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# EUV spectra from the NIST EBIT

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# Outline

Motivation

EBIT

- Experimental set up
- Collisional-radiative modeling of plasma

EUV Spectra

- Gadolinium
- Dysprosium
- Tungsten

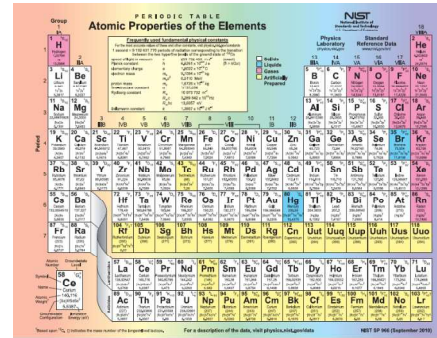
'Potential lowering' of  $4f^n$  ions

Summary

# Motivation

## Atomic and Plasma Theory

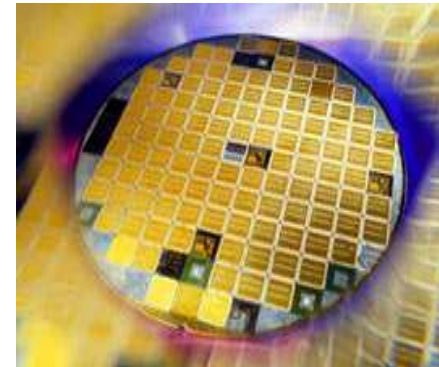
- Hf, Ta, W, Au ions  
advance atomic / plasma codes  
predict trends in atomic structure



A detailed periodic table of elements from NIST, titled "Atomic Properties of the Elements". It includes various physical and chemical properties for each element, such as atomic weight, ionization energy, and electron configuration. The table is color-coded by groups and includes a legend for element types (Metal, Nonmetal, Metalloid, and Unknown).

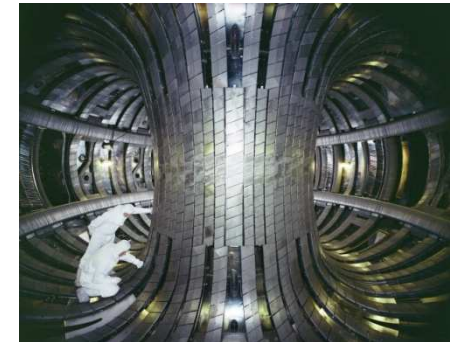
## Next-Generation Lithography

- Modeling of sources  
at 6.x nm



## ITER

- Diagnostics of hot  
plasmas in fusion  
devices



# NIST Electron Beam Ion Trap (EBIT)

## EBIT creates, traps and excites HCI

### Electron beam

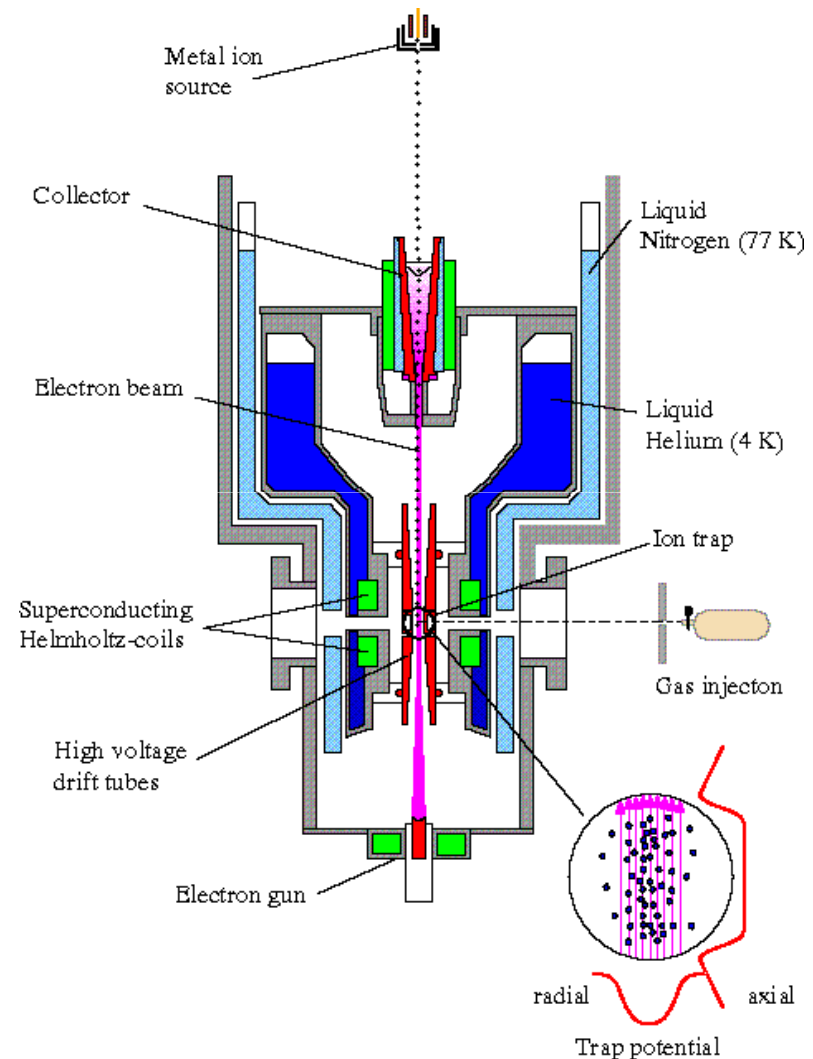
- collides with, ionizes and excites atoms
- monoenergetic, width  $\sim 60$  eV
- tuneable, 1 - 30 keV
- radius  $\sim 30$   $\mu\text{m}$
- density  $\sim 10^{11}$   $\text{cm}^{-3}$

