Atomic Data Needs for Laboratory & Astrophysical Plasma Research

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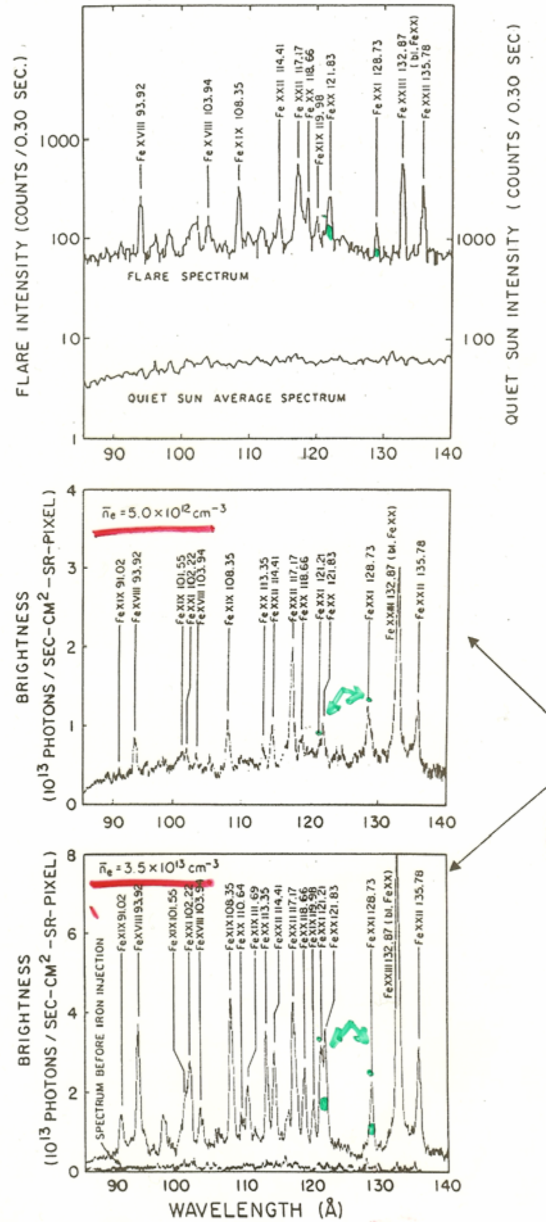
Content

- The link between laboratory and astrophysical plasma spectroscopy
- How do we establish the ‘needs’ for atomic data?
  - Atomic structure calculations
  - Ingredients for CR modeling
- Benchmarking of atomic data and CR models

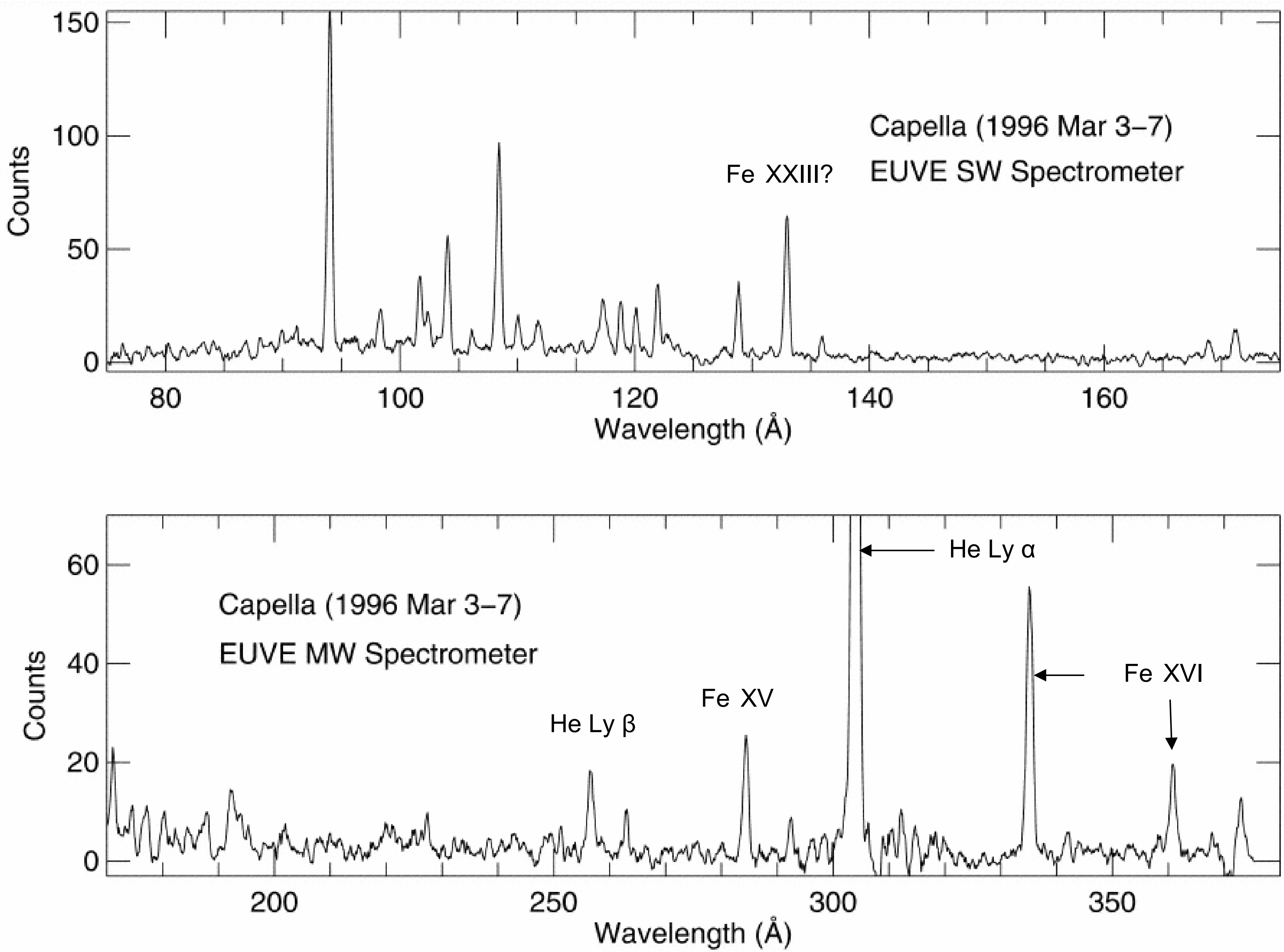
Collaborators

- Kevin Fournier and Stephanie Hansen
  - Lawrence Livermore National Laboratory
- Mario Mattioli
  - Consortio RFX, Assoc. Euratom ENEA, Padova, Italy
- Randall Smith
  - Goddard Space Flight Center, Greenbelt, MD
- Rudolf Neu and Thomas Pütterich
  - Max Planck – Institut für Plasmaphysik, Garching, Germany
- Danilo Pacella – ENEA, Frascati, Italy



