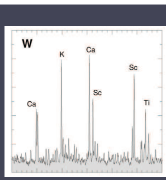
Atomic Spectroscopic Data and Spectra Modeling for Highly-Charged High-Z Ions



Yuri Ralchenko

National Institute of Standards and Technology
Gaithersburg, MD 20899, USA

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  - C. Bowen
  - H.A. Scott
  - …

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Plan

- NIST Atomic Database(s)
- EBIT spectra and modeling
  - X-ray
  - EUV
  - Dielectronic resonances
- Validation and verification of CR models
- Conclusions

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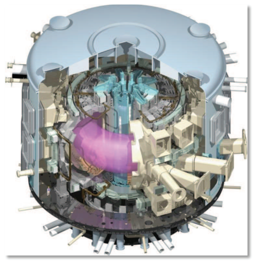
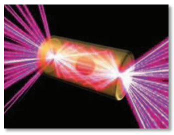
Why highly-charged high-Z elements?



ITER: **W** plates in the divertor

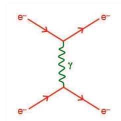


Au hohlraums, National Ignition Facility

EUV lithography **Sn^{10+}, Gd^{20+}**

New atomic clocks of exceptional accuracy

QED tests



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HCI atomic physics: peculiarities

- **Atomic structure**
  - ***nl*** electrons become more "***hydrogenic***" with ion charge increase…
  - …but "*highly-charged*" may still mean "***many-electron***"
    - W^{50+}: $3s^23p^63d^6$
  - Effect of **correlations** is still very important
    - Complex (same *n*)!
  - **Relativistic** and **QED** effects
  - **Forbidden** transitions become stronger
  - **MCDHF, RRPA, RMBPT, RMP (FAC, HULLAC),…**
- **Atomic collisions**
  - **Perturbative** methods (distorted waves, Coulomb-Born) work very well
  - **Relativistic** effects may become important
  - **Dielectronic recombination** becomes the most important recombination channel
  - **Charge exchange** with neutrals in laboratory plasmas may be important
  - **RMP (FAC, HULLAC), RDW, CB,…**

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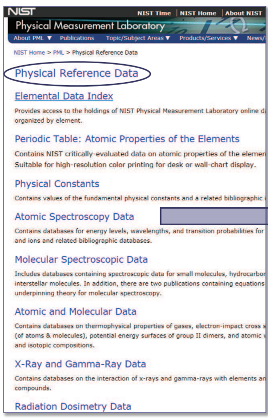
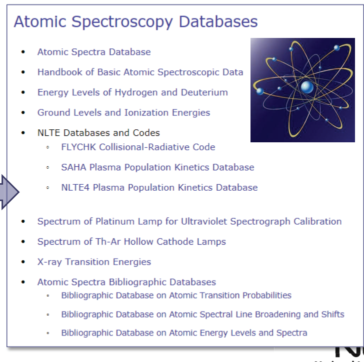
Atomic and plasma data services at NIST



http://pml.nist.gov/data



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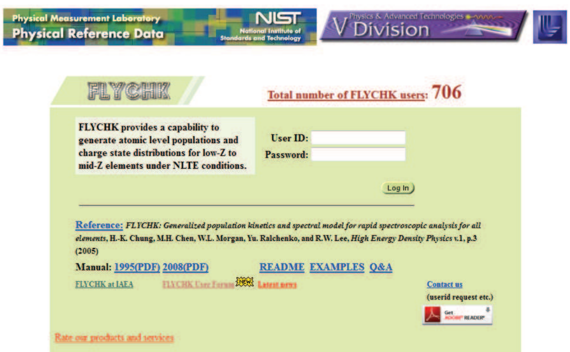
FLYCHK: online CR code at http://nlte.nist.gov/FLY/