### Ions are trapped

- radially by space charge
- axially by electrodes and magnetic field

### EUV radiation

- from the ions is observed with a flat field grazing incidence spectrometer



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# Collisional-Radiative Modeling

All important physical processes in the EBIT plasma

## Atomic Data –

### Flexible Atomic Code (FAC)

- Relativistic potential to solve the Dirac eqn (CI and QED):  
energy levels, radiative decay rates,  
radiative recombination cross sections
- $e^-$  ion collisions are treated with distorted wave/Coulomb Born-exchange approx:  
electron impact excitation,  
de-excitation, ionization cross sections

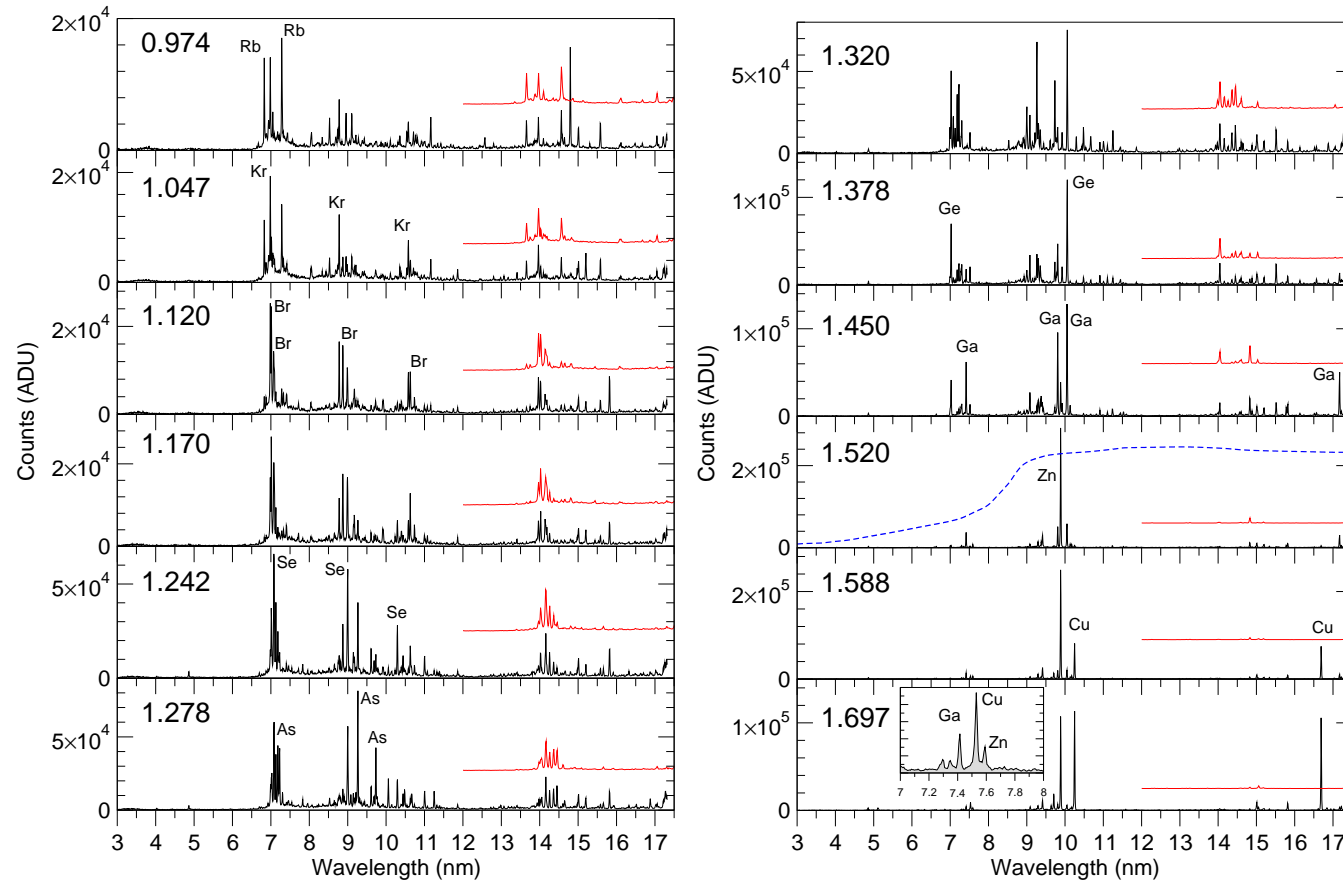