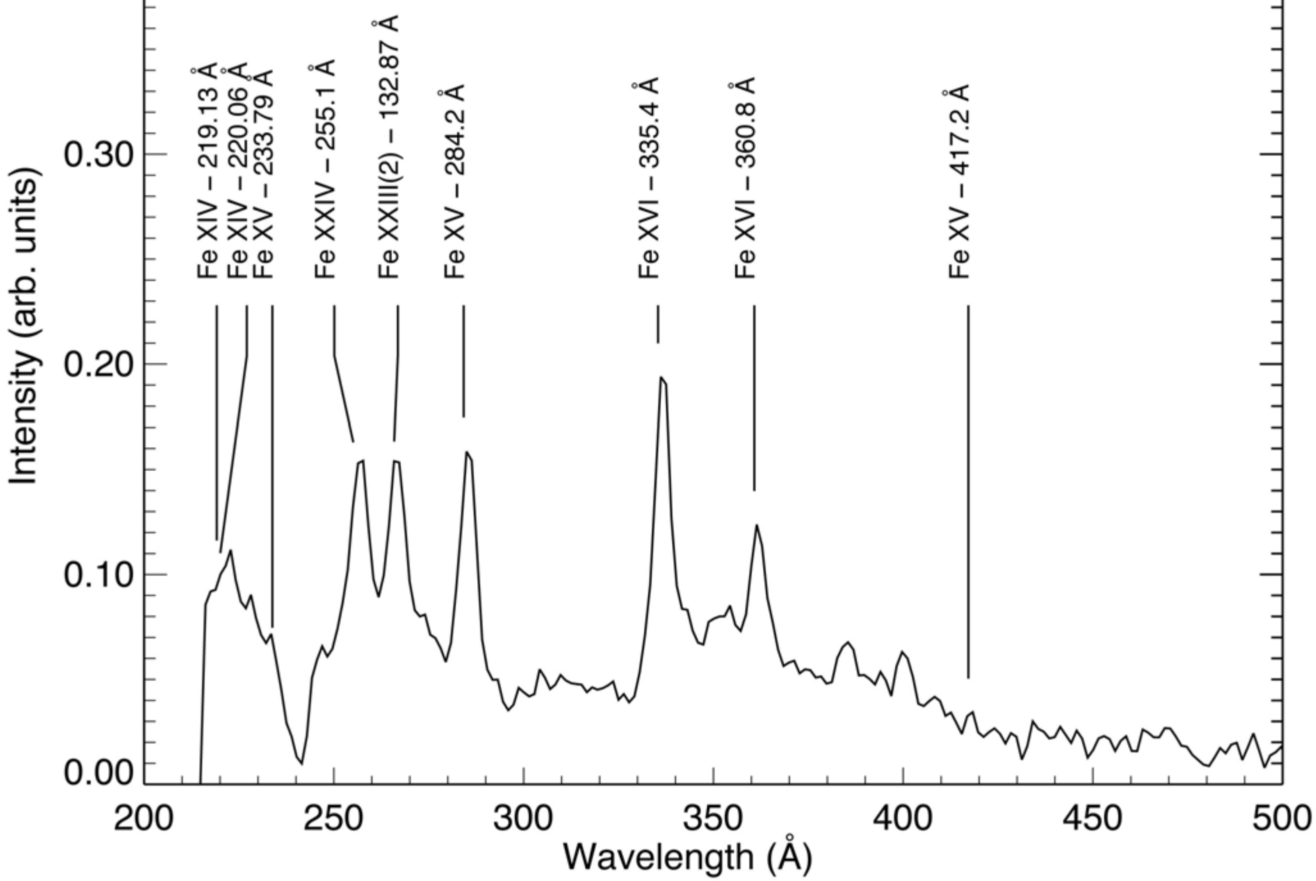
Solar spectra

Tokamak spectra

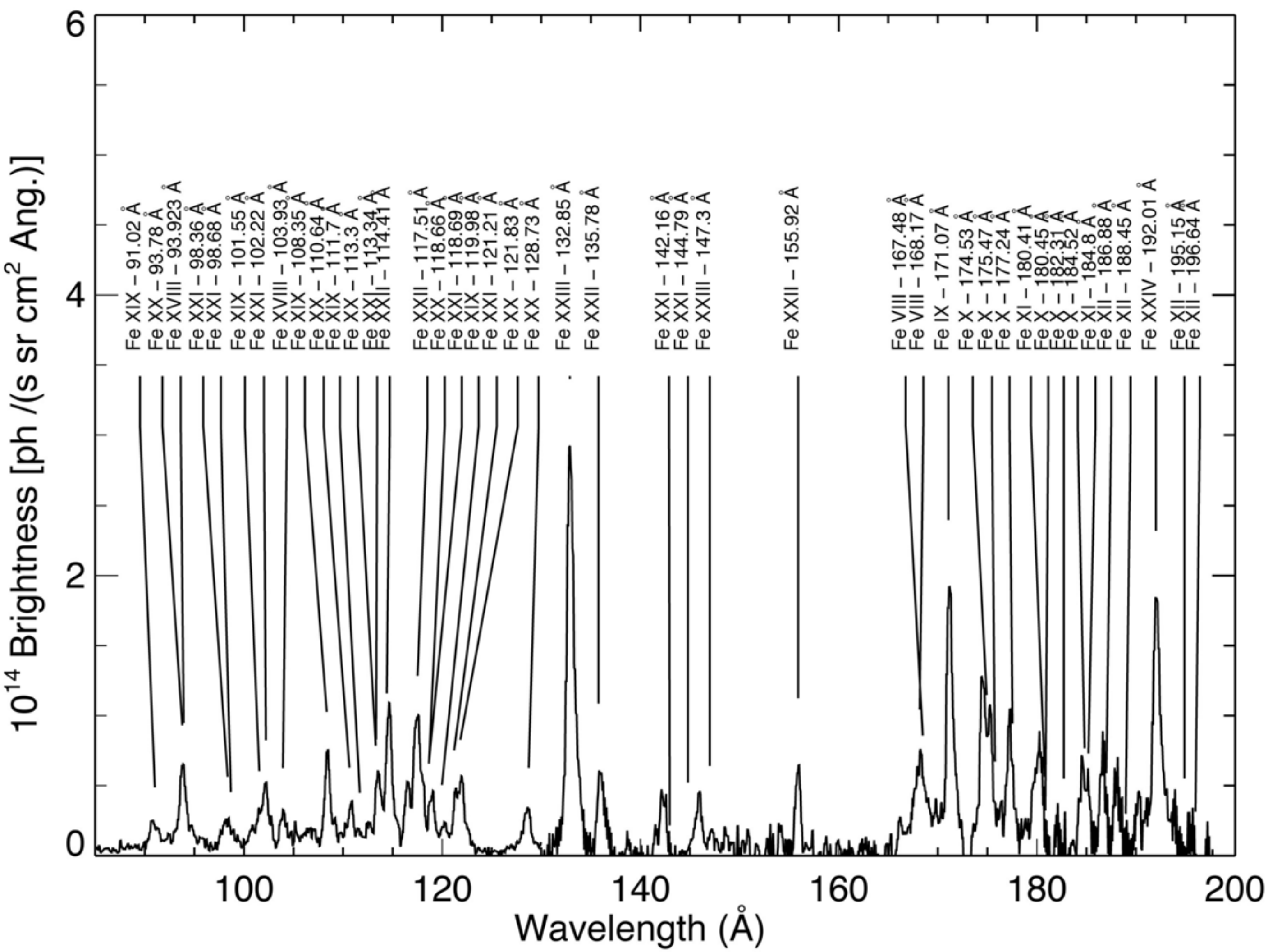


Capella (1996 Mar 3–7)
EUVE SW Spectrometer
Fe XXIII?
Counts
Wavelength (Å)
Capella (1996 Mar 3–7)
EUVE MW Spectrometer
He Ly α
Fe XVI
Fe XV
He Ly β
Counts
Wavelength (Å)

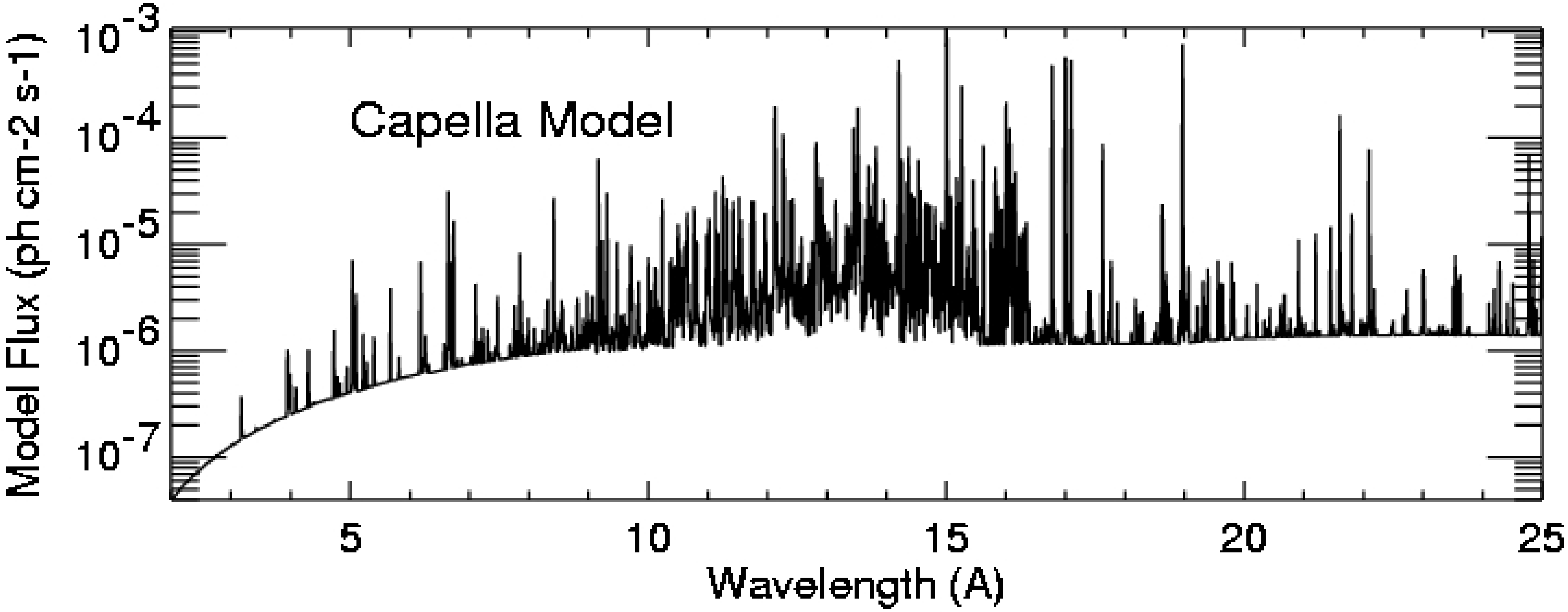
M-shell Fe spectrum emitted by tokamak plasma (FTU, Frascati)



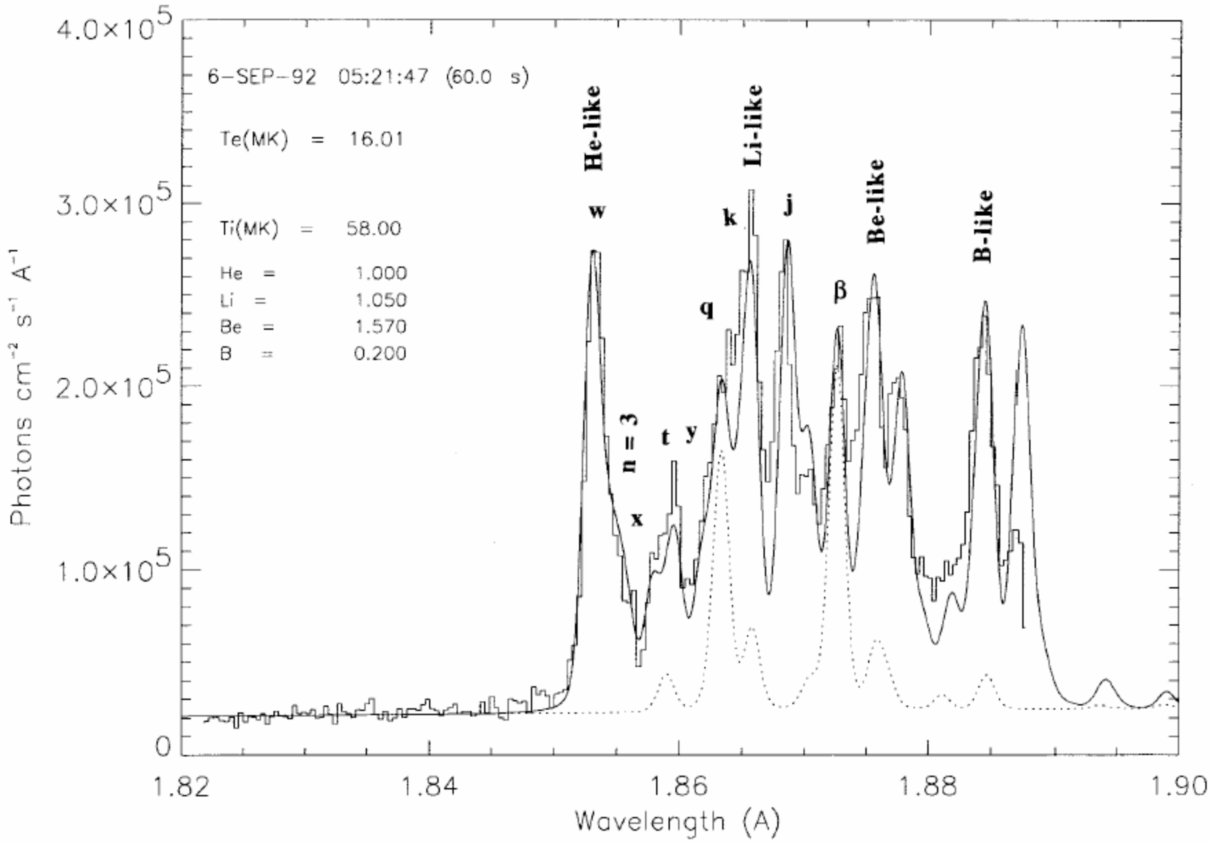
L-shell Fe spectrum from tokamak plasma, 100 – 200A