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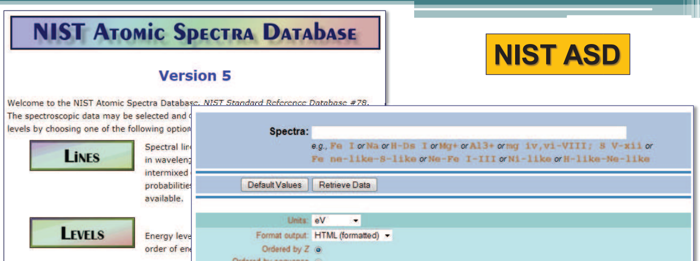
NIST ASD



At. Num.	Ion Charge	El. name	Isoel. Seq.	Ground Shells [a]	Ground Level	Ionized Level	Ionization Energy [b] (eV)	References
14	0	Silicon	Si	$[Ne]3s^23p^2$	$^3P_0$	$3p\ ^2P^\circ_{1/2}$	8.151683(30)	L5815
14	+1	Silicon	Al	$[Ne]3s^23p$	$^2P^\circ_{1/2}$	$3s^2\ ^1S_0$	16.34585(4)	L5815
14	+2	Silicon	Mg	$[Ne]3s^2$	$^1S_0$	$3s\ ^2S_{1/2}$	33.49300(9)	L5815
14	+3	Silicon	Na	$[Ne]3s$	$^2S_{1/2}$	$2p^6\ ^1S_0$	45.14179(7)	L5815
14	+4	Silicon	Ne	$1s^22s^22p^6$	$^1S_0$	$2p^5\ ^2P^\circ_{3/2}$	166.767(3)	L3934
14	+5	Silicon	F	$1s^22s^22p^5$	$^2P^\circ_{3/2}$	$2p^4\ ^3P_2$	[205.267(19)]	L5815
14	+6	Silicon	O	$1s^22s^22p^4$	$^3P_2$	$2p^3\ ^4S^\circ_{3/2}$	[246.32(10)]	L11770
14	+7	Silicon	N	$1s^22s^22p^3$	$^4S^\circ_{3/2}$	$2p^2\ ^3P_0$	[303.66(17)]	L11770
14	+8	Silicon	C	$1s^22s^22p^2$	$^3P_0$	$2p\ ^2P^\circ_{1/2}$	[351.10(8)]	L11770
14	+9	Silicon	B	$1s^22s^22p$	$^2P^\circ_{1/2}$	$2s^2\ ^1S_0$	[401.38(4)]	L11770
14	+10	Silicon	Be	$1s^22s^2$	$^1S_0$	$2s\ ^2S_{1/2}$	[476.18(8)]	L11770
14	+11	Silicon	Li	$1s^22s$	$^2S_{1/2}$	$1s^2\ ^1S_0$	(523.415(7))	L16264c99
14	+12	Silicon	He	$1s^2$	$^1S_0$	$1s\ ^2S_{1/2}$	(2 437.65804(20))	L12128
14	+13	Silicon	H	$1s$	$^2S_{1/2}$		(2 673.1774(3))	L7188

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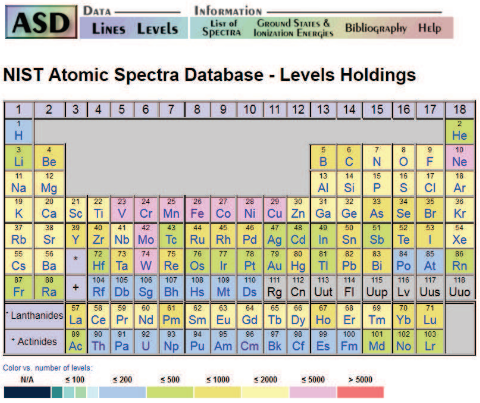
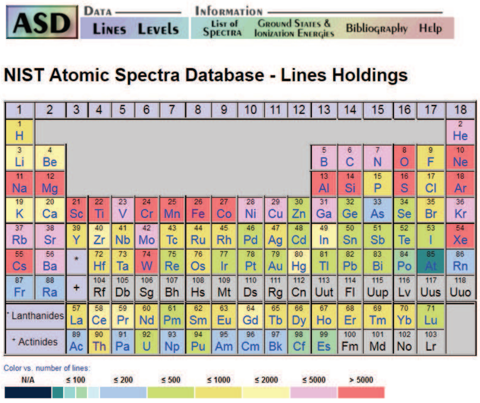


