Spectroscopic investigations on energy, angular and atomic level distribution functions of sputtered tungsten

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EUROfusion

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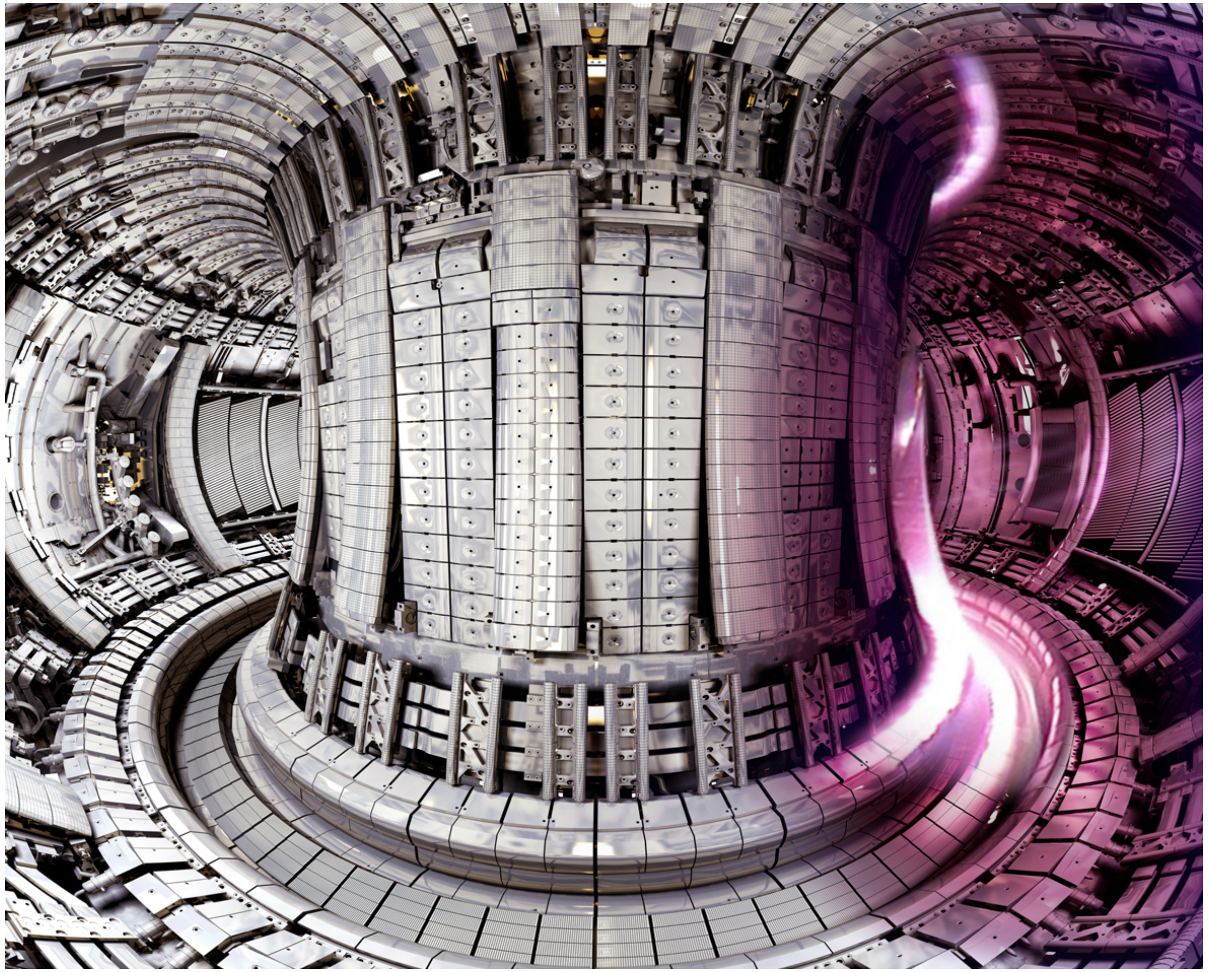
MOTIVATION

- Tungsten (W) proposed as PFM in divertor (ITER, DEMO) and main chamber (DEMO)
- Lifetime of PFM determined by sputtering
- Erosion of W leads to cooling of plasma and needs to be monitored
- Spectroscopy as tool to monitor W gross erosion

→ Understanding of the atomic data and the ongoing processes is essential

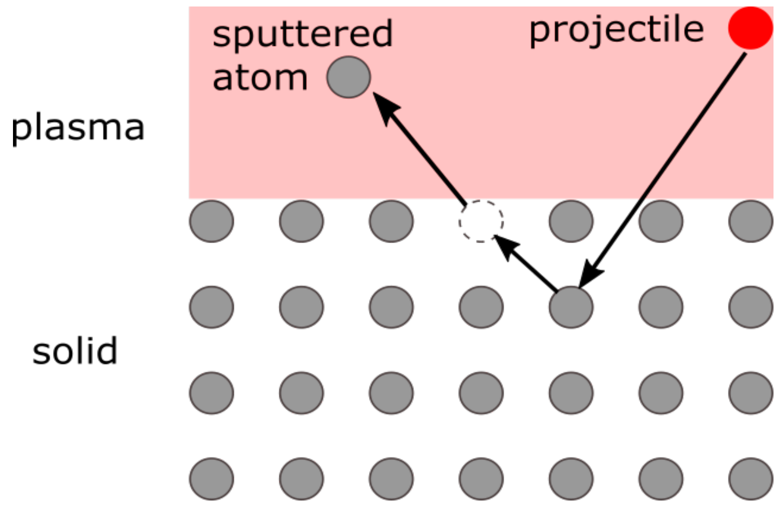


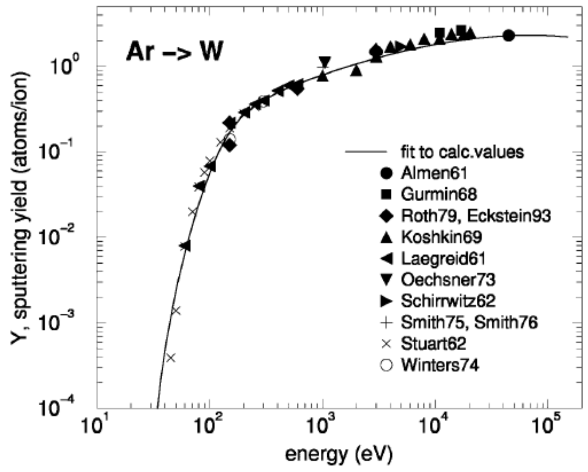
[1] www.euro-fusion.org/devices/jet/

MOTIVATION

Physical sputtering

- Occurs at solid surfaces at plasma boundary
- Depends on impact energy and incident angle of incoming particles
- Sputtering at high impact energies well understood
- In fusion research impact energy in the range of 100 eV
- **Energy and angular distribution of sputtered atoms remains open question**
- **Sputtering in ground and/or excited level**



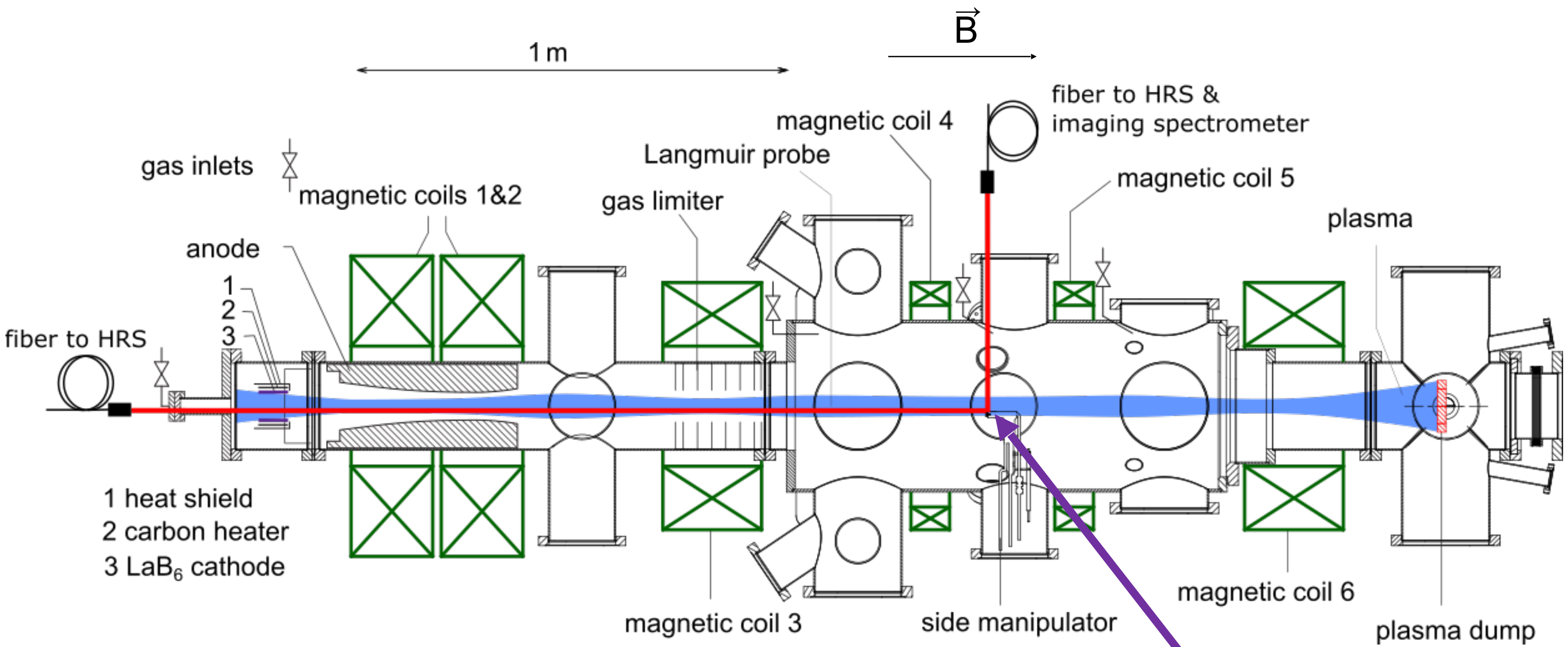


[2]

