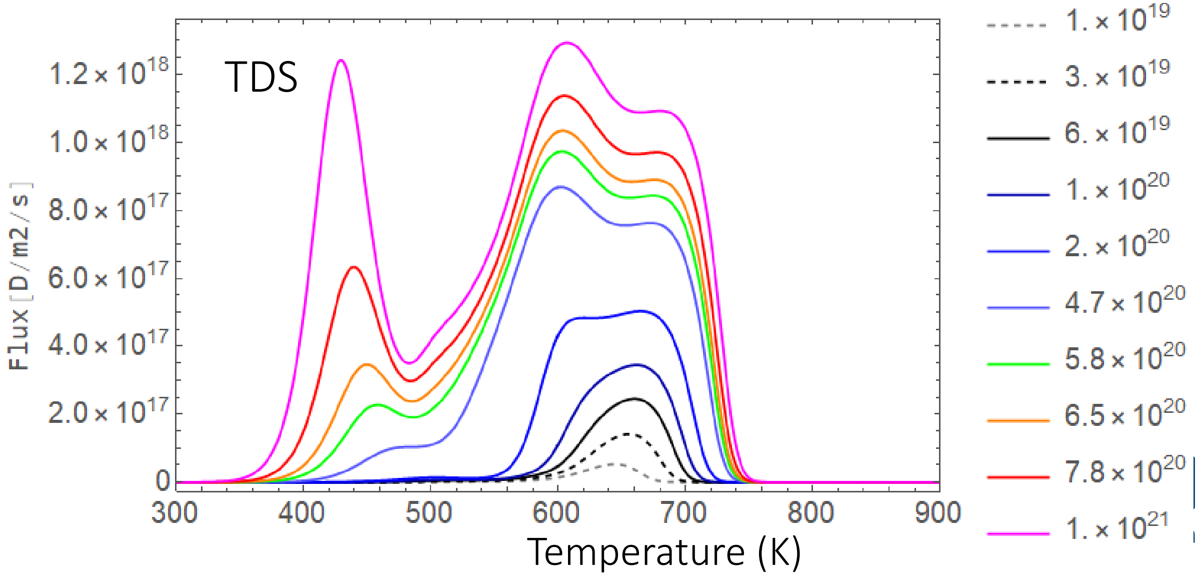
D, V and SIA - Gaussian sources based on SDTrimSP
SIA are very mobile, V are fixed (even empty V)

D is allowed to accumulate on the surface with effective surface area x100 the nominal area

With SIA + all VH_j recombination → suggestion from *DFT-NEB by Y. Ferro*

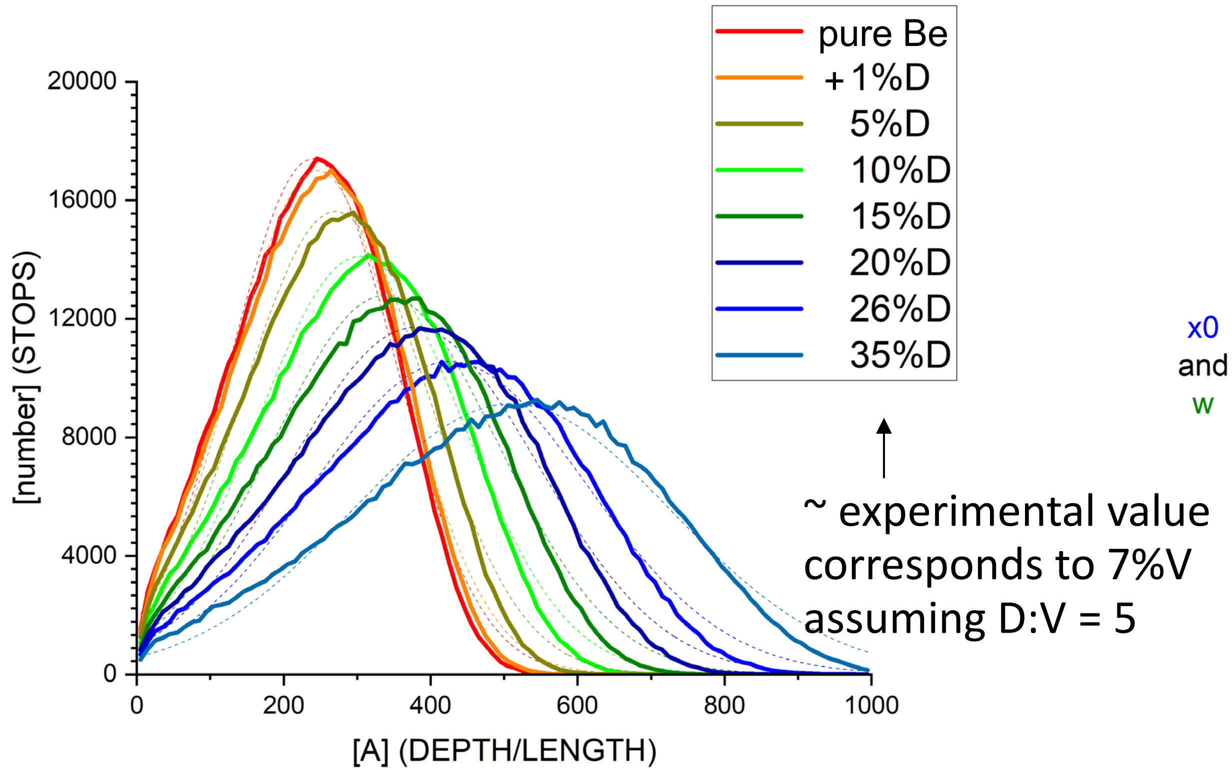
- Vacancy survival continuously
- Still no complete saturation of HT peak
- Other effects (V clustering?) must be at play
- Surface population from about 10^{21} D/m^2
- Better agreement with experiment
- Indirect confirmation of DFT results:
  SIA + VH_j recombine w/o energy barrier