Fe L-shell from CXO observation (Behar)



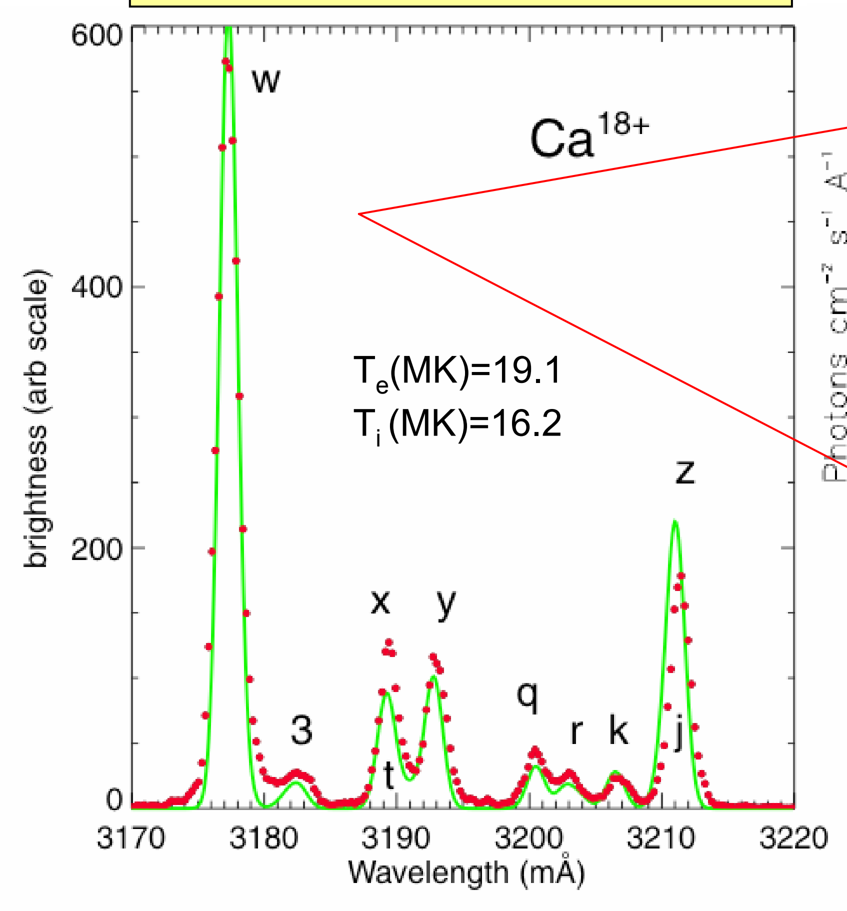
K-shell Fe spectrum from recombination phase of a solar flare



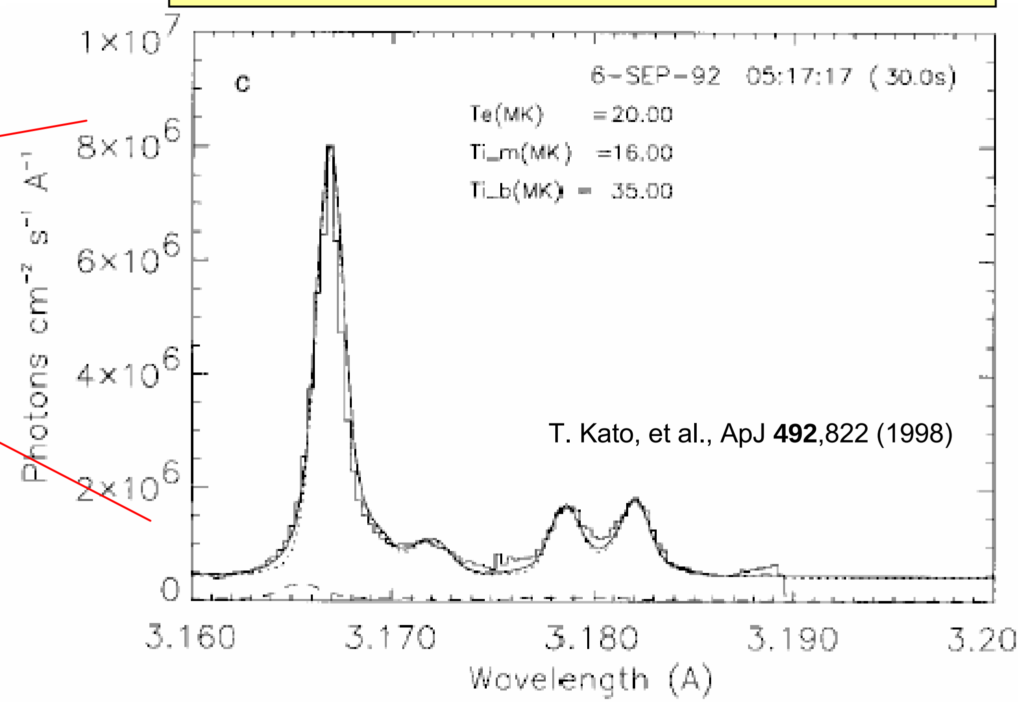
T. Kato, et al., ApJ **492**, 822 (1998)

High-resolution and good detection gives access to other diagnostic line ratios

Ca injection in Alcator C-Mod



Yohkoh blue shifted flare spectrum

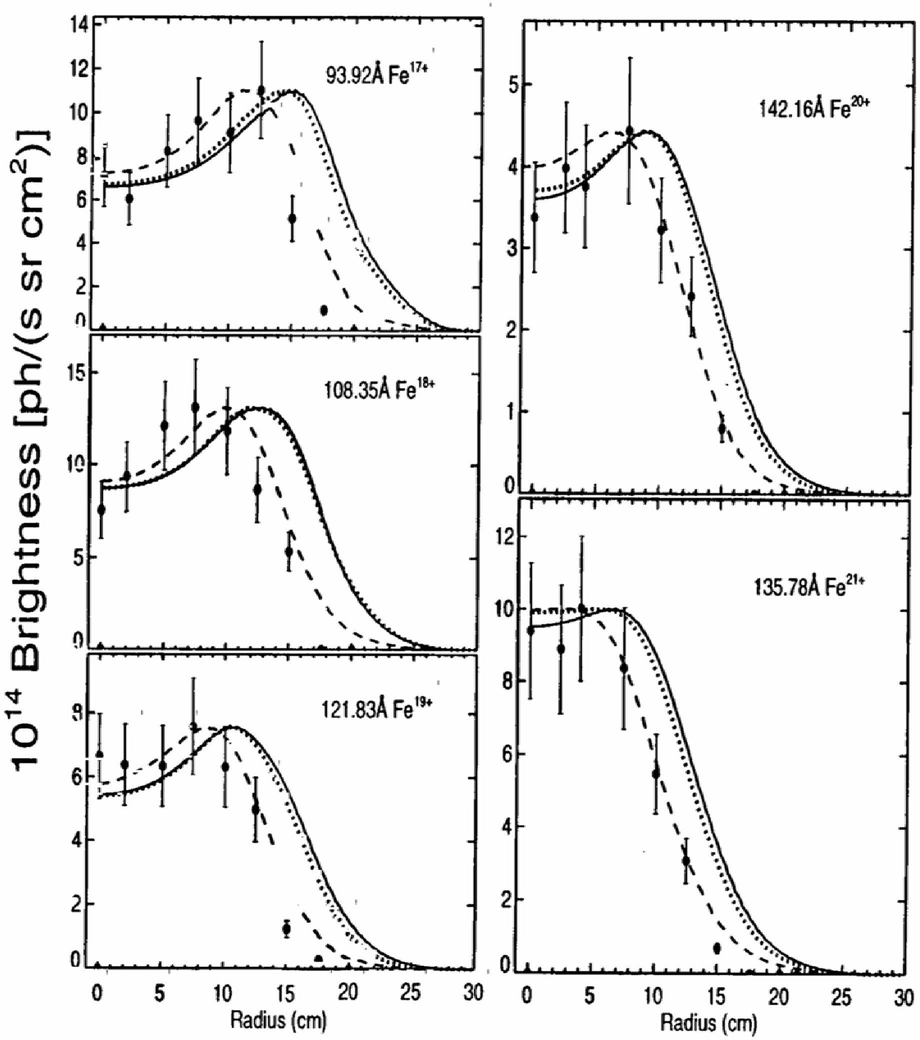


Electron temperatures during solar flares are drived by looking at the *n*=3 to W line ratio, also observed in Alcator C-Mod spectra