## CR model –

### NOMAD

- non-Maxwellian time-dependent CR plasma code
- $\sim 10^3$  levels/ion  
typically 6-8 ions  
several million transitions  
runs in minutes
- **one free parameter** – charge exchange CX between ions and neutrals

# EBIT Spectra of Gd

## Rb-like to Cu-like gadolinium ion spectra



Ion	IP (eV)
Rb-like	936
Kr-like	1100
Br-like	1142
Se-like	1189
As-like	1233
Ge-like	1320
Ga-like	1369
Zn-like	1481
Cu-like	1531

# EBIT Spectra of Gd

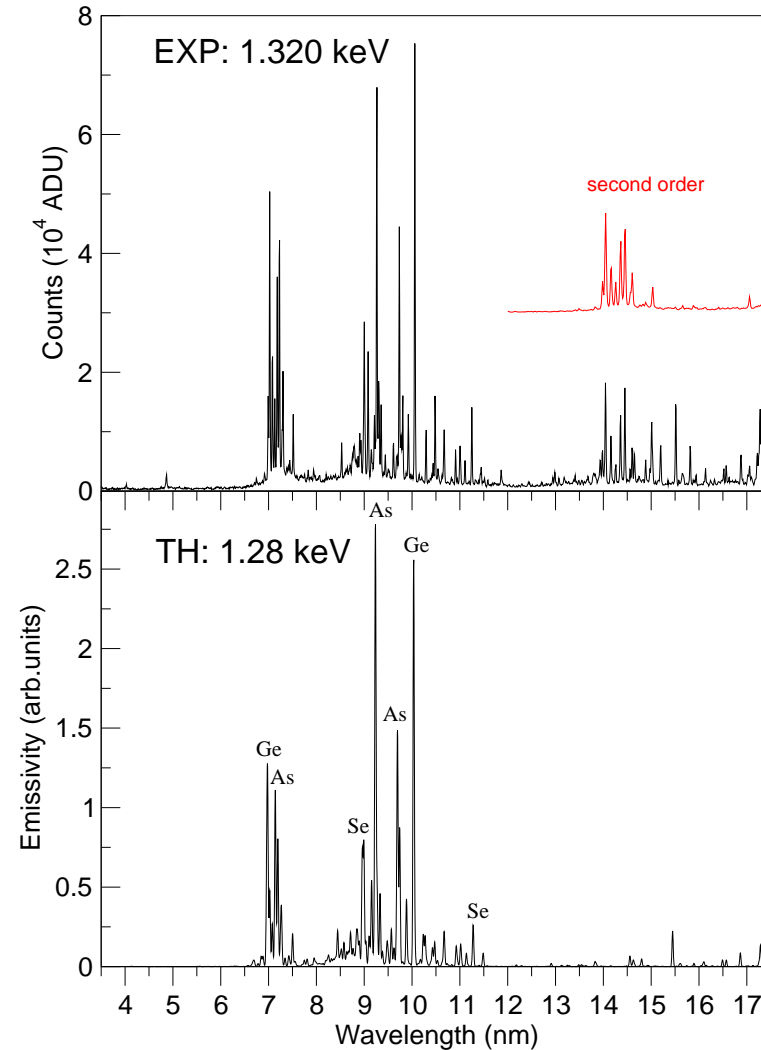
## Ge-like Gd ion

CR database of singly + doubly excited  
 $4s^24p^2$ ,  $4p^4$ ,  $4s^24d^2$ ,  $4s4p^3$ ,  $4s^24p4d$ ,  
 $4s^24p4f$ ,  $4s4p^24d$ ,  $4s4p^24f$ ,  $4s^24p5l$ ,  
 $4s4p^25l$ ,  $4s^24p6l$ ,  $4s4p^26l$