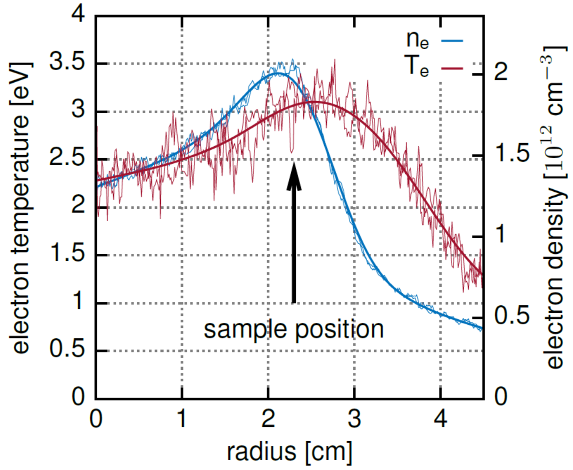
[2] R. Behrisch and W. Eckstein "Sputtering by Particle Bombardment", Springer-Verlag (2007)

MOTIVATION

Experimental facility PSI-2



conditions	argon plasma
T_e	≈ 3 eV
n_e	≈ $1 \cdot 10^{12}$ cm^{-3}
E_{imp}	Up to 150 eV
B	92 mT
T_{surf}	300 K



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OUTLINE

I. Line shape of sputtered atoms

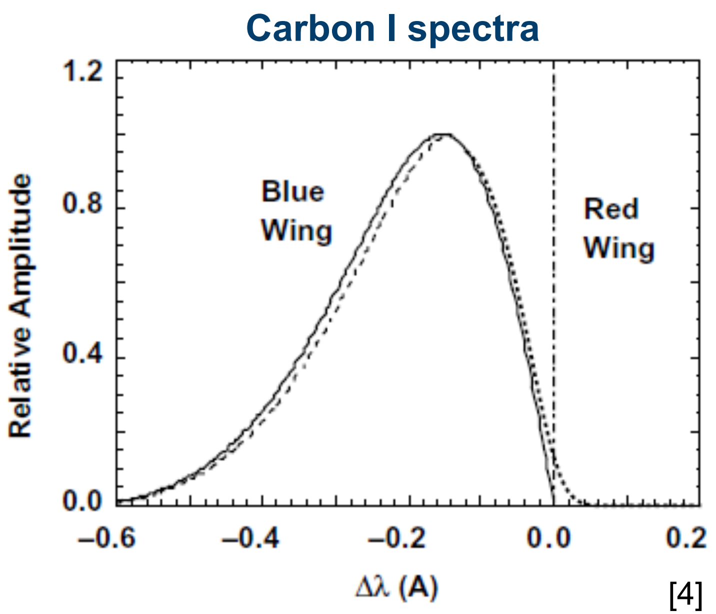
II. Atomic level population of sputtered tungsten

I. LINE SHAPE OF SPUTTERED ATOMS

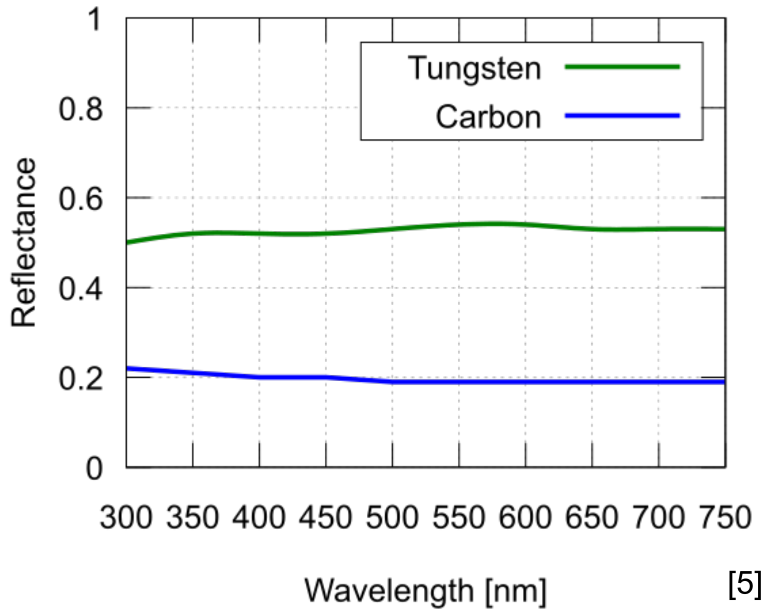
I. LINE SHAPE OF SPUTTERED ATOMS

Motivation

- Knowledge of absolute intensity I_{tot} is essential to determine the gross erosion
- Light reflection impacts the measured intensity values and line shape
- Light reflection in a carbon machine was investigated in [4], research on reflection of metallic walls (W) is needed



[4]



[5]

[4] N.H. Brooks et al. 2005 J. Nucl. Mater. 227–231
[5] refractiveindex.info for W: Werner et al. 2009 DFT calculations; for C : Larruquert et al. 2013

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I. LINE SHAPE OF SPUTTERED ATOMS

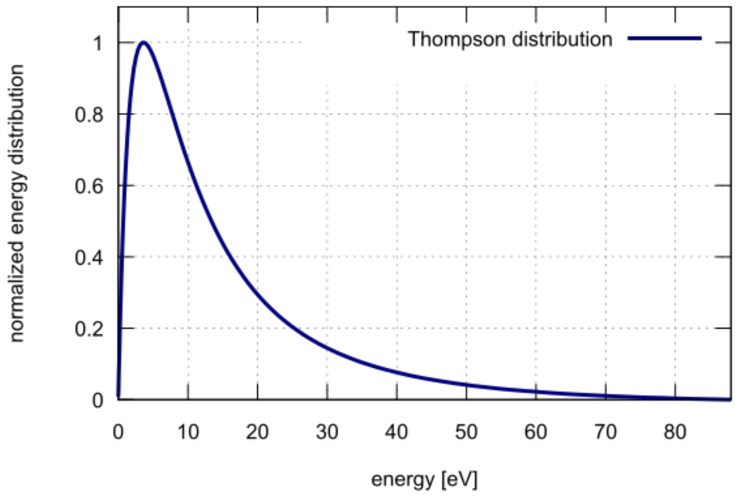
Motivation: Energy and angular distribution of sputtered atoms

<u>High ion impact energy [6]:</u>

Thompson energy distribution $F(E)$ [7]:

$$F(E) = \frac{E}{(E+E_\mathrm{b})^{n+1}}\left(1-\sqrt{\frac{E}{E_\mathrm{max}}}\right)$$

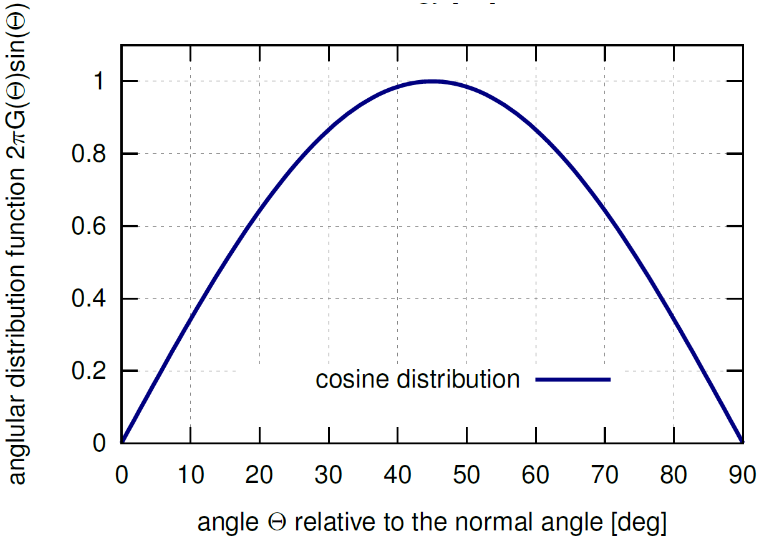
$$\begin{aligned} E &= \text{Energy of sputtered atoms,}\\ E_\mathrm{b} &= \text{surface binding energy,}\\ E_\mathrm{max} &= \text{ maximum energy of sputtered atoms,}\\ n &= 2 \text{ (scaling parameter).}\end{aligned}$$



Cosine angular distribution $G(\Theta)$:

$$G(\Theta) \propto \cos^b(\Theta)$$

$$\begin{aligned} \Theta &= \text{polar angle,}\\ b &= 1 \text{ (scaling parameter).}\end{aligned}$$