J. Rice, et al., Phys. Plasmas **7**, 1825 (2000)

Experimental and modeled spatial profiles for Iron in FTU Tokamak

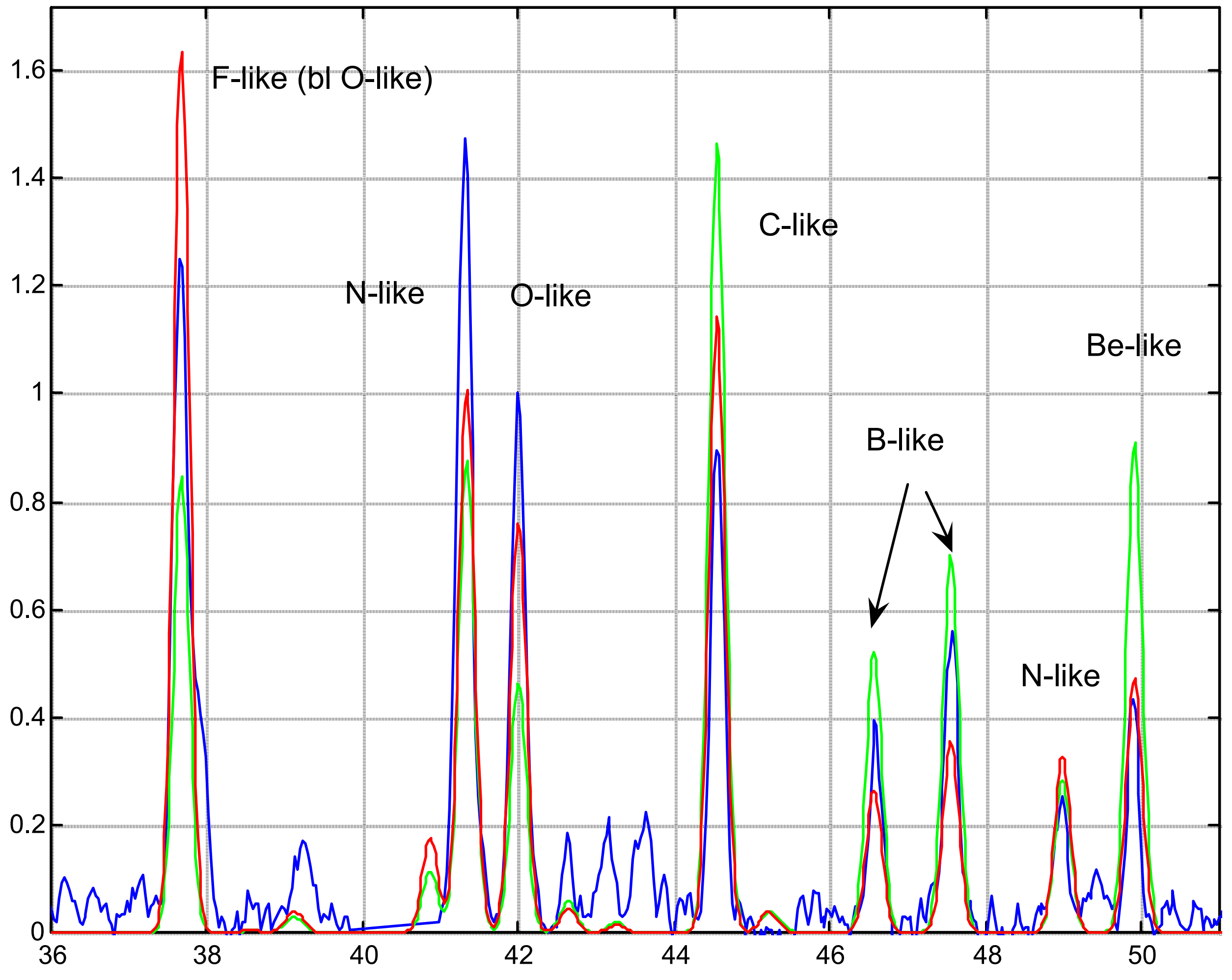
JOHNS HOPKINS



- Measured Fe^{17+} (F-like), Fe^{18+}, Fe^{19+} Fe^{20+}, and Fe^{21+} profiles as a function of position and temperature ($T_e(0) \sim 2keV$)
- MIST simulations with Mazzotta and AR92 atomic physics rates are not adequate to reproduce the experiment
- DR rates (F->Ne like to B->C) must be x2 to recover experiment

········	AR92
—	Mazzotta
----	Mazzotta DR x2

Comparison between experimental and modeled L-shell Molybdenum spectrum (Mattioli et al.)



Motivation for Tokamak/MCF

First Solution: Choice of First Wall

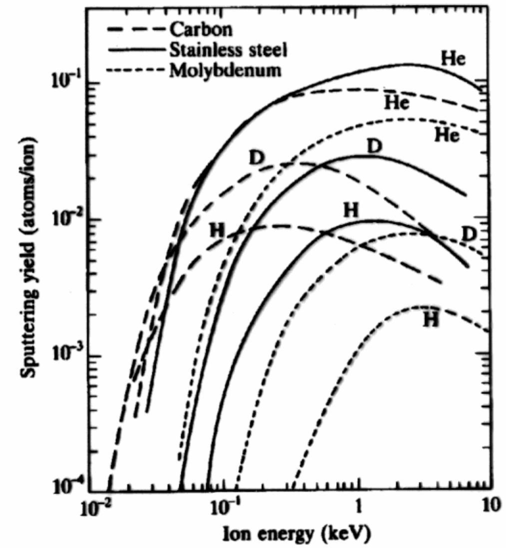
Low Z: (C, Be, Li)

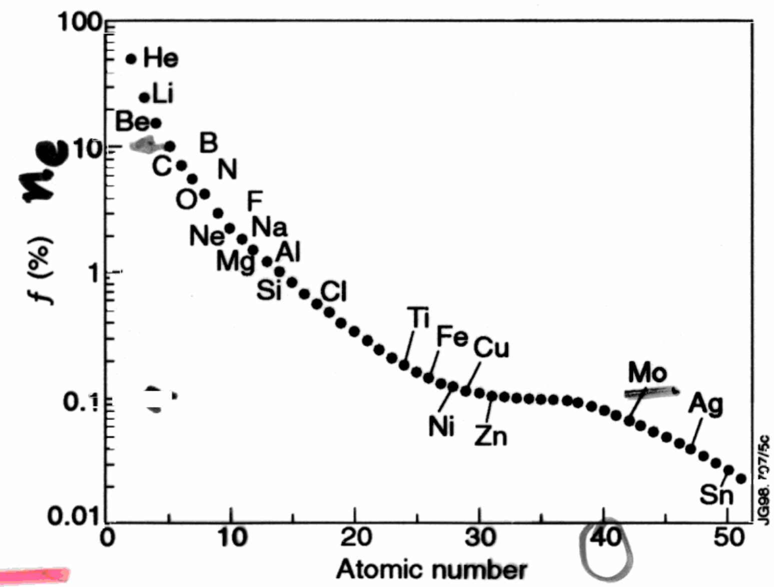
- Significant sputtering problem
- Minimal radiation problem

High Z: (Mo, W)

- Low sputtering
- Significant radiator can reduce core temperature thus reducing fusion yields
- Critical concentration of high Z impurities to have an acceptable Lawson Criterion

$n\tau \sim 10^{14}\ cm^{-3}\ sec$





Ionization Balance Simulations for Kr

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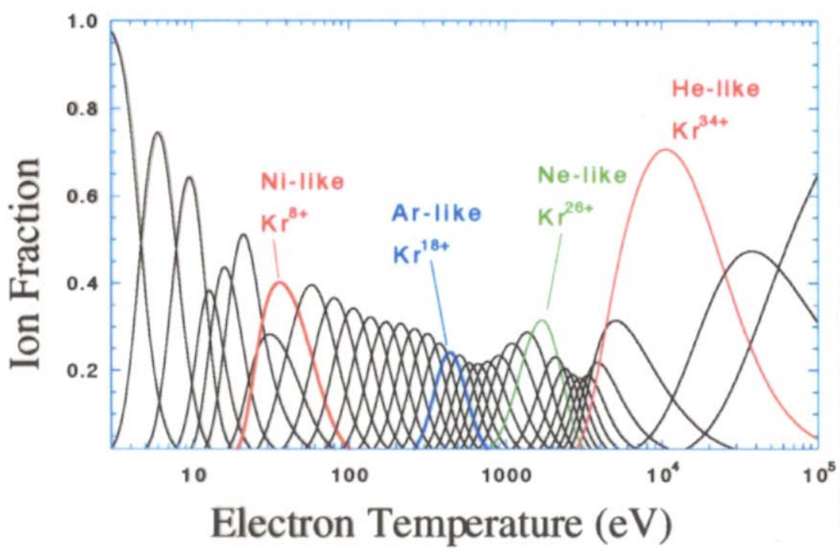
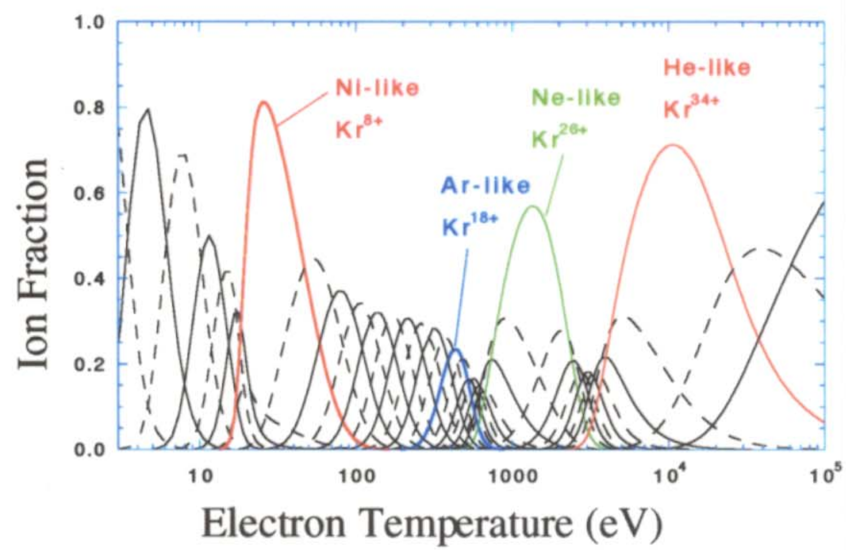
AdPak Model for Kr