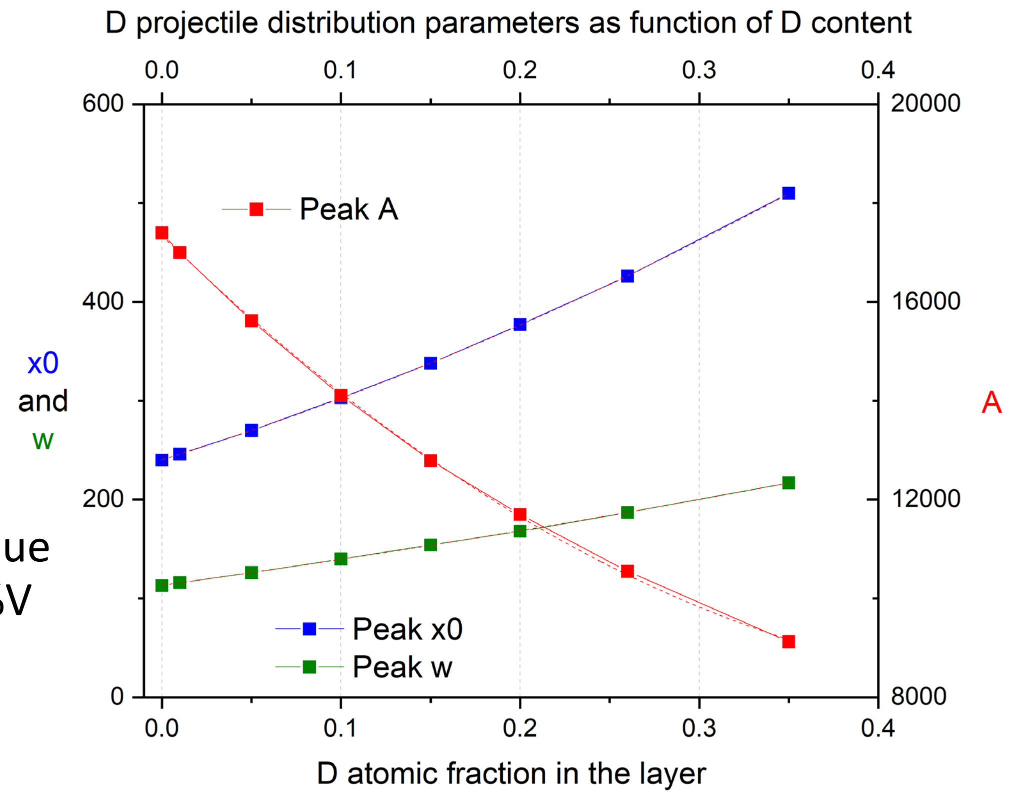




Additional effects

1) Consider increase of D penetration depth and V creation depth with D content in the surface (SDTrimSP)