<u>Low ion impact energy:</u>

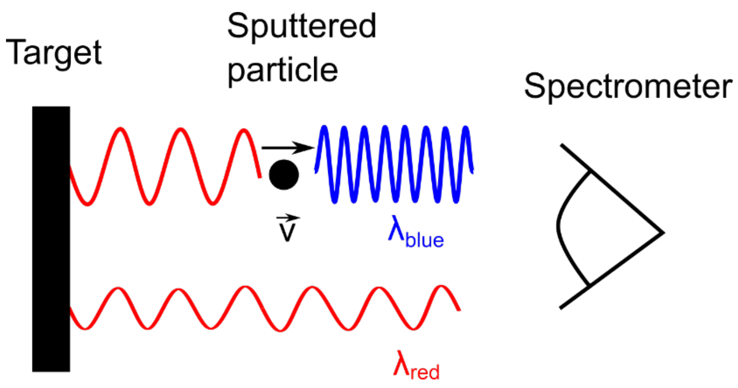
Deviations from Thompson energy (n>2) and cosine angular (heart shape) distribution are reported

[6] R. Behrisch and W. Eckstein "Sputtering by Particle Bombardment", Springer-Verlag, 2007
[7] M W Thompson 1968 Phil. Mag. 18 377–414

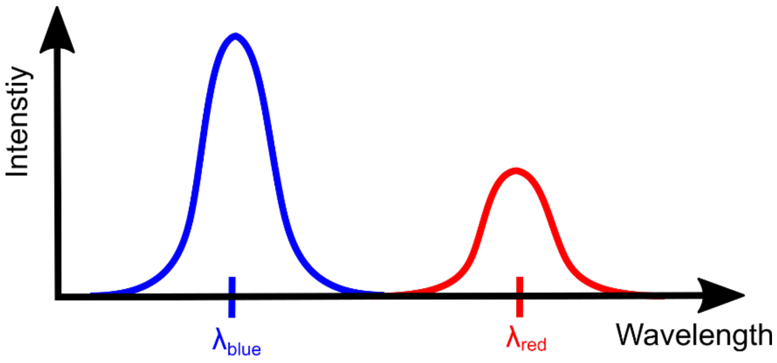
I. LINE SHAPE OF SPUTTERED ATOMS

Method

Doppler effect



Obtained spectra

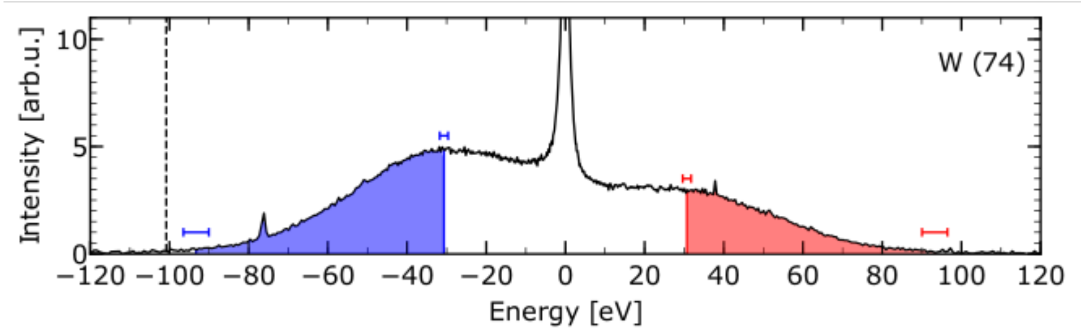


Doppler shift:

$$\lambda = \lambda_0 \sqrt{\frac{c-v}{c+v}}$$

$\lambda =$ detected wavelength,
$\lambda_0 =$ emitted wavelength,
$c =$ speed of light,
$v =$ particle velocity.

Effect has been observed for fast H atoms in PSI-2 [8]



[8] S. Dickheuer et al. 2018 Rev. Sci. Instrum. **89** 063112

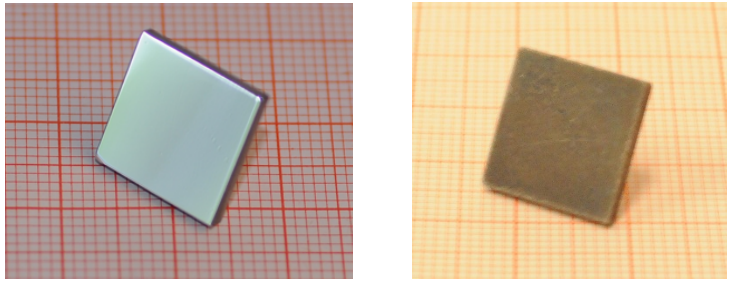
I. LINE SHAPE OF SPUTTERED ATOMS

Experimental results

- Stronger line shape deformation for Al than for W (proof of principle)

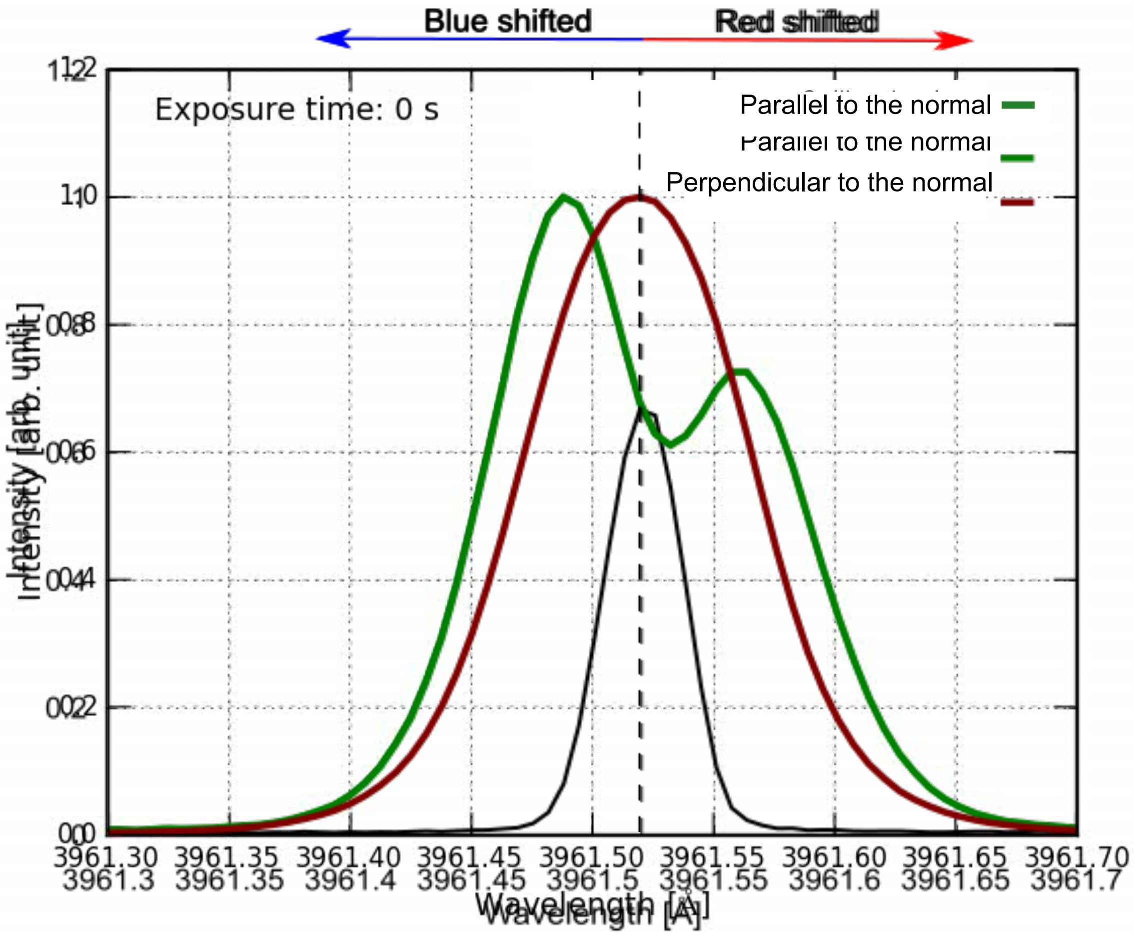
$$\frac{\Delta\lambda}{\lambda} \propto \sqrt{\frac{2E_{kin}}{m}}$$

- Only explanation is light reflection
- Erosion of surface leads to decrease in reflection



Al-target before and after exposure

Al-target in argon plasma $E_{impact} \approx 110$ eV



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I. LINE SHAPE OF SPUTTERED ATOMS

Model

<u>Doppler-shifted emission model based on [9]:</u>

- Point source approximation
- Cosine angular distribution $G(\Theta) \propto \cos^b(\Theta)$
- Light reflection at the surface