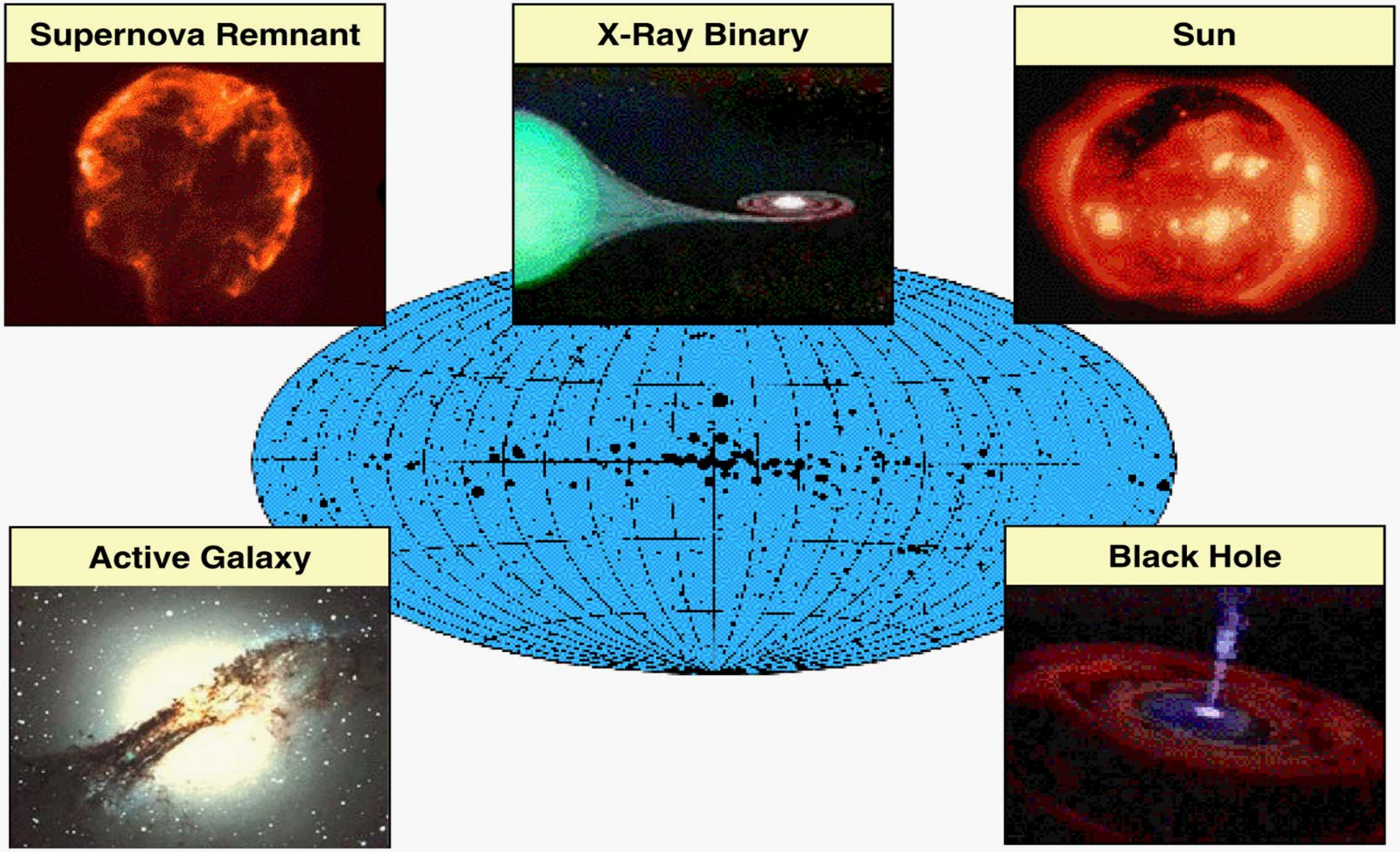


HULLAC Model for Kr



Detailed treatment of excitation-autoionization and dielectronic recombination shows significant impact on the charge state distribution

The universe is x-ray active



FeIX (171Å) is an important temperature diagnostic of the solar chromosphere

EIT SOHO image of the sun at 171Å

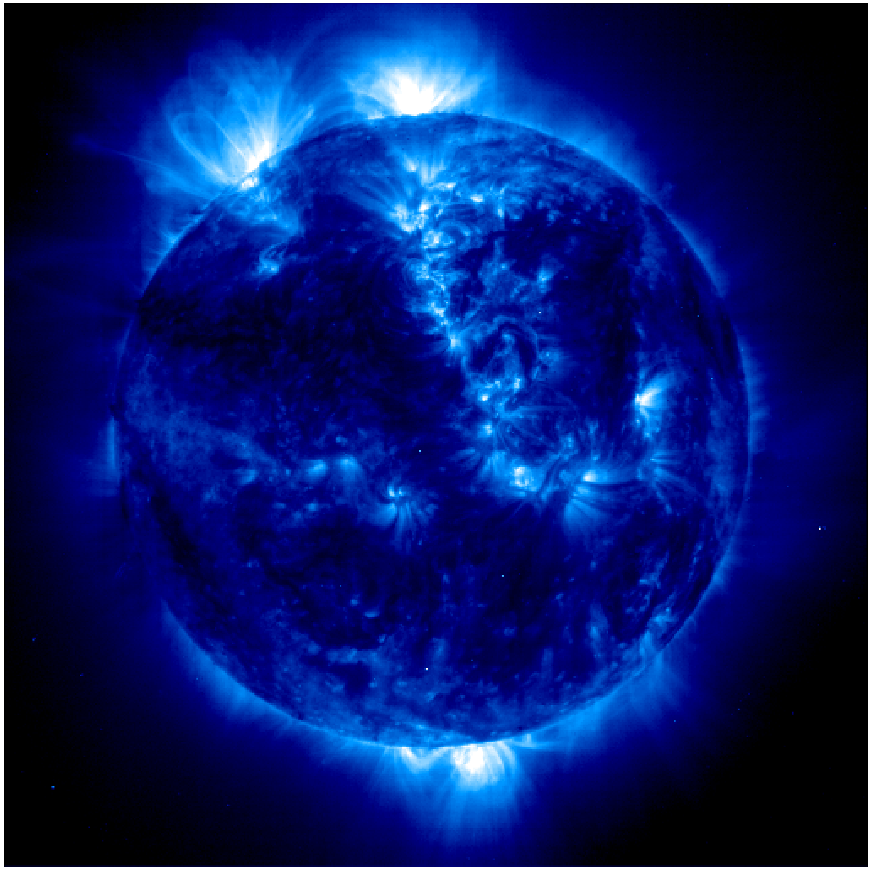
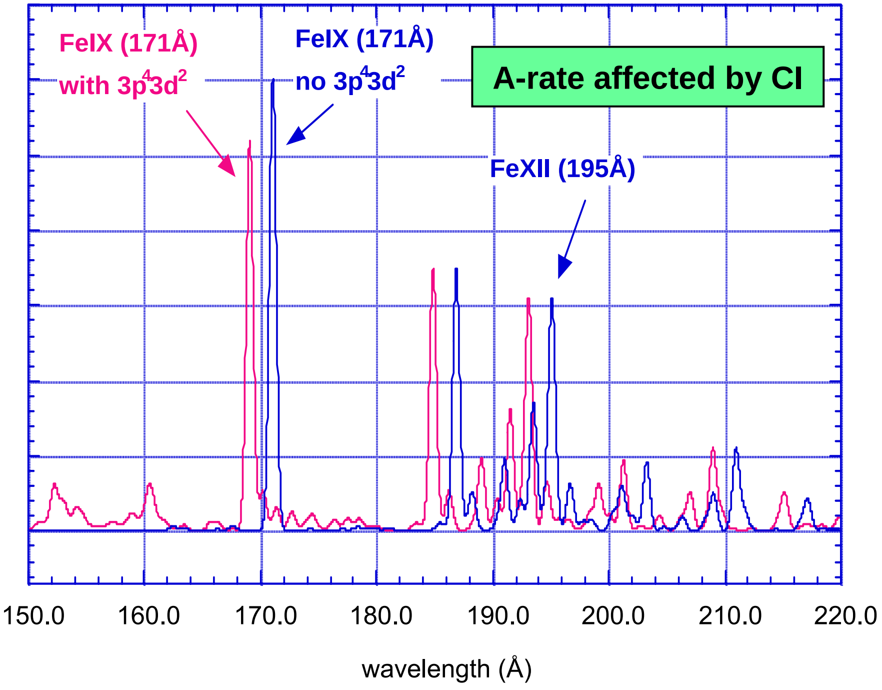


Image from http://umbra.nascom.nasa.gov/eit/eit_full_res.html
07Dec1999 19:00:15
SOHO - Extreme Ultraviolet Imaging Telescope

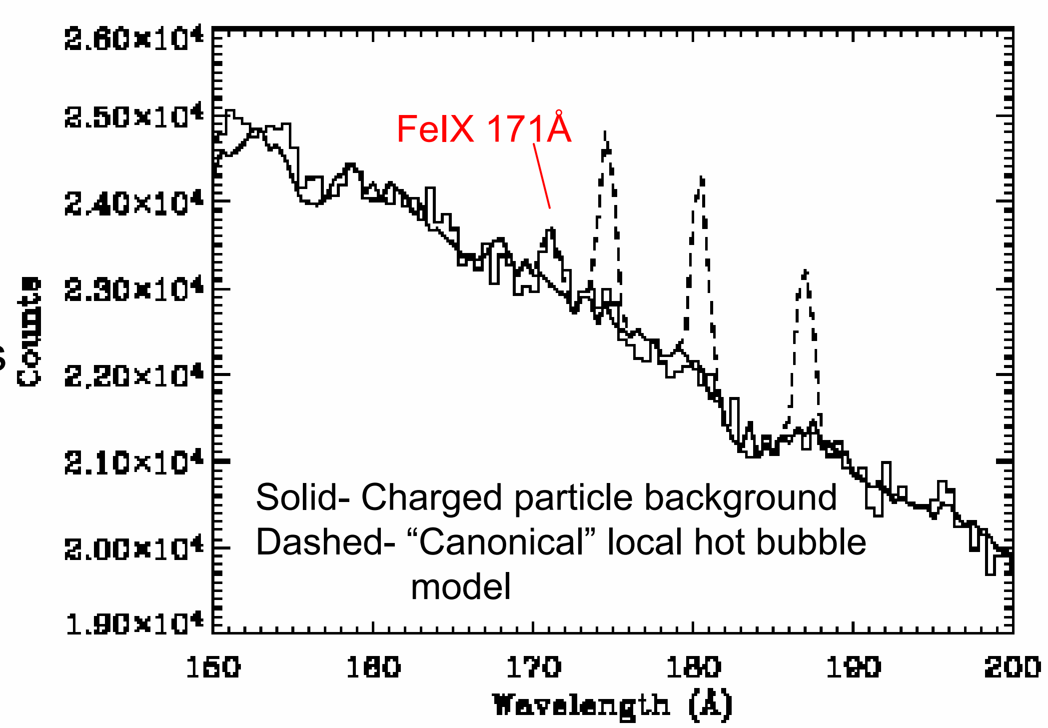


Neglect of $3p^43d^2$ in models leads to a 20% overestimate of the 171Å/195Å ratio

Recent CHIPS observations of FeIX soft x-ray emission indicate local ISM is out of equilibrium