Energy levels of all singly, doubly, triply  
and quadruply excited  $n=4$  complex  
 $4s4d^3$ ,  $4s4f^3$ ,  $4d^4$ ,  $4f^4$ ,  $4p^24d^2$ ,  $4p^24f^2$  and  
 $4p^24d4f$

CR database is updated with new  
energies of the lowest levels

**Excellent agreement** between  
measured and simulated spectra e.g.  
Se, As, Ge-like



# Gadolinium Data Tables

59 new lines:  
**4s-4p, 4p-4d and  
 4d-4f transitions**  
 ranging from  
 6.630 nm to  
 17.279 nm  
 (mostly E1)

Ion	Lower level		Upper level		Experiment		Theory	
	Conf.	State	Conf.	State	Current	Previous	Current	Previous
Gd <sup>33+</sup> [Ga]	4s <sup>2</sup> 4p [1]	(4p <sub>-</sub> ) <sub>1/2</sub>	4s4p <sup>2</sup> [7]	((4s <sub>+</sub> ,4p <sub>-</sub> ) <sub>1,4p<sub>+</sub></sub> ) <sub>1/2</sub>	9.807	9.811(20) <sup>f</sup>	9.7664	9.655 <sup>f</sup>
Gd <sup>34+</sup> [As]	4s <sup>2</sup> 4p <sup>3</sup> [1]	(4p <sub>+</sub> ) <sub>3/2</sub>	4s4p <sup>4</sup> [9]	(4s <sub>+</sub> ,4p <sub>+</sub> <sup>2</sup> ) <sub>3/2</sub>	9.732		9.6954	
Gd <sup>28+</sup> [Kr]	4p <sup>6</sup> [1]	(4p <sub>+</sub> <sup>+</sup> ) <sub>0</sub>	4p <sup>5</sup> 4d [7]	(4p <sub>+</sub> <sup>3</sup> ,4d <sub>+</sub> ) <sub>2</sub>	9.726		9.6932	
Gd <sup>35+</sup> [Cu]	4p [3]	(4p <sub>+</sub> ) <sub>3/2</sub>	4d [5]	(4d <sub>+</sub> ) <sub>5/2</sub>	9.704	9.7026(15) <sup>d</sup> , 9.7074(15) <sup>c</sup>	9.6999	9.6962 <sup>d</sup> , 9.6958 <sup>n</sup>
Gd <sup>30+</sup> [Se]	4s <sup>2</sup> 4p <sup>4</sup> [1]	(4p <sub>+</sub> <sup>2</sup> ) <sub>2</sub>	4p <sup>3</sup> 4d [11]	(4p <sub>+</sub> ,4d <sub>+</sub> ) <sub>4</sub>	9.684		9.6719	
Gd <sup>35+</sup> [Cu]	4d [5]	(4d <sub>+</sub> ) <sub>5/2</sub>	4f [7]	(4f <sub>+</sub> ) <sub>7/2</sub>	9.636	9.6349(15) <sup>d</sup> , 9.6398(15) <sup>c</sup>	9.6598	9.6419 <sup>n</sup> , 9.6426 <sup>d</sup>