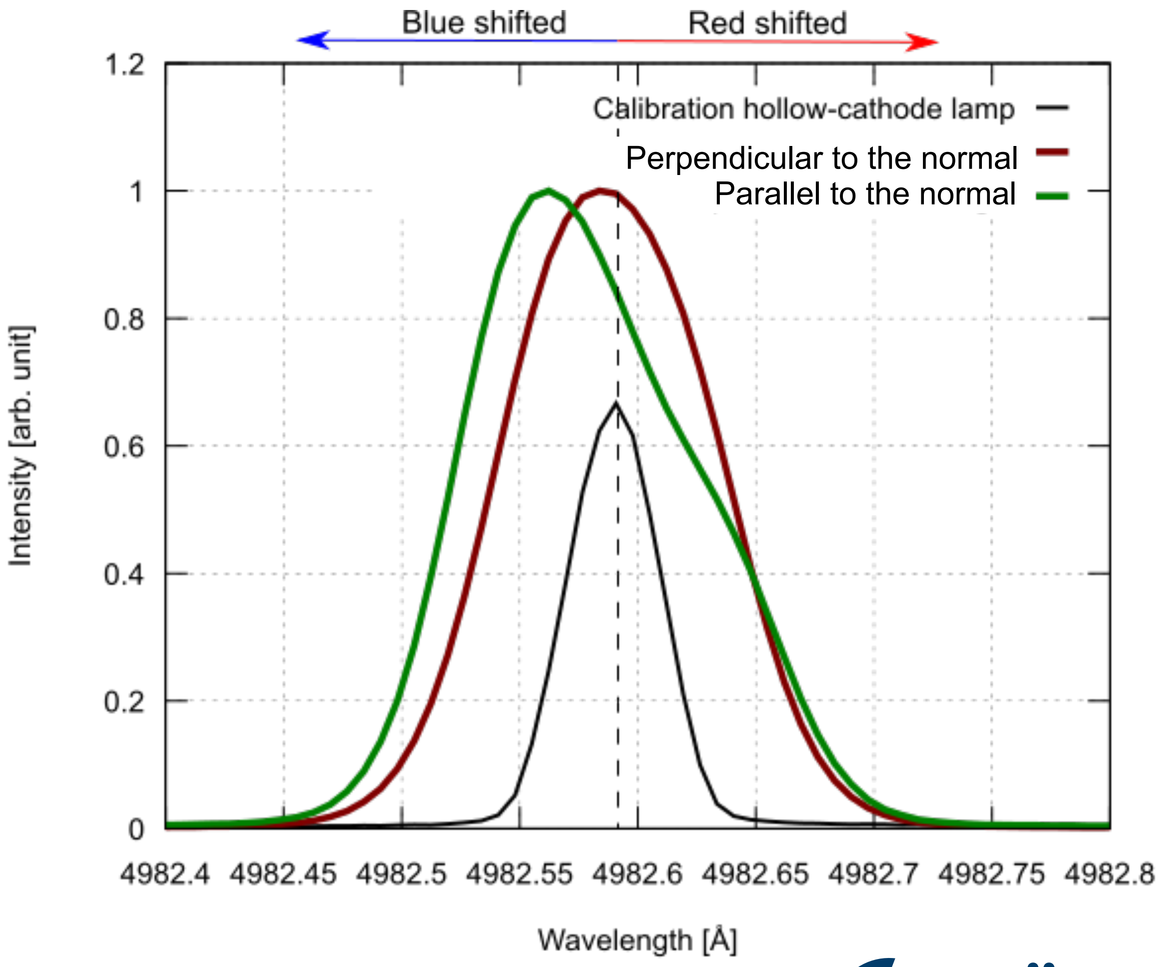
<u>Adapted:</u>

- Energy distribution = Thompson energy distribution

<u>Expanded:</u>

- Zeeman-effect
- Instrumental broadening

W-target in argon plasma $E_{impact} \approx 110eV$



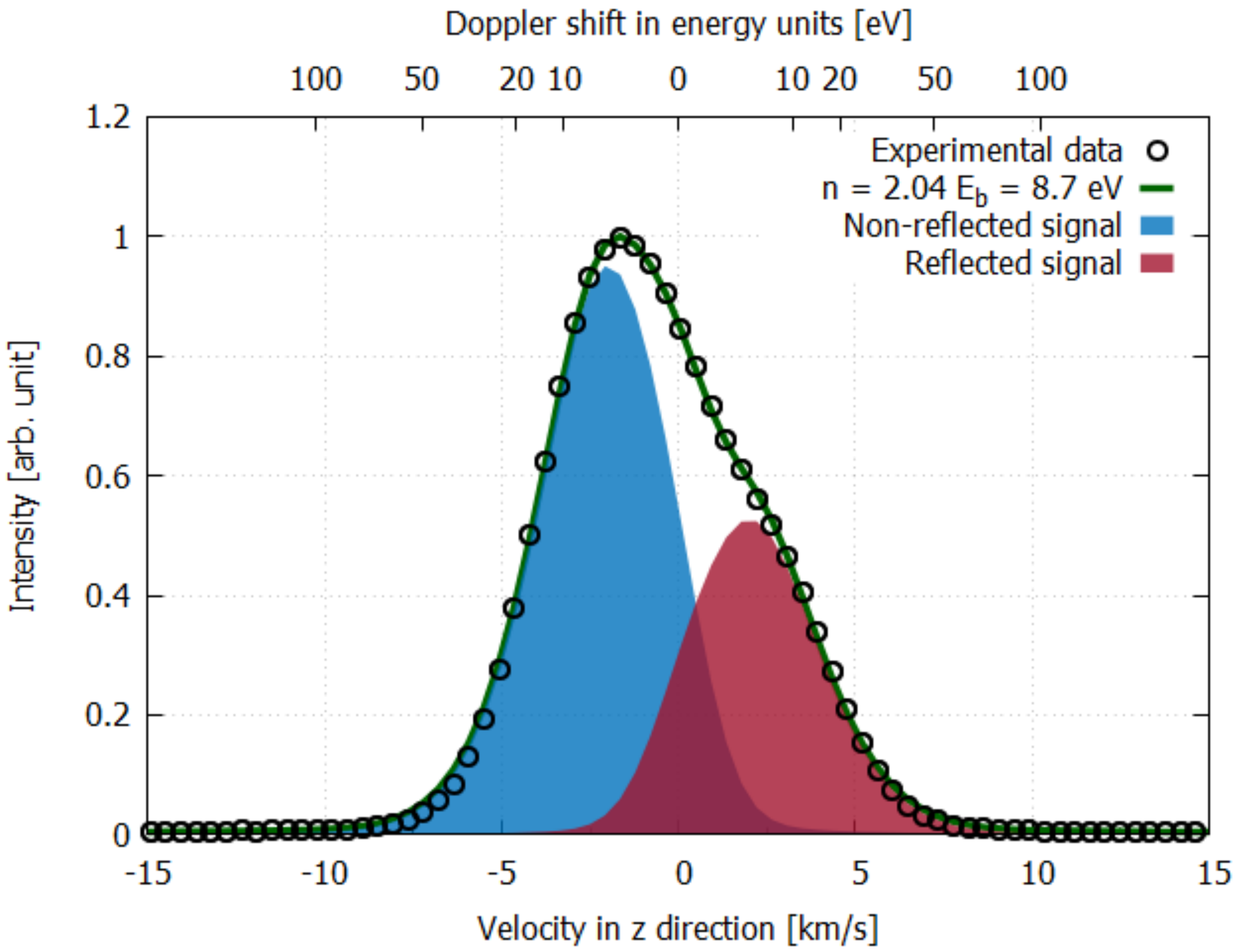
[9] S. Dickheuer et. al Physics of Plasmas **26**, 073513 (2019)

I. LINE SHAPE OF SPUTTERED ATOMS

Results

Findings for Ar ions at 110 eV according to cosine distribution $(b = 1)$:

Reflection = 55% (Literature = 53% [5])
Thompson energy distribution:
n = 2.04; E_b= 8.7 eV [6]



[5] W. S. M. Werner et al. J. Phys Chem Ref. Data 38, (2009) 1013-1092
[7] R. Behrisch and W. Eckstein "Sputtering by Particle Bombardment", Springer-Verlag, 2007

I. LINE SHAPE OF SPUTTERED ATOMS

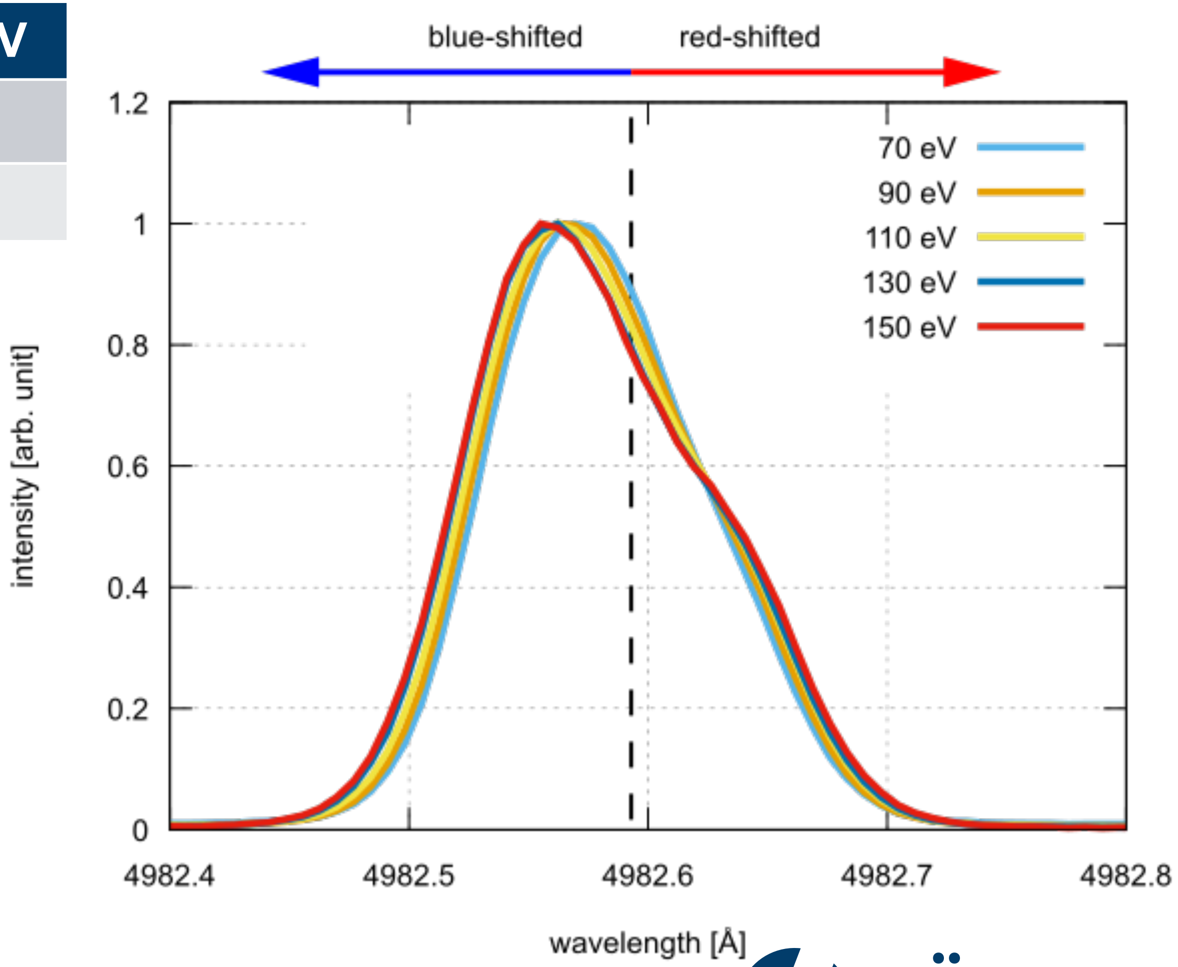
Results

Impact energy	70 eV	90 eV	110 eV	130 eV	150 eV
n	2.17	2.12	2.04	2.00	1.99
Reflection [%]	54	53	54	55	55