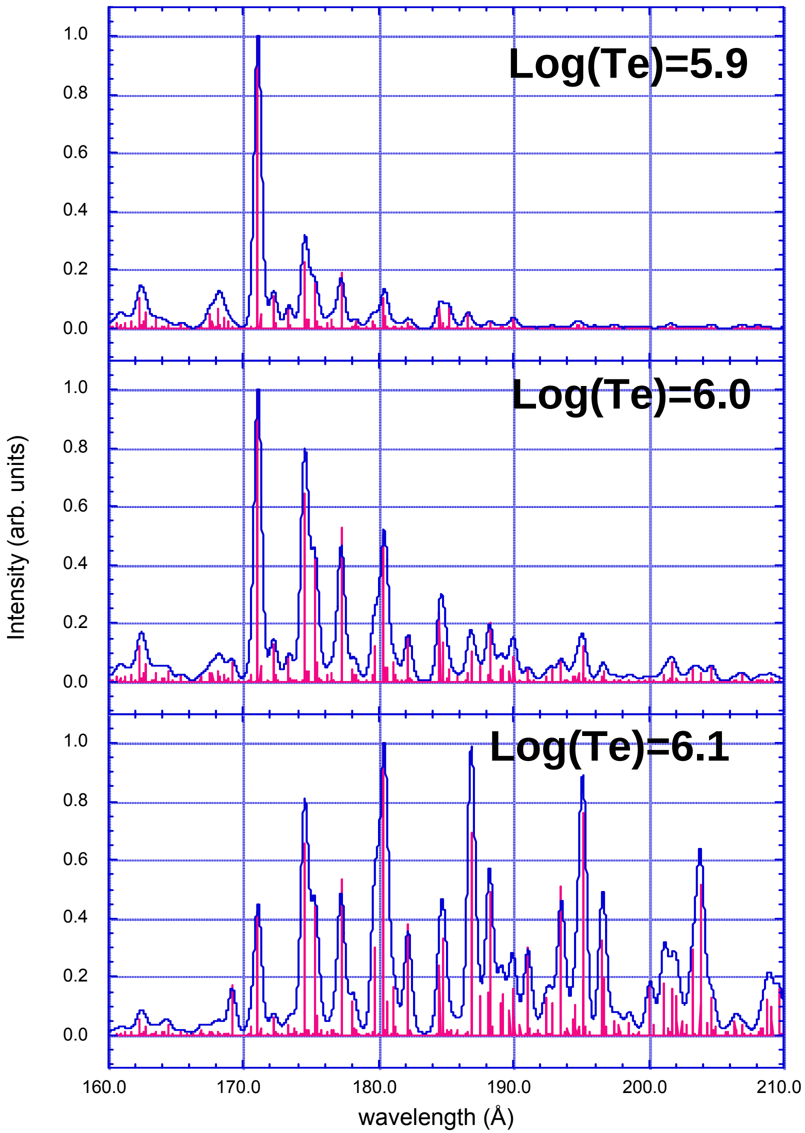
Recent work of Hurwitz, Sasseen and Sirk:

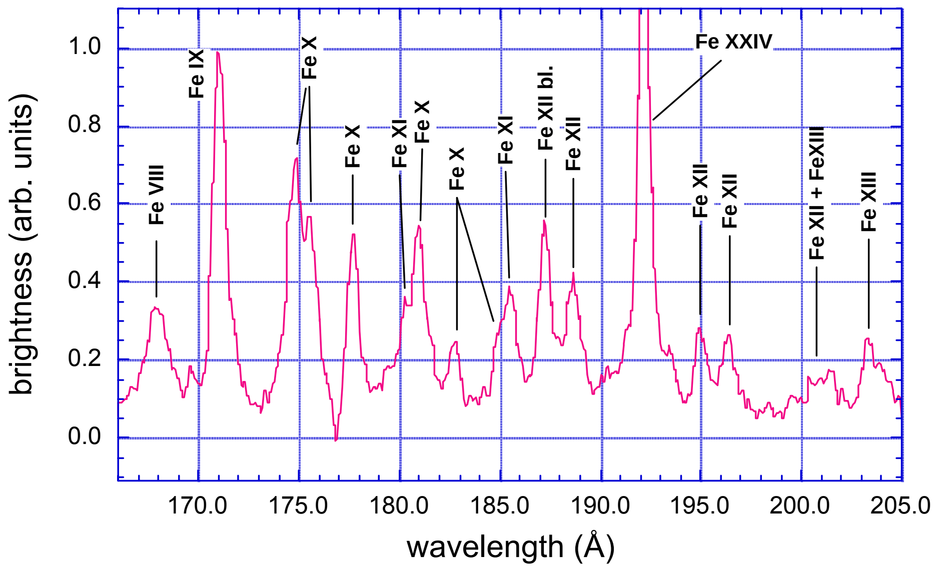
- Canonical models have the local bubble as a CIE gas at XXX K.
- Diffuse x-ray emission is supports this picture.
- Substantial counts above the background in the bins covering FeX - FeXII should be seen.
- As a result, the soft x-ray emitting gas must be at a temperature below XXXK.



ApJ Letter preprint at http://chips.ssl.berkeley.edu/AAS1.pdf

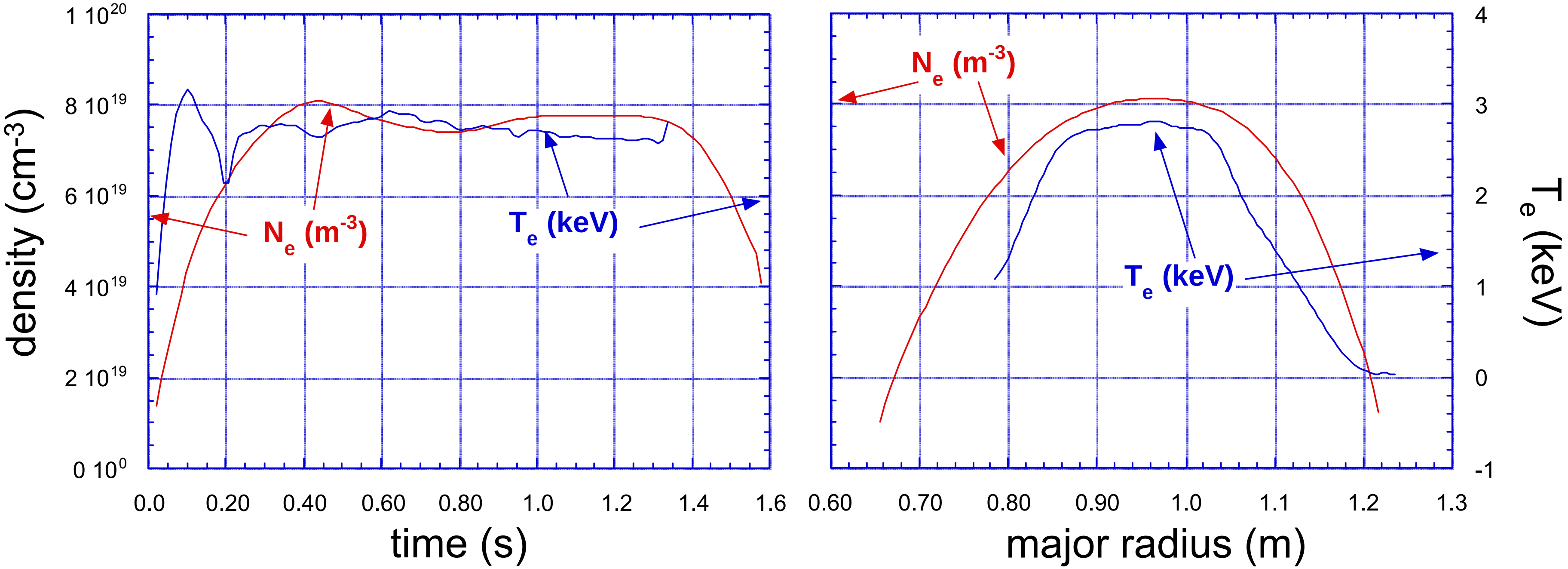
Measured M-shell iron spectrum is a sensitive thermometer



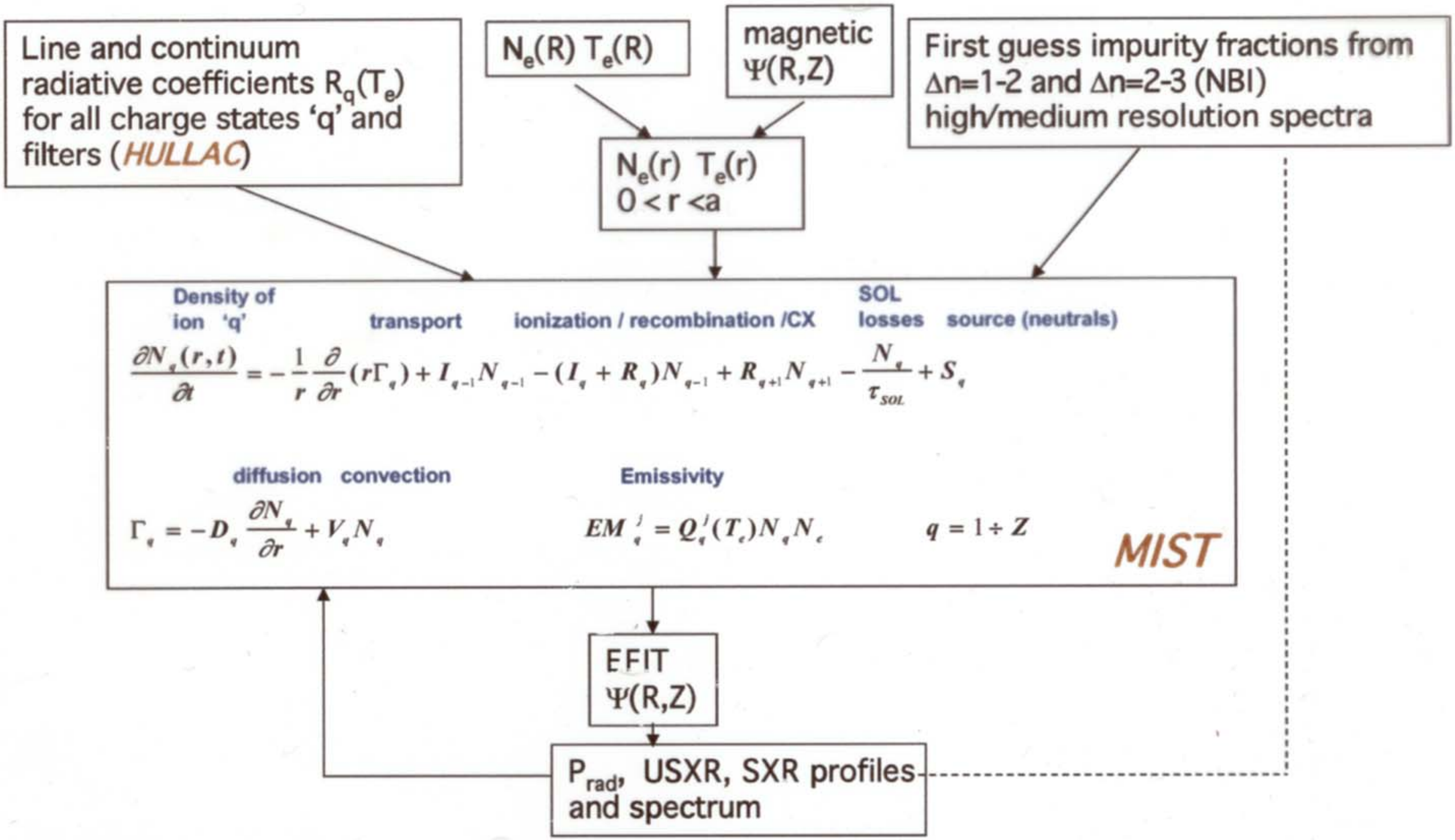


- Ramp-down plasma temperature profile is measured to be nearly single valued
- Ionization equilibration times are 10's of μs, much faster than changes in plasma conditions
- Measured volume-averaged temp $\langle T_e \rangle = 75 \pm 30$ eV ($\log(T_e) = 5.94$).