v.5.2

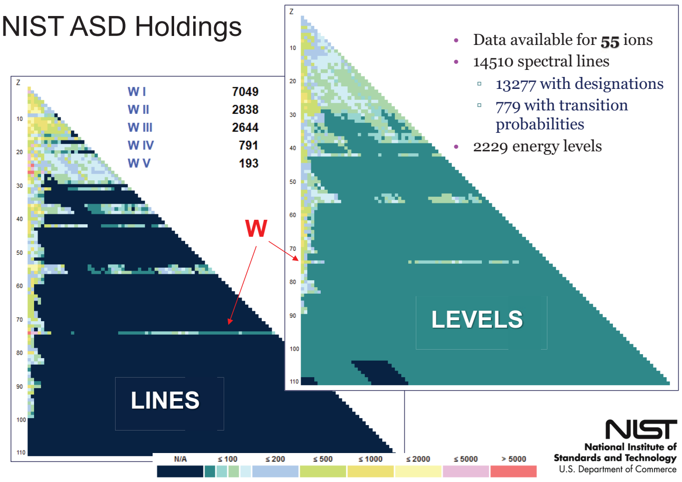
Current total number of levels: 107260



v.5.2

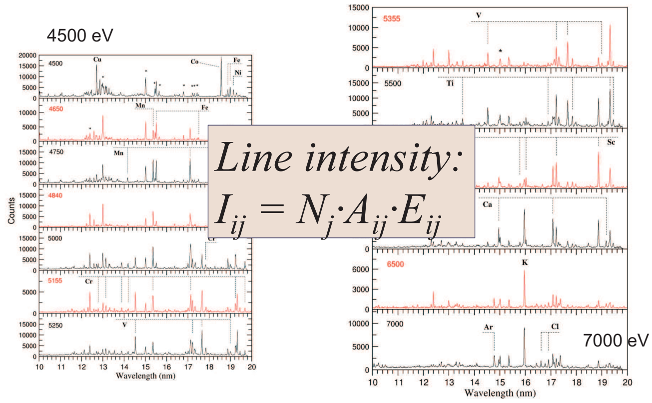
Current total number of lines: 227477

NIST ASD Holdings



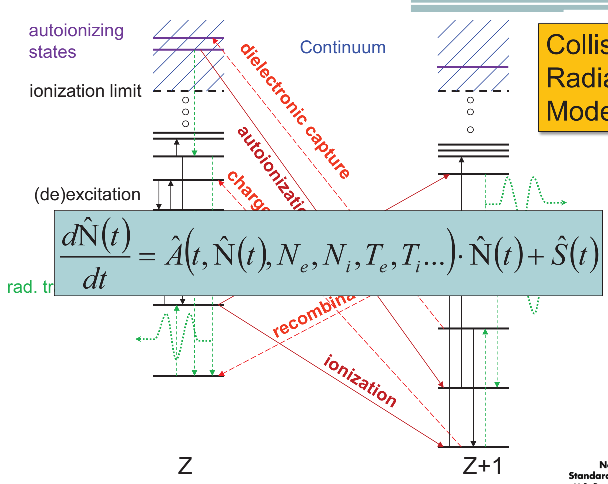
- Data available for **55** ions
- 14510 spectral lines
  - 13277 with designations
  - 779 with transition probabilities
- 2229 energy levels