- Good agreement using Thompson energy and cosine angular distribution
→ Same as for high impact energies

- Good agreement for literature values of reflection ≈ 53% [5]

W-target in argon plasma: Variation of impact energy



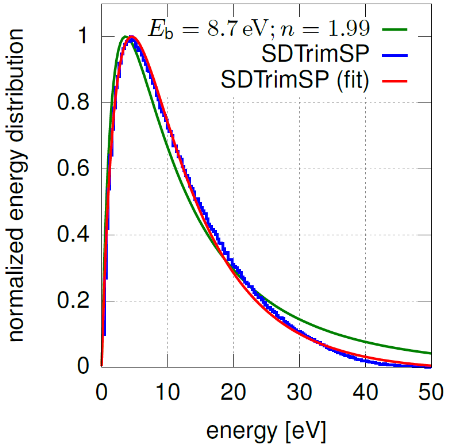
[5] W. S. M. Werner et al. J. Phys Chem Ref. Data 38, (2009) 1013-1092

I. LINE SHAPE OF SPUTTERED ATOMS

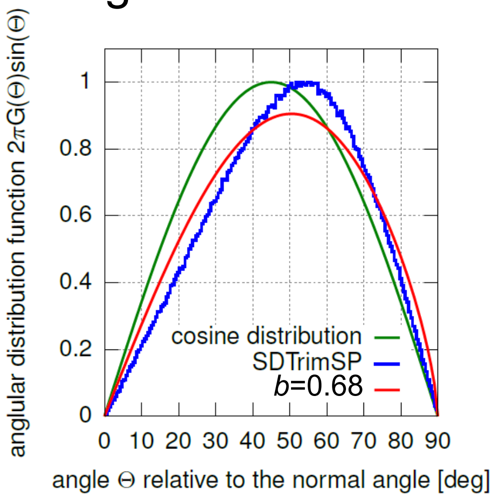
Results

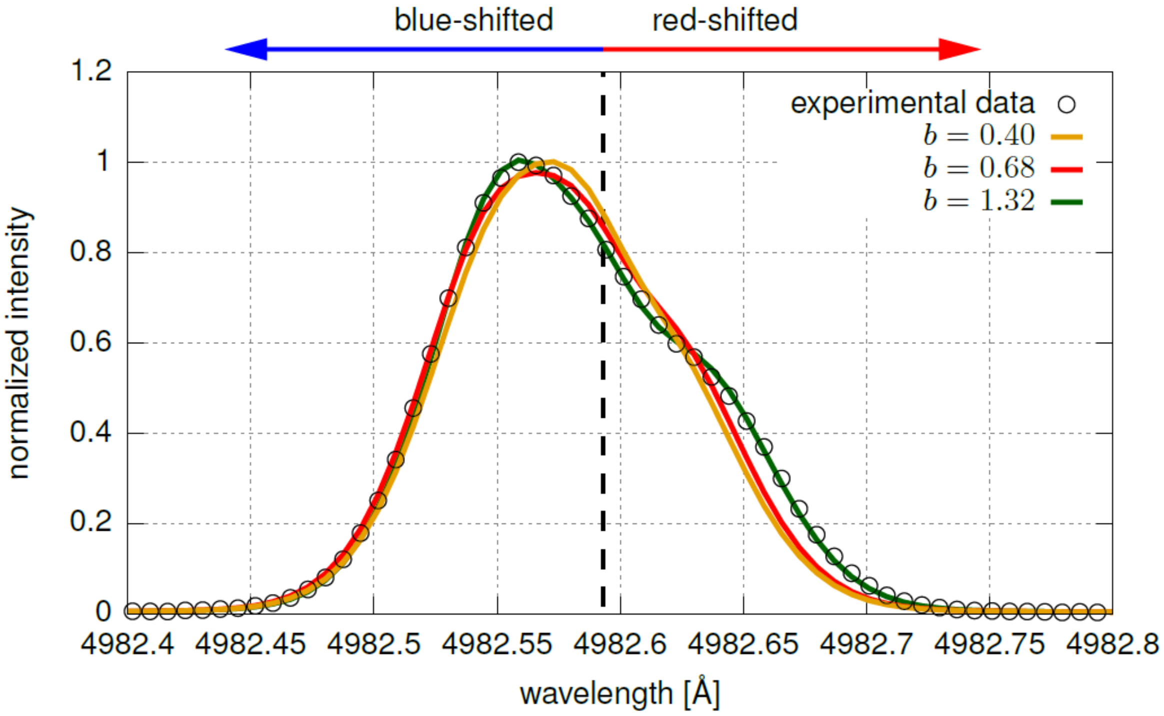
SDTrimSP simulations [10] for Ar ions at $E_{\mathrm{imp}} = 150\,\mathrm{eV}$

Energy distribution



Angular distribution





Energy distribution of SDTrimSP:
good agreement only for over-cosine (b>1) in angular distribution

Especially for high energetic part of the spectrum

[10] A. Mutzke et al. IPP-Report 2019-02, (2019)

I. LINE SHAPE OF SPUTTERED ATOMS

Summary

- Proof of light reflection in the line shape of sputtered atoms
- In-situ light reflection measurements by modeling
- Energy distribution modeled from line shape
- Good agreement for Thompson energy and cosine angular distribution
- SDTrimSP energy distribution only good agreement for over-cosine

Outlook

- Expand model to 2D source for angular and energy distribution modeling
- Benchmark angular distribution with spatial intensity development
- Investigation of impact of surface morphology on angular and energy distribution

II. Atomic level population of sputtered tungsten

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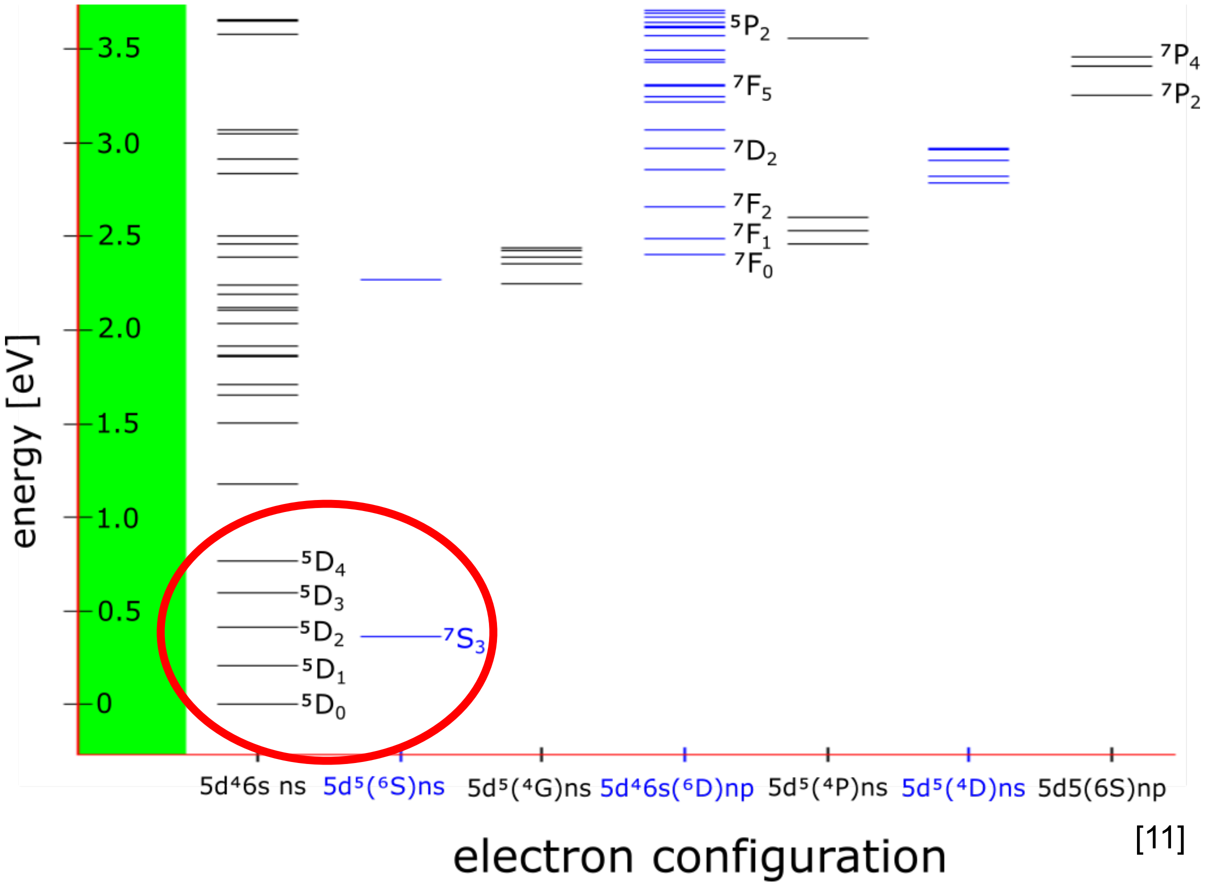
Motivation