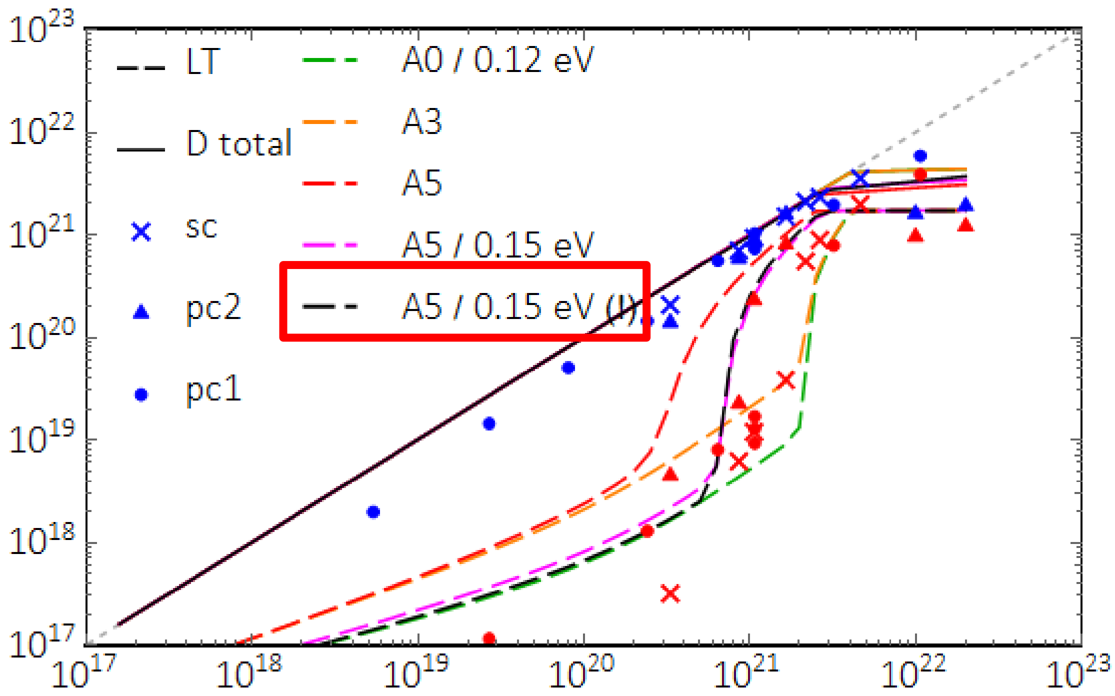




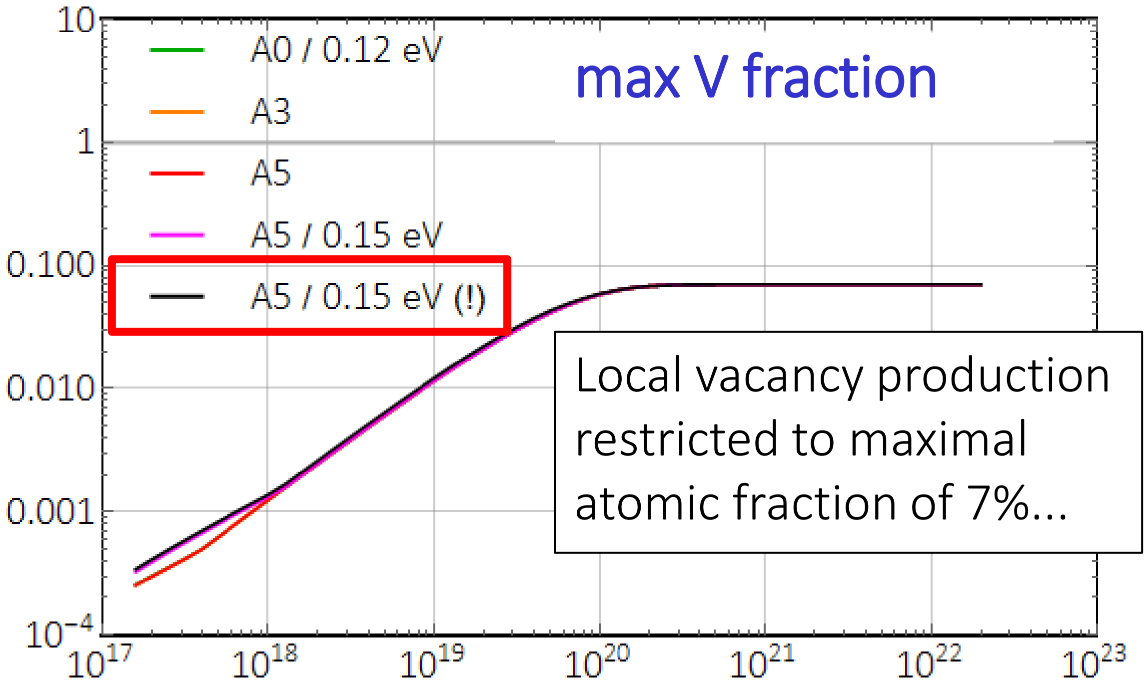
2) Consider imposed maximal V fraction such that locally no V can be created (for 7%V → 35%D ~ experiment)

Comparison to experiment

Retention, D/m²



Fluence, D/m²



Fluence, D/m²

the case with varying depth profiles for source terms

Conclusions

- The reaction-diffusion model implementation was used to model vacancy dynamics during D implantation accounting for multiple trapping, kinetic de-trapping and variable source profiles
- Qualitative description of reduction of the net vacancy production rate with implanted fluence
- V and trapped D concentrations exceed the values of several at.% for fluences above 10^{21} m^{-2}. At such concentrations bulk material properties of Be and hydrogen transport and retention parameters (from DFT) probably no longer hold. Formation of vacancy clusters can be expected. This fluence range nicely corresponds to emergence of low temperature release in experiment.
- Low temperature release stage with multiple sharp peaks can potentially be attributed to release from gas-filled cavities of different sizes with faceted surfaces

Thank you for your attention