Electron temperature and density profiles and histories for a typical FTU discharge



Impurity transport modeling



- **Cross-field particle flux (D,V) varied to match complete experimental data set**
- **Self-consistent transport solution obtains from time-dependent computations**

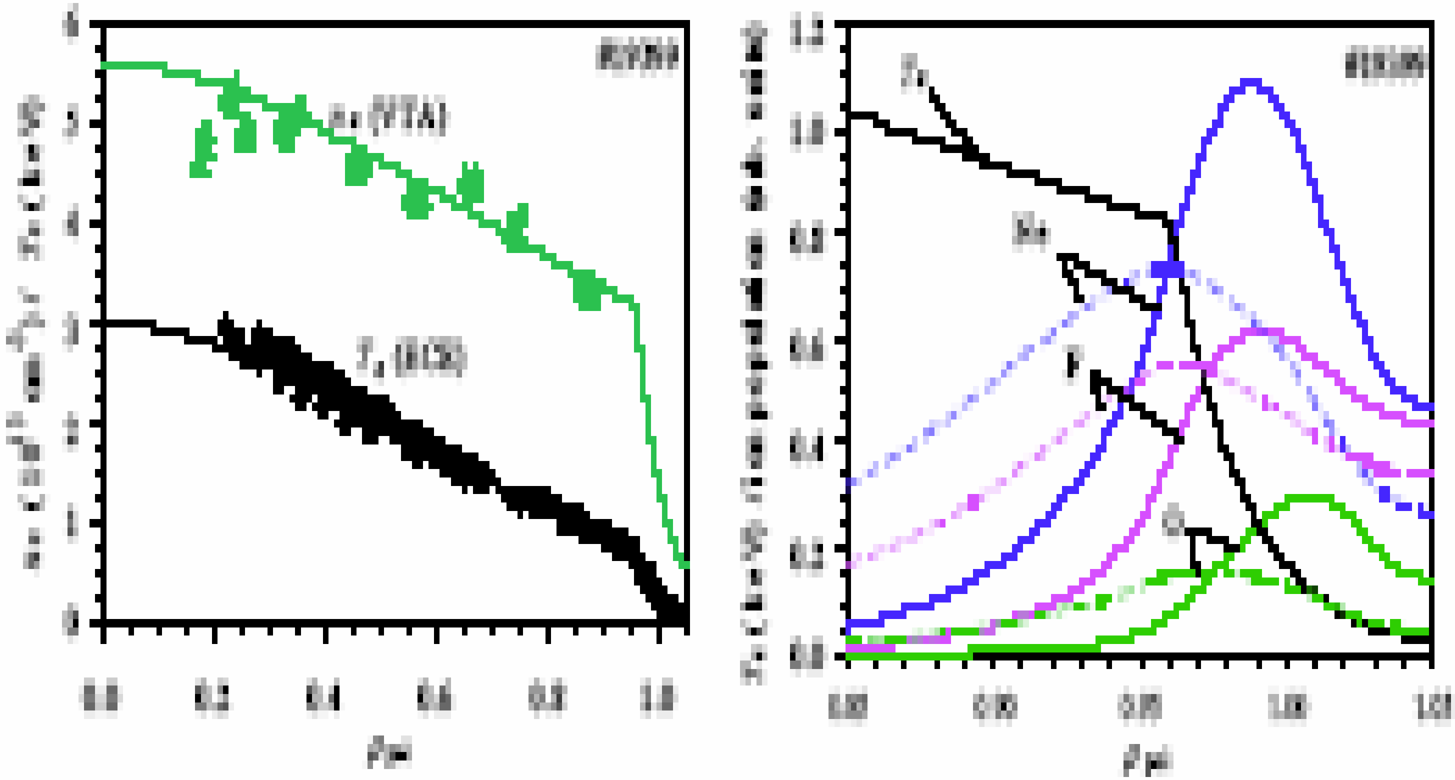
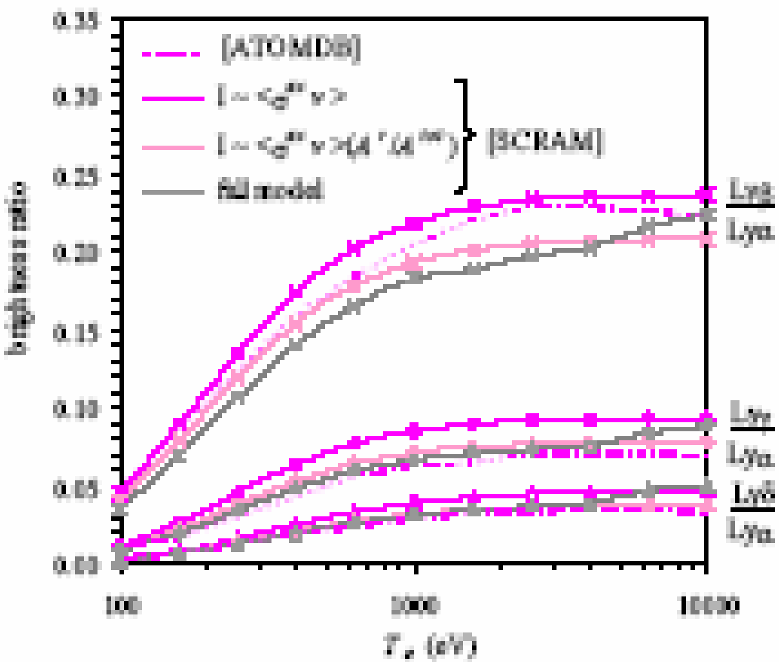


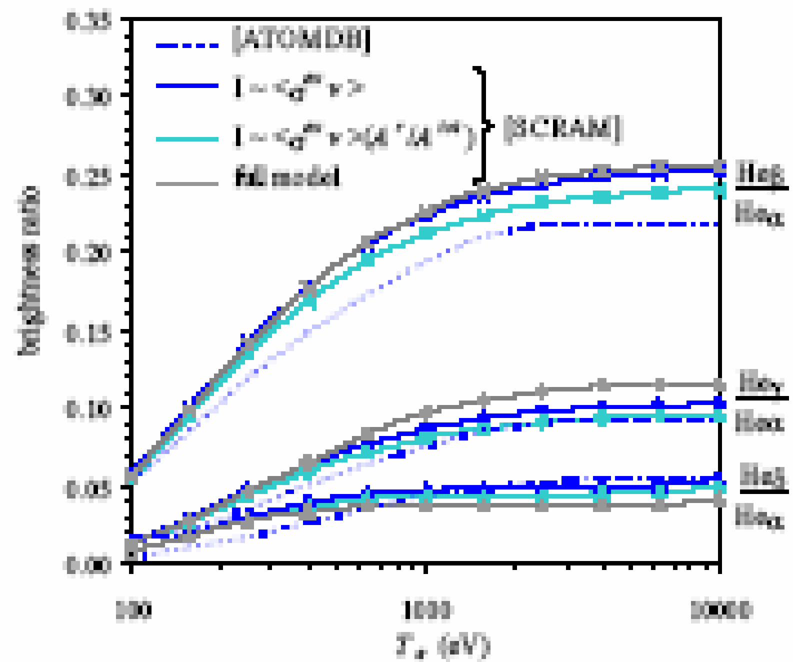
Fig. 1.— Left: measured n_e and T_e along the poloidal axis. Right: He-like (solid) and H-like (dashed) ion populations from STRAHL in the radiating region $\rho_{pol} = 0.85 - 1.06$.