- **Initial atomic energy level population distribution of sputtered W is unknown**
  - important for analysis of spectroscopic data
  - not well understood
    - TEXTOR experiments:
      population according to effective temperature T_W
      led to unphysical electron temperature T_e (1 eV) [12]
    - Ion beam experiments using different materials:
      population in the ground level (>95 %) [13]

Grotrian diagram of W



[11] nist.gov (visited on 24.11.2020)
[12] I. Beigman et al. Plasma Phys. Control. Fusion (2007) 49 1833
[13] A. P. Yalin et. al. Applied optics (2005) Vol. 44 6496

II. Atomic level population of sputtered tungsten

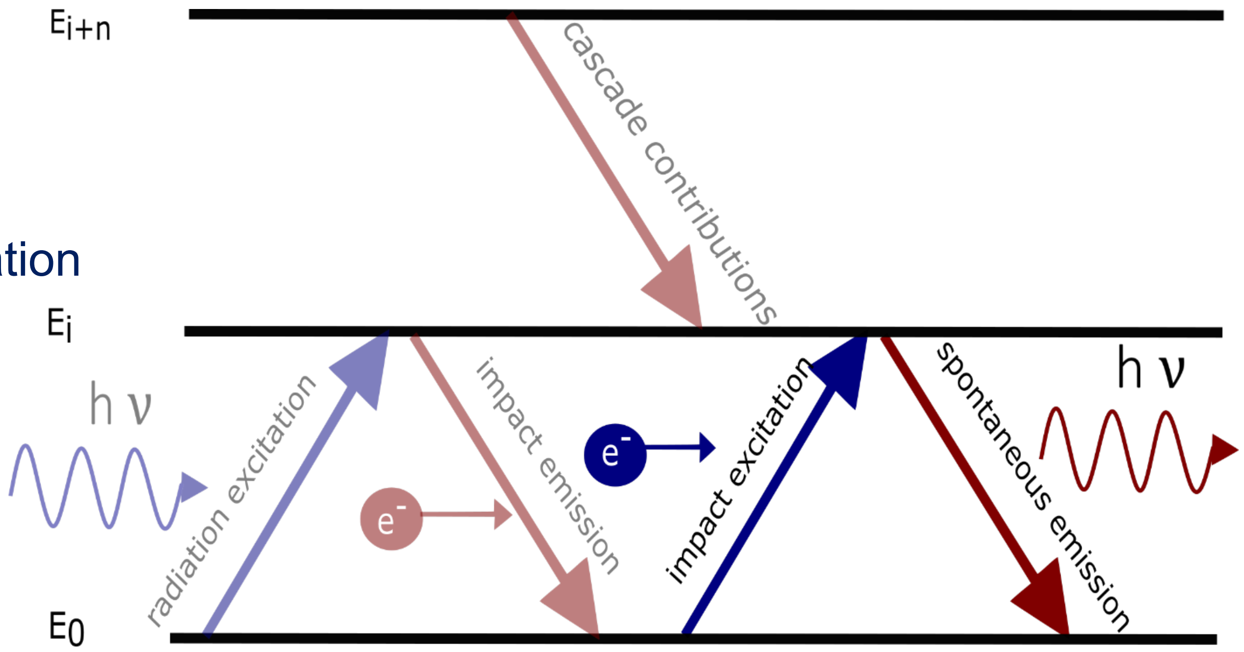
Method

Corona equilibrium:

$$\frac{dN_i}{dt} = -\sum_{j<i} N_i A_{ij} + n_e N_0 \langle v_e \sigma_X \rangle$$

Spontaneous emission Electron impact excitation

$$\begin{aligned} N_i &= \text{population of level i}, \\ A_{ij} &= \text{Einstein coefficient between level i and j}, \\ \langle v_e \sigma_X \rangle &= \text{excitation coefficient}, \\ n_e &= \text{electron density}. \end{aligned}$$



II. Atomic level population of sputtered tungsten

Method

$$\frac{dN_i}{dt} = -\sum_{j<i} N_i A_{ij} + n_e N_0 \langle v_e \sigma_X \rangle$$

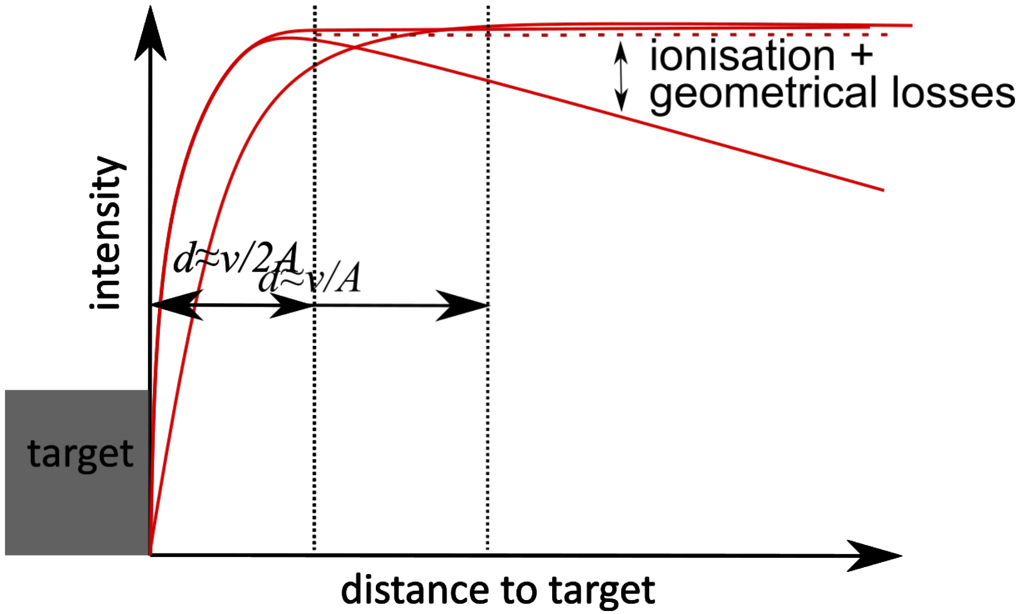
- Position of maximum line intensity is proportional to velocity and reciprocal Einstein coefficient:

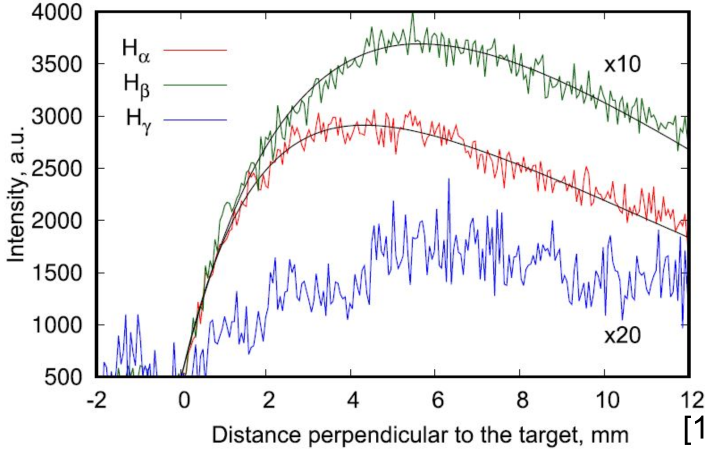
$$d = v \cdot \tau = \frac{v}{\sum A_{ij}}$$

- Angular distribution of sputtered particles leads to:

$$d \approx \frac{v}{2\sum A_{ij}}$$

- Ionisation and geometrical losses lead to decreasing intensity





[14]

[14] O. Marchuk et. al. J. Phys. B: At. Mol. Opt. Phys (2018) Vol.51 025702

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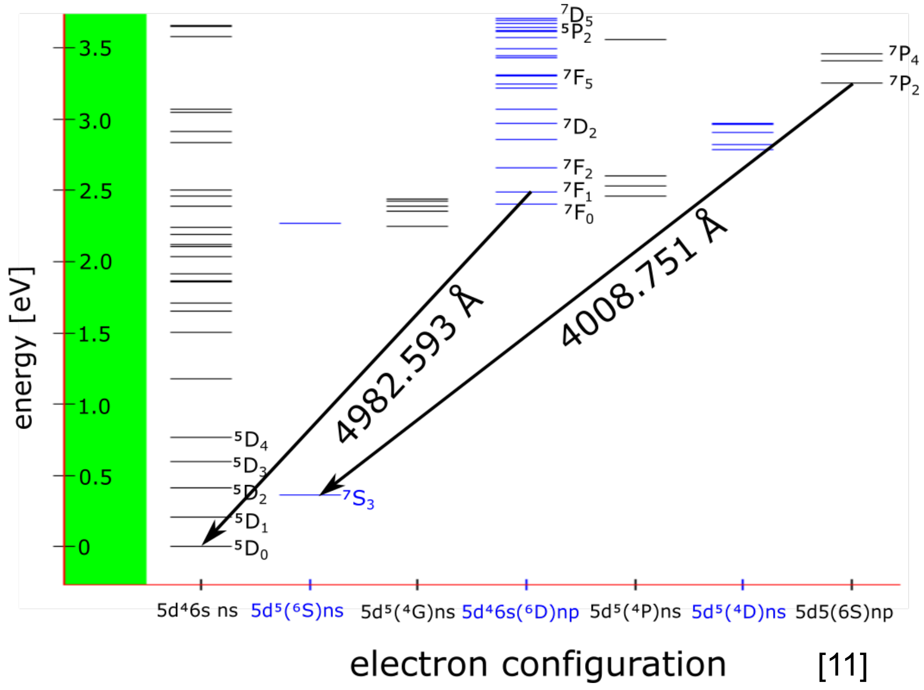
II. Atomic level population of sputtered tungsten