Gd <sup>30+</sup> [Se]	4s <sup>2</sup> 4p <sup>4</sup> [1]	(4p <sub>+</sub> <sup>2</sup> ) <sub>2</sub>	4s4p <sup>5</sup> [12]	(4s <sub>+</sub> ,4p <sub>+</sub> <sup>3</sup> ) <sub>1</sub>	9.609		9.5688	
Gd <sup>34+</sup> [Zn]	4s4p [5]	(4s <sub>+</sub> ,4p <sub>+</sub> ) <sub>1</sub>	4s4d [14]	(4s <sub>+</sub> ,4d <sub>+</sub> ) <sub>2</sub>	9.409	9.4085(20) <sup>c</sup>	9.3897	9.3651 <sup>c</sup>
Gd <sup>33+</sup> [Ga]	4s <sup>2</sup> 4p [2]	(4p <sub>+</sub> ) <sub>3/2</sub>	4s4p <sup>2</sup> [11]	(4s <sub>+</sub> ,4p <sub>+</sub> <sup>2</sup> ) <sub>3/2</sub>	9.376		9.3183	
Gd <sup>32+</sup> [Ge]	4s4p <sup>3</sup> [7]	(4s <sub>+</sub> ,4p <sub>+</sub> ) <sub>1</sub>	4s4p <sup>2</sup> 4d [33]	(4s <sub>+</sub> ,4d <sub>+</sub> ) <sub>2</sub>	9.352		9.3317	
Gd <sup>32+</sup> [Ge]	4s <sup>2</sup> 4p <sup>2</sup> [3]	(4p <sub>-</sub> ,4p <sub>+</sub> ) <sub>2</sub>	4p4d [15]	(4p <sub>-</sub> ,4d <sub>+</sub> ) <sub>3</sub>	9.300		9.2711	
Gd <sup>31+</sup> [As]	4s <sup>2</sup> 4p <sup>3</sup> [1]	(4p <sub>+</sub> ) <sub>3/2</sub>	4p <sup>2</sup> 4d [10]	(4d <sub>+</sub> ) <sub>5/2</sub>	9.262		9.2345	
Gd <sup>29+</sup> [Br]	4p <sup>5</sup> [1]	(4p <sub>+</sub> <sup>3</sup> ) <sub>3/2</sub>	4p <sup>4</sup> 4d [11]	(4p <sub>+</sub> <sup>2</sup> ,4d <sub>+</sub> ) <sub>1/2</sub>	9.172		9.1315	
Gd <sup>30+</sup> [Se]	4s <sup>2</sup> 4p <sup>4</sup> [2]	(4p <sub>+</sub> <sup>2</sup> ) <sub>0</sub>	4p <sup>3</sup> 4d [15]	(4p <sub>+</sub> ,4d <sub>+</sub> ) <sub>1</sub>	9.146		9.1050	
Gd <sup>27+</sup> [Rb]	4p <sup>6</sup> 4d [1]	(4d <sub>-</sub> ) <sub>3/2</sub>	4p <sup>5</sup> 4d <sup>2</sup> [23]	((4p <sub>+</sub> <sup>3</sup> ,4d <sub>-</sub> ) <sub>2,4d<sub>+</sub></sub> ) <sub>5/2</sub>	9.105		9.0503	