NIST EBIT spectra of $3d^n$ Ions of W: M1 lines



Line intensity: $I_{ij} = N_j \cdot A_{ij} \cdot E_{ij}$

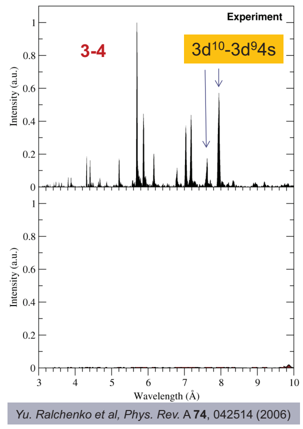
Yu.Ralchenko et al, *Phys. Rev. A* 83, 032517 (2011)



$$\frac{d\hat{N}(t)}{dt} = \hat{A}\left(t, \hat{N}(t), N_e, N_i, T_e, T_i \ldots\right) \cdot \hat{N}(t) + \hat{S}(t)$$

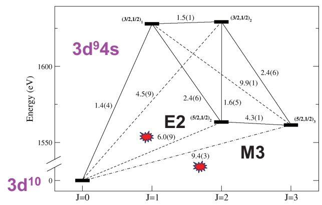
Collisional-Radiative Model

NIST EBIT X-ray measurements ($E_b \approx 4$ keV)



Yu. Ralchenko et al, *Phys. Rev. A* **74**, 042514 (2006)

Mainly Ni-like W^{46+}

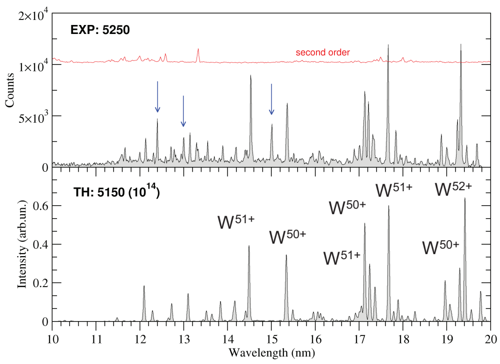


Data: **FAC** (Gu, 2003)

CR model: **NOMAD** (Ralchenko & Maron, 2001)

E2/M3 ratio: good for density diagnostics in fusion machines

Theory vs Experiment (E = 5.25 keV)

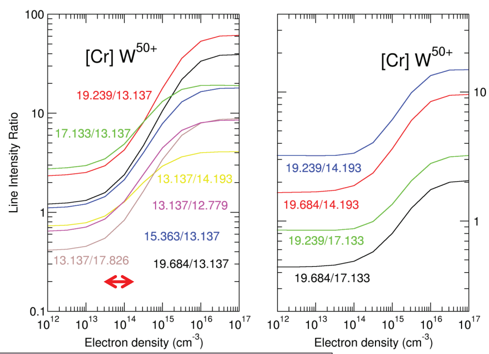


All lines: M1

Forbidden lines are often sensitive to density → good for diagnostics?..

Yu.Ralchenko et al, *Phys. Rev. A* 83, 032517 (2011)

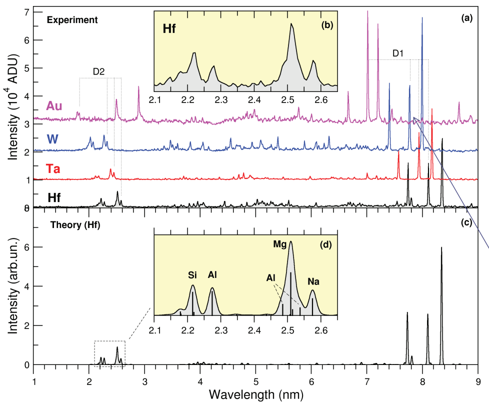
Density-Sensitive Ratios for Fusion Plasmas: W^{50+}



Collisional-radiative model for EBIT can be applied to Maxwellian fusion plasmas

Yu.Ralchenko et al, *Phys. Rev. A* 83, 032517 (2011)

D-doublet in Na-like W, Hf, Ta, and Au



J.D. Gillaspy et al, *Phys. Rev. A* **80**, 010501 (2009)