Results

Grotrian diagram of W



[11]

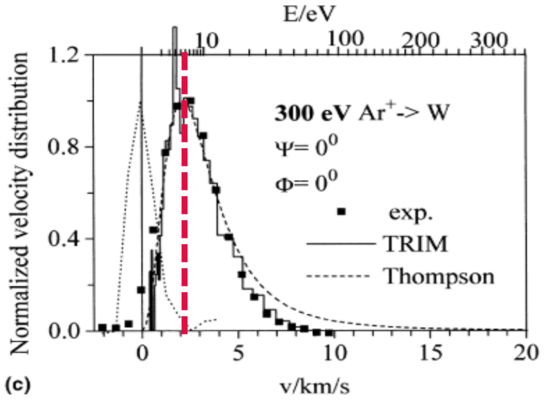
Wavelength (Å)	Lower level	Einstein coefficient (s^{-1})	Einstein coefficient upper level (s^{-1}) [11]	Relative proportion
4982.593	$^5D_0$	4.17E+5	5.31E+5	0.79
4008.751	$^7S_3$	1.63E+7	1.65E+7	0.99

[11] nist.gov (visited on 24.11.2020)

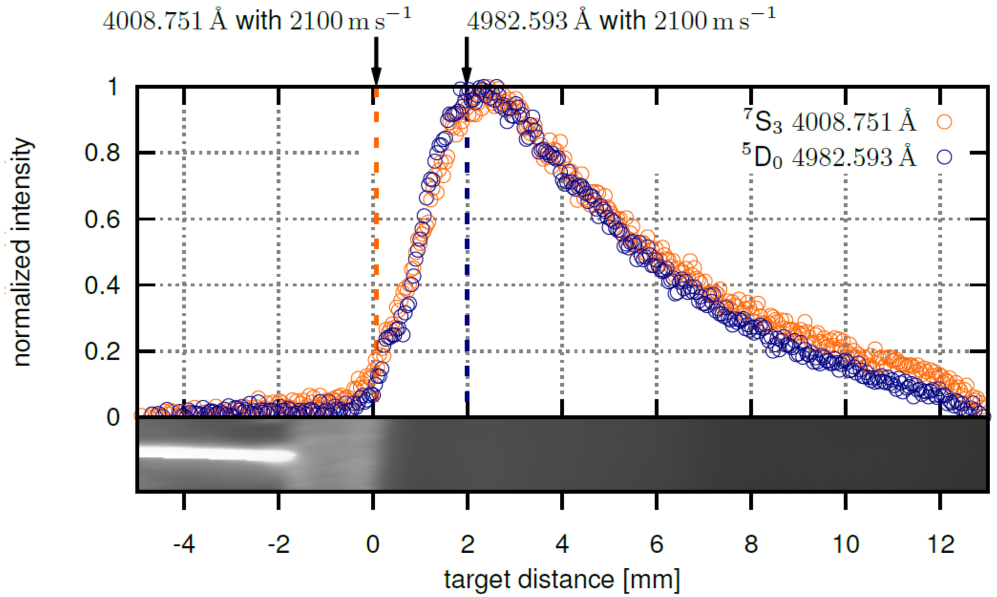
II. Atomic level population of sputtered tungsten

Results

- Experimental data: maximum of both lines at the same position
- $$d \approx \frac{v}{2\sum A_{ij}}$$
- According to Thompson energy distribution [7]: $v \approx 2100\,\mathrm{m\,s^{-1}}$
- Agreement only for ground term $^5D_0$



[12]



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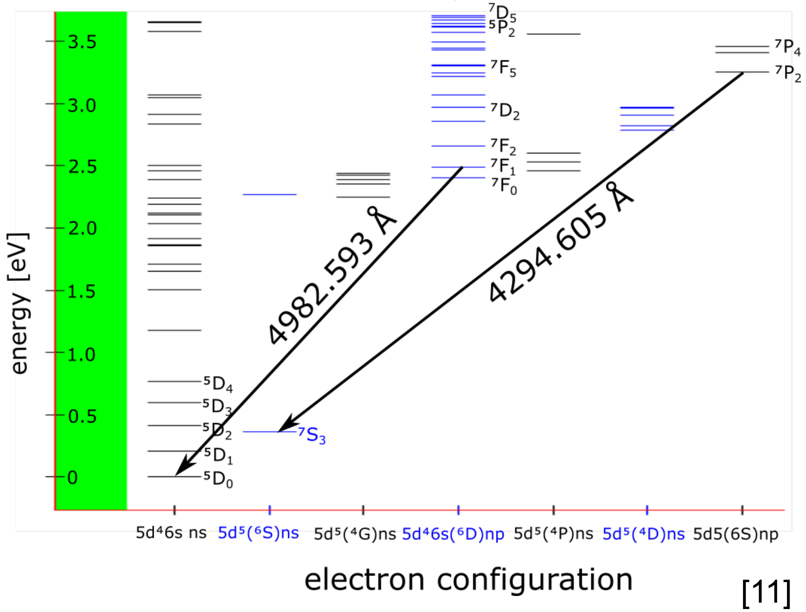
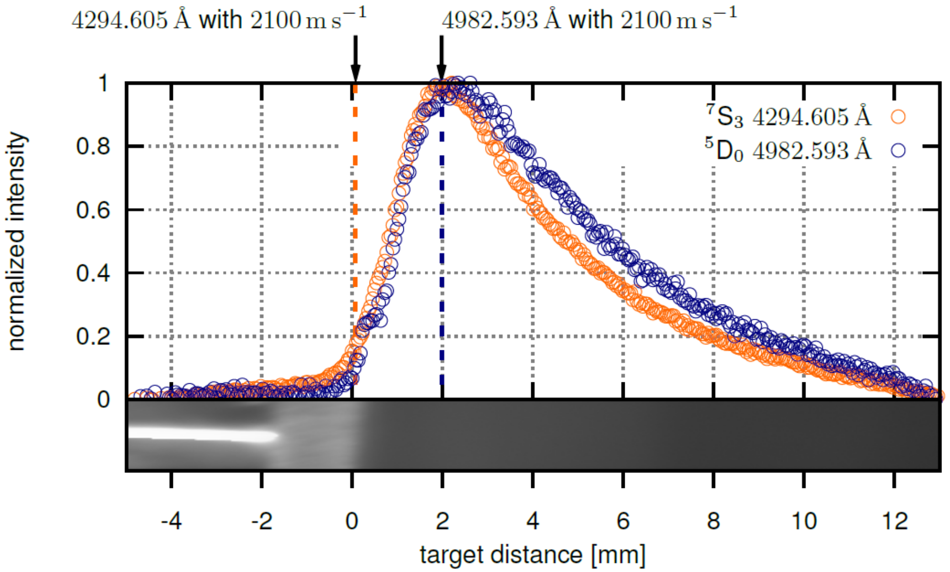
[7] M W Thompson 1968 Phil. Mag. 18 377–414
[12] A. Goehlich et. al. J. Nucl. Mater. 1999 Vol.266-269 501-506
[11] nist.gov (visited on 24.11.2020)

II. Atomic level population of sputtered tungsten

Results



[11]



Wavelength (Å)	Lower level	Position maximum (mm)	Einstein coefficient upper level (s^{-1}) [11]	Calculated velocity (m/s)	Relative proportion
4982.593	$^5D_0$	2.34	5.31E+5	1952	0.79
4294.605	$^7S_3$	2.21	1.32E+7	58212	0.94

[11] nist.gov (visited on 24.11.2020)