## 'Forbidden lines'

Kr-like (9.726 nm) (M2)

4p<sup>6</sup>(4p<sub>+</sub><sup>4</sup>)<sub>0</sub> – 4p<sup>5</sup>4d(4p<sub>+</sub><sup>3</sup>,4d<sub>+</sub>)<sub>2</sub>

Se-like (9.684 nm) (M2)

4s<sup>2</sup>4p<sup>4</sup>(4p<sub>+</sub><sup>2</sup>)<sub>2</sub> – 4p<sup>3</sup>4d(4p<sub>+</sub>,4d<sub>+</sub>)<sub>4</sub>

Se-like (7.826 nm) (M2)

4s<sup>2</sup>4p<sup>4</sup>(4p<sub>+</sub><sup>2</sup>)<sub>2</sub>  
 – 4p<sup>3</sup>4d((4p<sub>-</sub>,4p<sub>+</sub><sup>2</sup>)<sub>3/2</sub>,4d<sub>-</sub>)<sub>0</sub>

Spectra were calibrated with known lines of  
 Ba, Xe, C and O ions – accuracy 0.003 nm

## Cu-like lines

NIST EBIT

9.086 nm

7.527 nm

NIFS

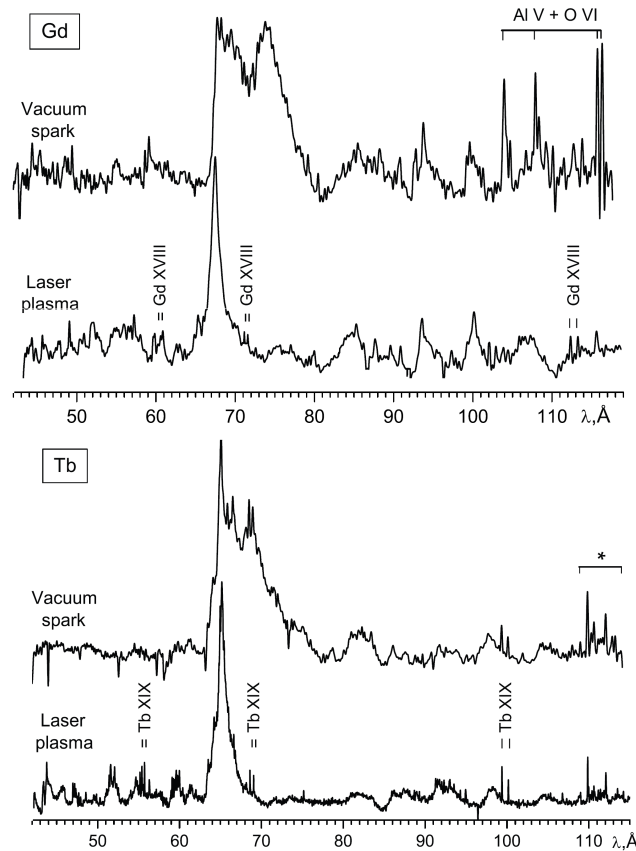
9.091(2) nm

7.524(2) nm



# Next-Generation EUV Lithography at 6.x nm

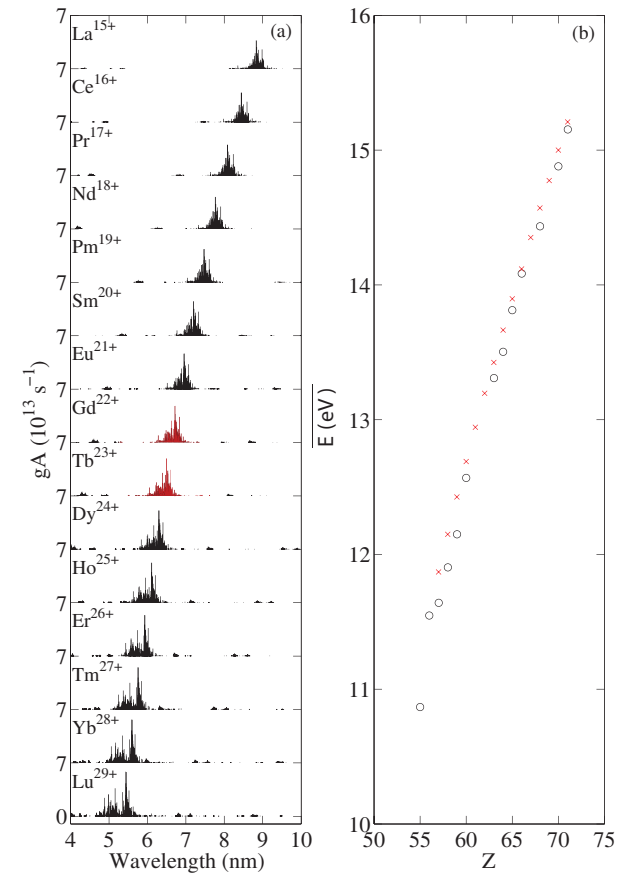
Churilov identified **Gd and Tb** in LPPs and spark discharges



Churilov *et al. Phys. Scr.* **80** 045303 (2009)

## 4d-4f + 4p-4d UTAs

Intense emission due to overlap of many open 4d and 4f subshell ions



Kilbane and O'Sullivan *Phys. Rev. A* **82** 062504 (2010)