$E_b \approx 12$ keV

D1: $3s_{1/2} - 3p_{1/2}$
D2: $3s_{1/2} - 3p_{3/2}$

Isoelectronic analysis

Three lines:
W^{61+}, W^{63+}, W^{62+}
T_e diagnostics

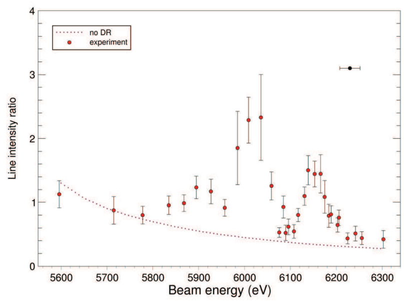
Ratios of M1 lines can be used to detect dielectronic resonances

- **DRs are normally not important/produced in nearly monoenergetic beams in EBITs: require precise match of energies to produce them**
- ***3d^n* ions in W: energies of high abundance are good for LMN ($2p\rightarrow3l$, $\varepsilon l\rightarrow4l'$) resonances**
- **DR shifts ionization balance that can be detected in M1 line ratios**
- **Goal: measure 10,000 eV resonances with ~80 eV M1 lines in EUV by scanning the beam energy**

Dielectronic resonances in W^{54+}

$$\frac{W^{54+}\ 3d^2{}_{J=2} - 3d^2{}_{J=3}}{W^{55+}\ 3d_{3/2} - 3d_{5/2}}$$

THEORY:
no DR

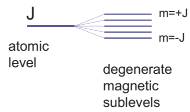


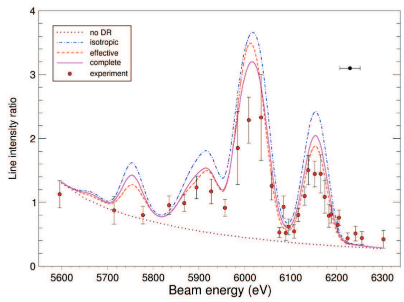
[Ca]/[K]

Non-Maxwellian (40-eV Gaussian) collisional-radiative model: **~18,000 levels + accurate account of anisotropy**

$$\frac{W^{54+}\ 3d^2{}_{J=2} - 3d^2{}_{J=3}}{W^{55+}\ 3d_{3/2} - 3d_{5/2}}$$

THEORY:
no DR
isotropic DR
anisotropic DR



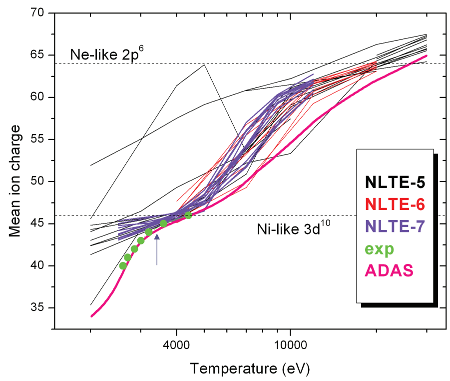


Impact beam electrons are monodirectional

Non-LTE Code Comparison Workshops

- GOAL: **validation and verification of collisional-radiative codes**
- Pre-workshop calculation of plasma population kinetics parameters and spectra for the same plasma conditions
- Pinpoint problems and discuss possible explanations of differences
- 7 workshops since 1996
- Typically more than 15 codes
- Very different structure
  - Averaged atom
  - Superconfiguration
  - Configuration
  - Hybrid
  - Detailed level accounting
- Different sources of atomic data and different approximations

W at NLTE workshops: example



Conclusions

- **Significant progress in production and evaluation of basic atomic spectroscopic data for W and other high-Z elements**
- **Collisional-radiative modeling of highly-charged high-Z ions is currently capable of providing very detailed analysis of measured spectra**
- **Evaluation of atomic structure data for fusion is in jeopardy because of the lack of funding**