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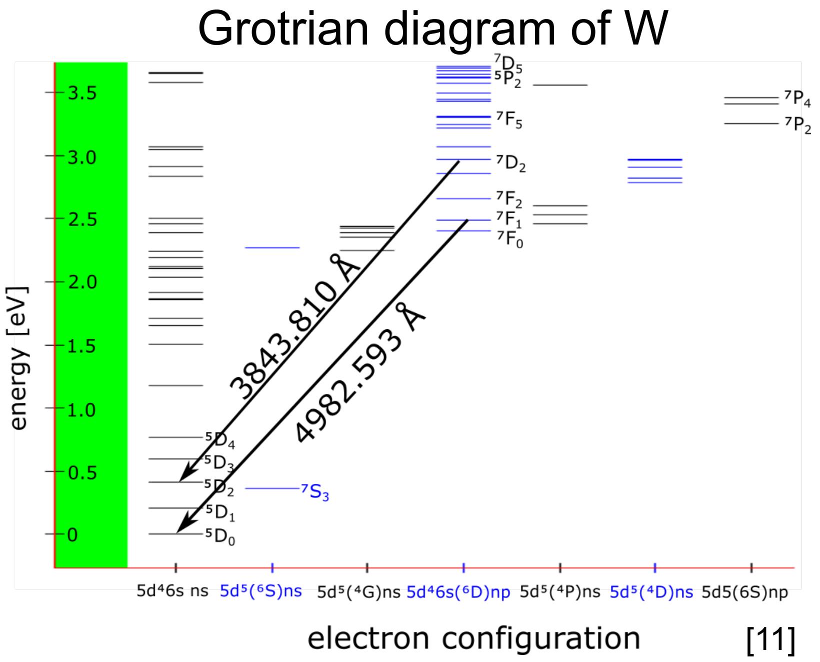
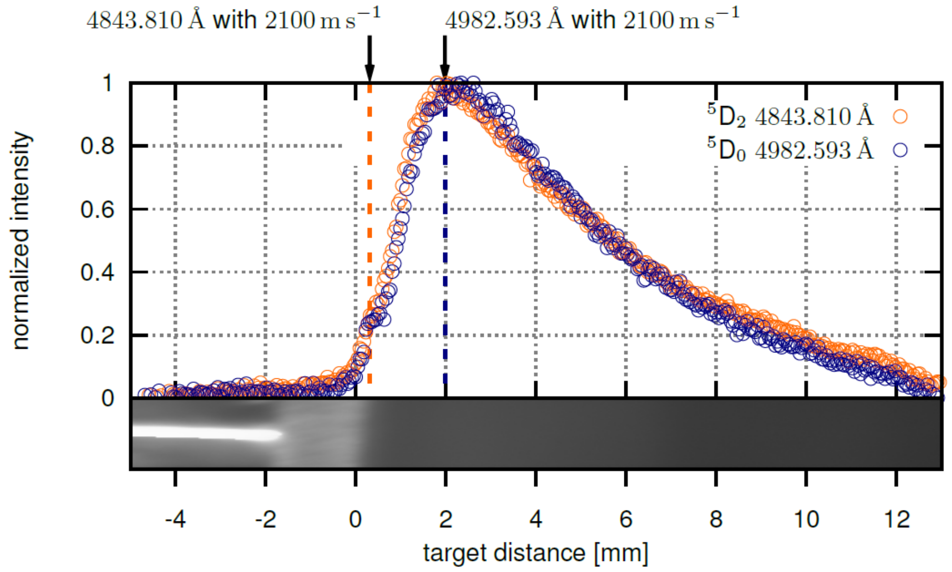
II. Atomic level population of sputtered tungsten

Results





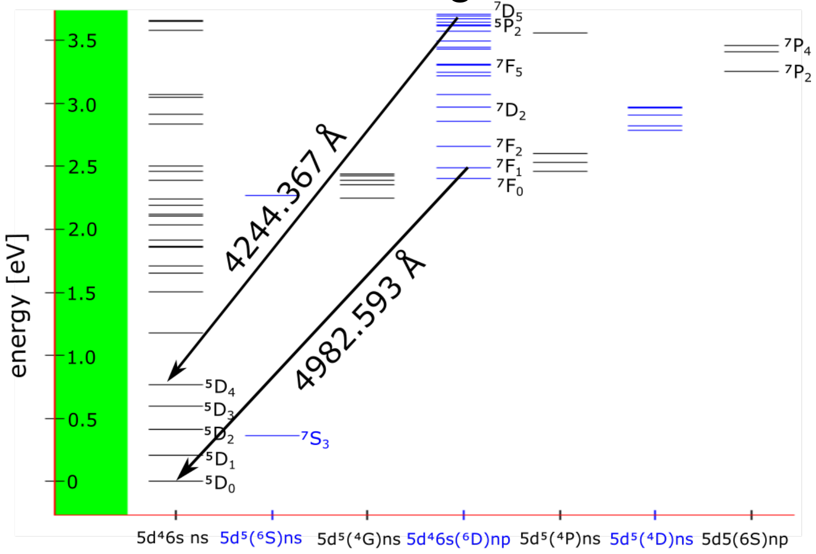
Wavelength (Å)	Lower level	Position maximum (mm)	Einstein coefficient upper level (s^{-1}) [11]	Calculated velocity (m/s)	Relative proportion
4982.593	$^5D_0$	2.34	5.31E+5	1952	0.79
4843.810	$^5D_2$	1.80	3.37E+6	12132	0.56

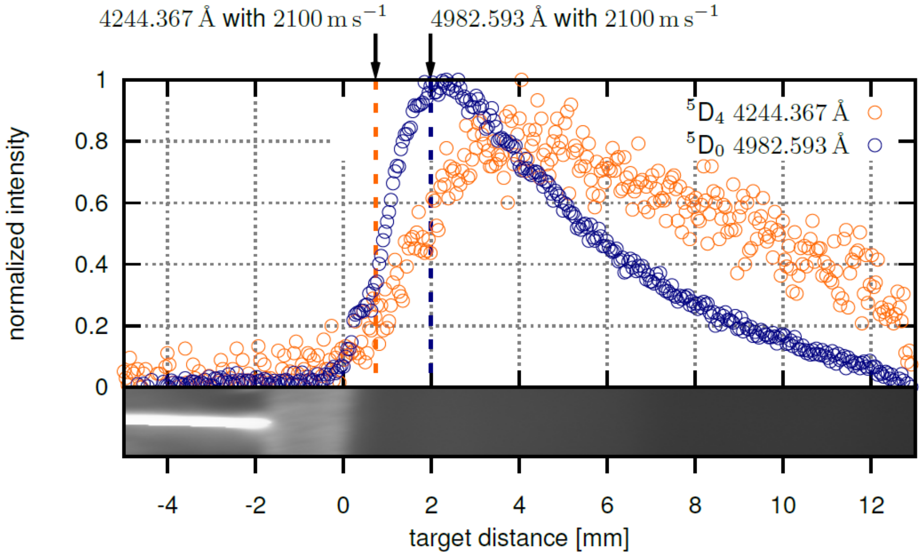
[11] nist.gov (visited on 24.11.2020)

II. Atomic level population of sputtered tungsten

Results

Grotrian diagram of W





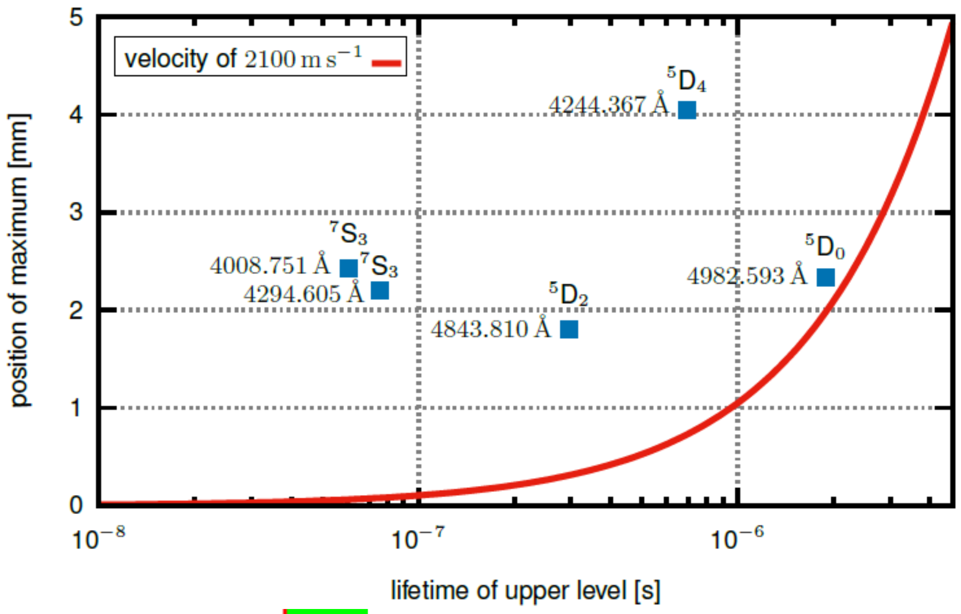
Wavelength (Å)	Lower level	Position maximum (mm)	Einstein coefficient upper level (s^{-1}) [11]	Calculated velocity (m/s)	Relative proportion
4982.593	$^5D_0$	2.34	5.31E+5	1952	0.79
4244.367	$^5D_4$	4.05	1.44E+6	11664	0.96

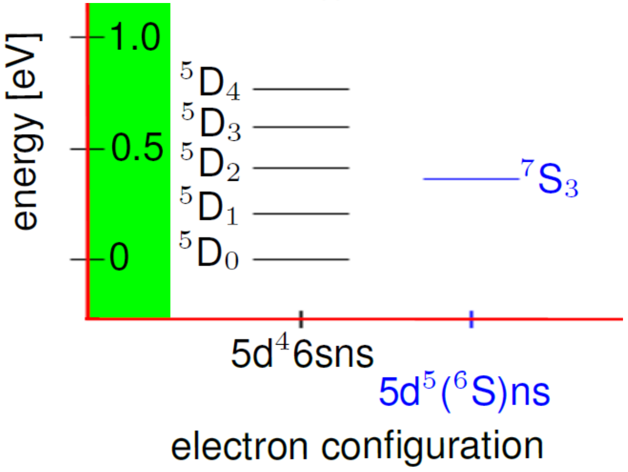
[11] nist.gov (visited on 24.11.2020)

II. Atomic level population of sputtered tungsten

Summary

- High spatial resolution spectroscopy measurements
- For a cold target (T_{surf}= 300 K) and mono-energetic incident ions in the order of 100 eV, W atoms are sputtered in the ground state $^5D_0$
- Exited levels $^7S_3$ and $^5D_{x>0}$ are not populated during sputtering





Outlook

- Further investigation with different lines, target temperatures, gases and plasma parameters
- Laser absorption measurements and Laser induced fluorescence (LIF) measurements in front of the target (direct measurements of population)

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