# Spectra of Gd and Dy at 6.x nm

## Gadolinium

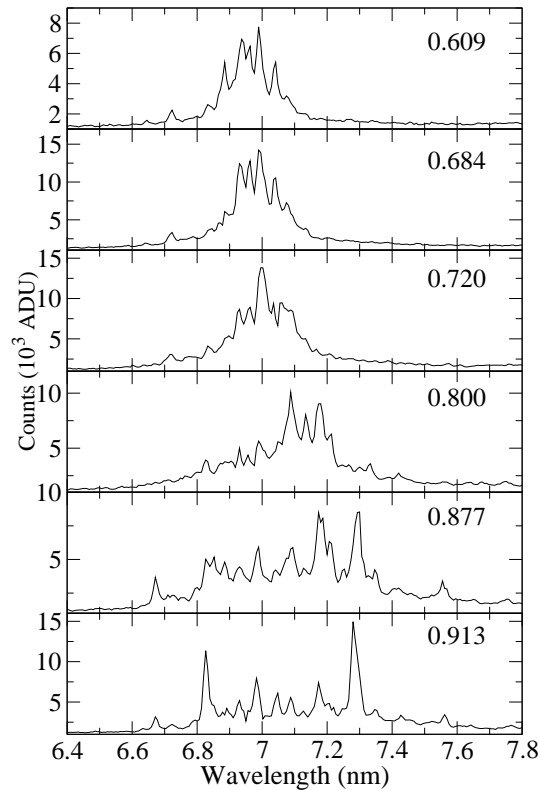
### Ag-like

$4d^{10}4f - 4d^94f^2$   
6.7423, 6.7465,  
6.7884 nm

### Pd-like

$4d^{10} - 4d^94f$   
6.7636 nm

Gd Ion	IP (eV)
Ag-like	358
Pd-like	565
Rh-like	601



## Dysprosium

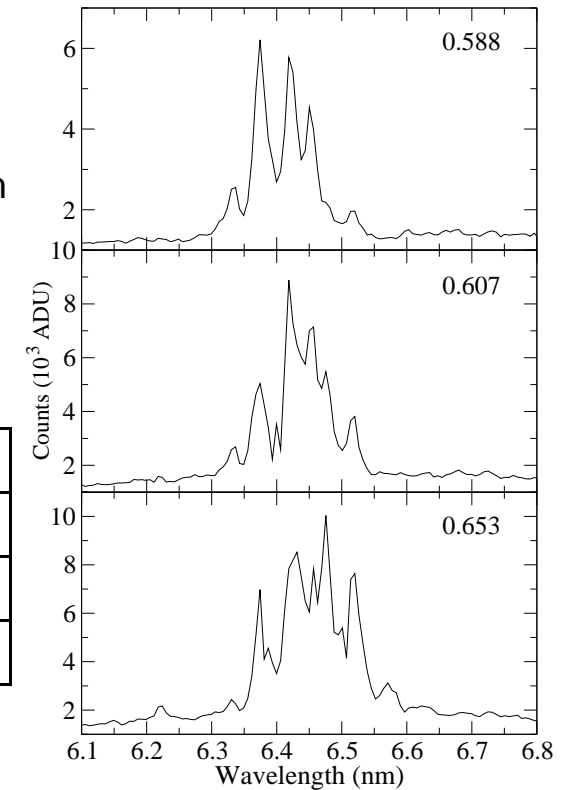
### Ag-like

$4d^{10}4f - 4d^94f^2$   
6.6437, 6.5967,  
6.2587, 6.3125 nm

### Pd-like

$4d^{10} - 4d^94f$   
6.2778 nm

Dy Ion	IP (eV)
Ag-like	423
Pd-like	664
Rh-like	702



Note: Very low current ~5 mA at 0.609 keV

**Absence of strong resonant transitions**

Sugar *et al. J. Opt. Soc. Am. B* **10** 799, 1321, 1977 (1993)

Rodrigues *et al. At. Data Nucl. Data Tables* **86** 117 (2004)

# Spectra of W

Ag-like  $4d^{10}4f - 4d^94f^2$   
5.1457, 5.0895, 4.8729,  
4.9403 nm

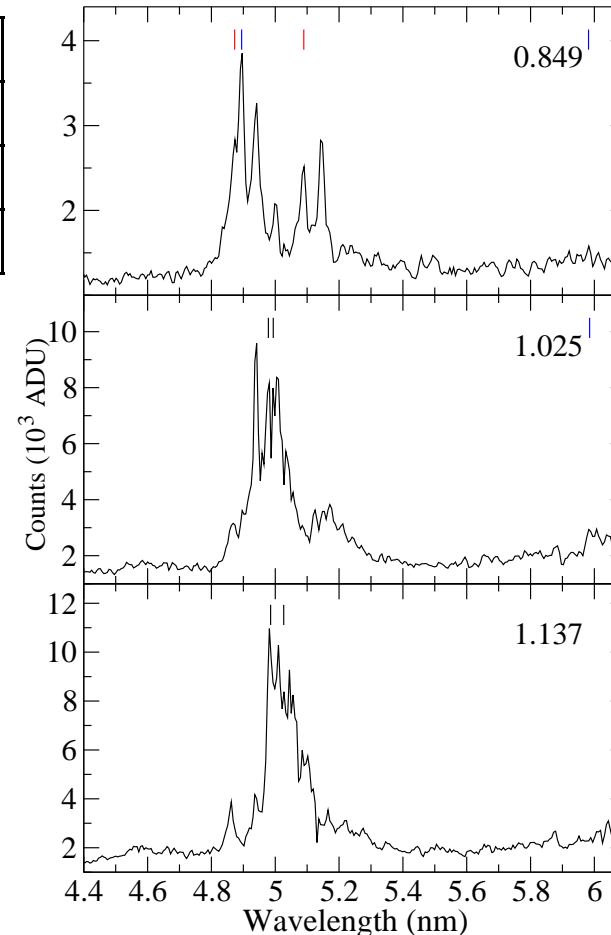
Pd-like  $4d^{10} - 4d^94f$   
4.8948, 5.9852 nm

Rh-like  $4d^9 - 4d^84f$   
4.9856, 4.9785, 4.9938,  
5.0265 nm

W Ion	IP (eV)
Ag-like	881.4
Pd-like	1132.2
Rh-like	1179.9

**Strong resonant transitions observed  
at lower beam energies in Pd-like ions**

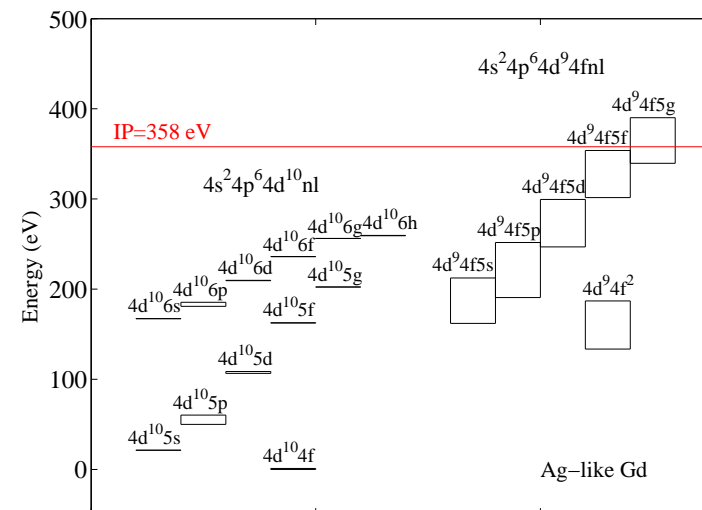
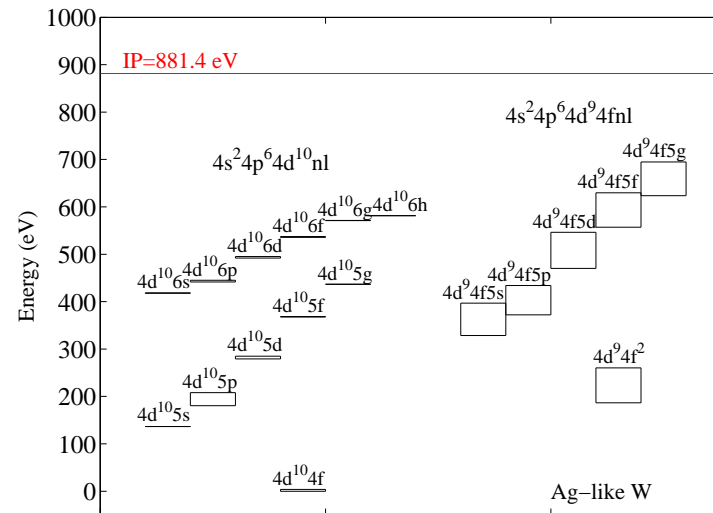
Note: Feature observed at  $\sim 4.5$  nm at 1.03 and  
1.15 keV at the Berlin EBIT is absent



# 'Potential Lowering' of $4f^n$ ions

## Metastable states

- Many low lying excited states of Ag-like ions are populated by collisions
- These metastable states remain well populated
- Beam energy required to generate excited states of Pd-like ions is reduced



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# Summary

## **EUV spectra of Gd, Dy and W ions from the NIST EBIT**

- 59 new lines identified in Rb-like to Cu-like gadolinium
- ‘Potential lowering’ observed in  $4f^n$  ions
- Uses:
  - validate atomic / plasma codes  
predict trends in atomic structure
  - model EUV sources for next-generation lithography
  - diagnostics of hot plasmas in fusion devices such as ITER

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# Thanks

## The Atomic Spectroscopy Group at NIST

### Acknowledgement:

This work was supported by Science Foundation Ireland under grant number 07/IN.1/I1771 and in part by the Office of Fusion Energy Sciences of the U.S. Department of Energy.



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