Model dependence of $(np - 1s)/(2p - 1s)$ ratios

H-like Ne



He-like Ne

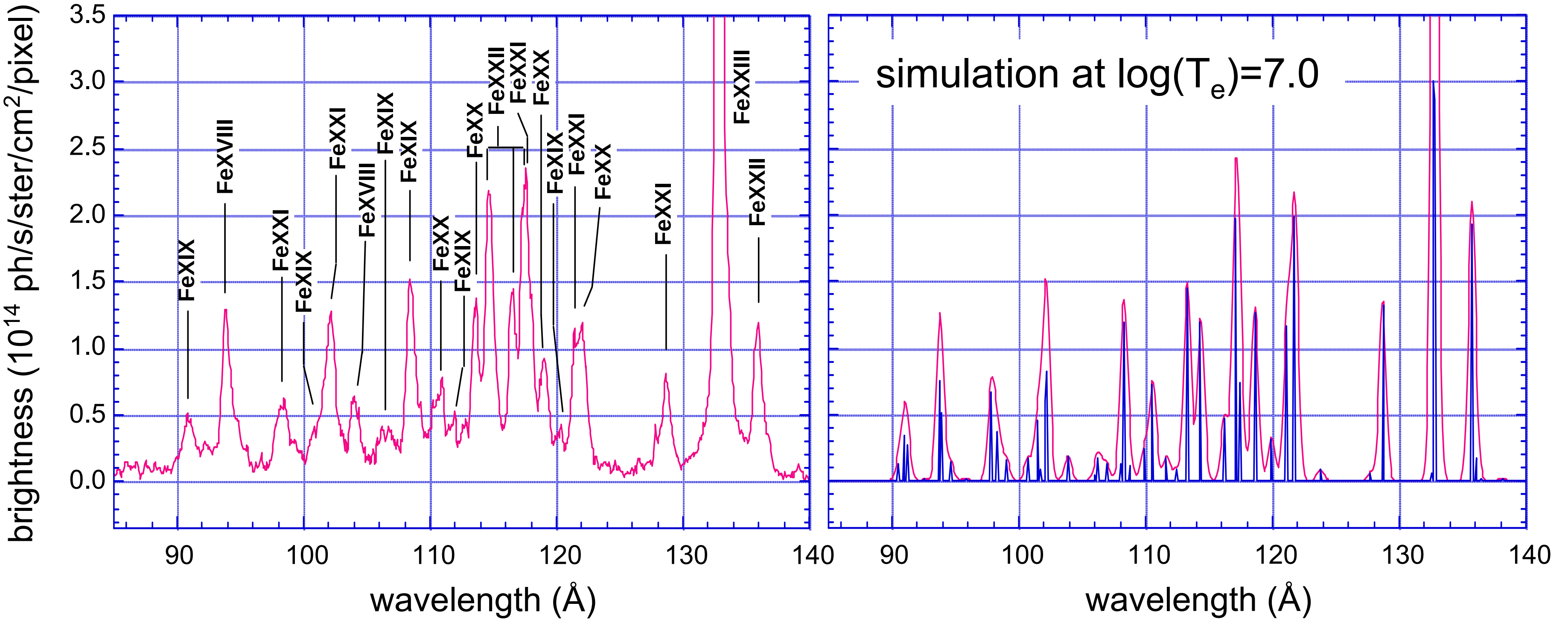


In the coronal approximation (Intensity ~ $<\sigma^{ex}v>$), intensities are limited by collisional excitation rates. Branching ratios A^r/A^{tot}, kinetic effects (cascades, recombination…), and the underlying model structure also affect line intensities.

Observed L-shell lines serve as local density diagnostics in stellar coronae

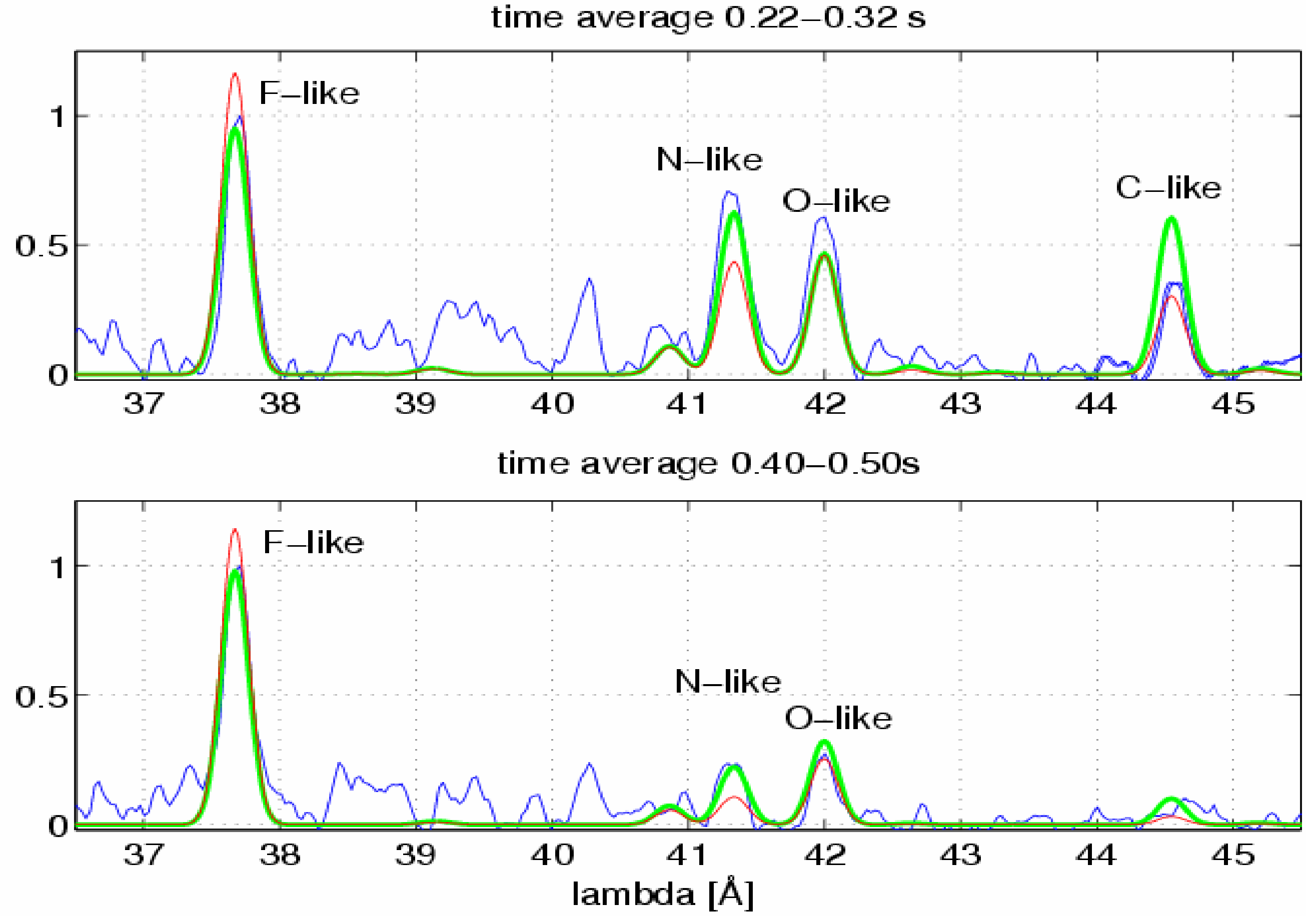
Fe L-shell Δn=0 spectra (absolute units)

HULLAC simulation at resolution



Pre-injection background signal subtracted from data

K.B. Fournier, et al., ApJ **561**, 1144 (2001)



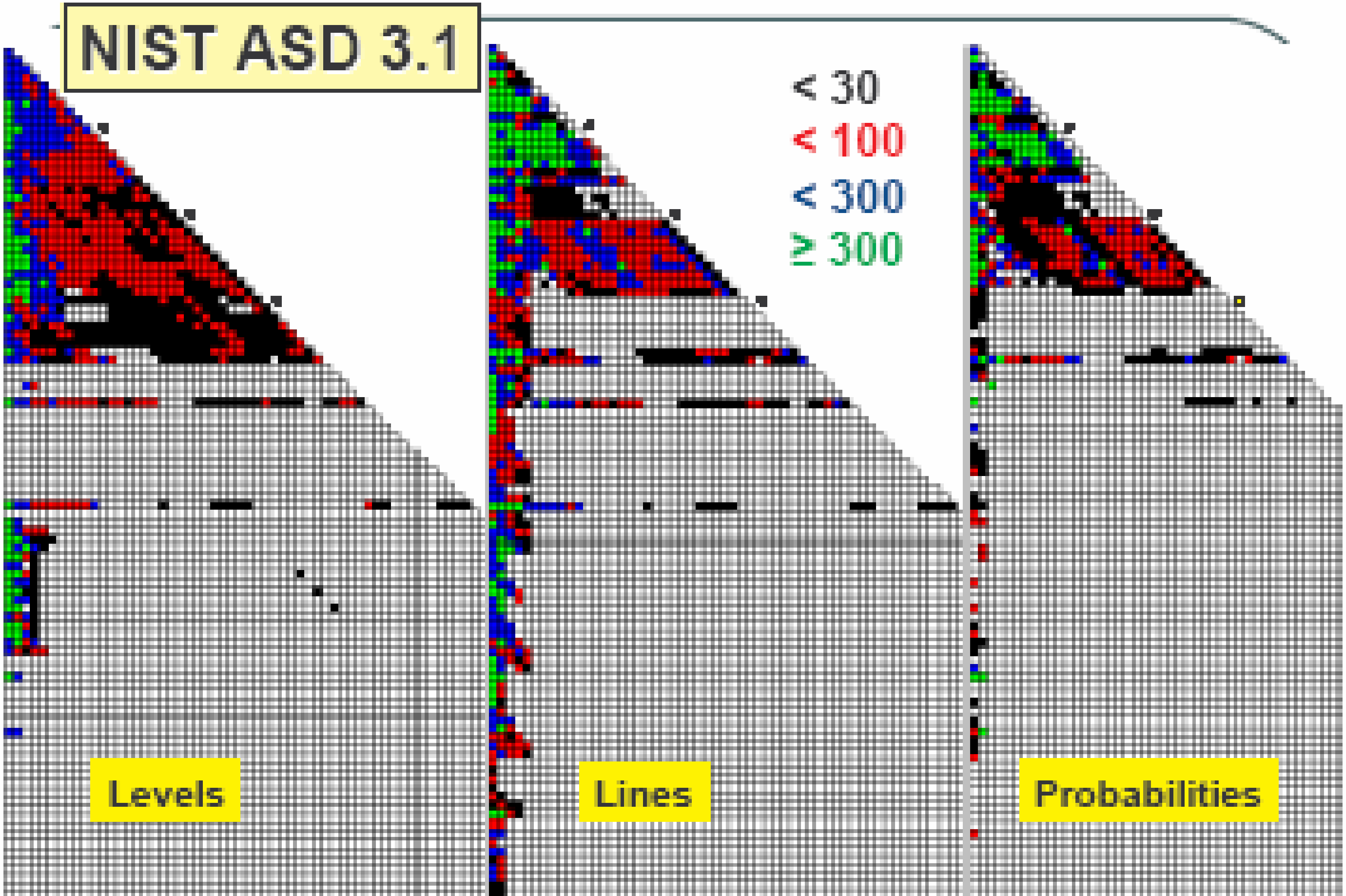
Comparison between experimental and computed
L-shell Mo spectra emitted from FTU tokamak

Atomic Processes Involved in Modeling

- Ionization
  - Electron/proton collisions
  - Photoionization
  - Innershell ionization
- Excitation/De-excitation
  - Electron/proton collisions
  - Photoexcitation
  - Radiative decay/cascades
- Recombination
  - Dielectronic
  - Radiative
  - Charge exchange
  - 3-body

- **Laboratory observations have the capabilities to**
  - catolog lines and study/deconvolve line blends
  - benchmark N_e and T_e diagnostic lines and ratios
  - look at ionization-equilibria emisison spectra
  - look at non-thermal effects

NIST ASD 3.1

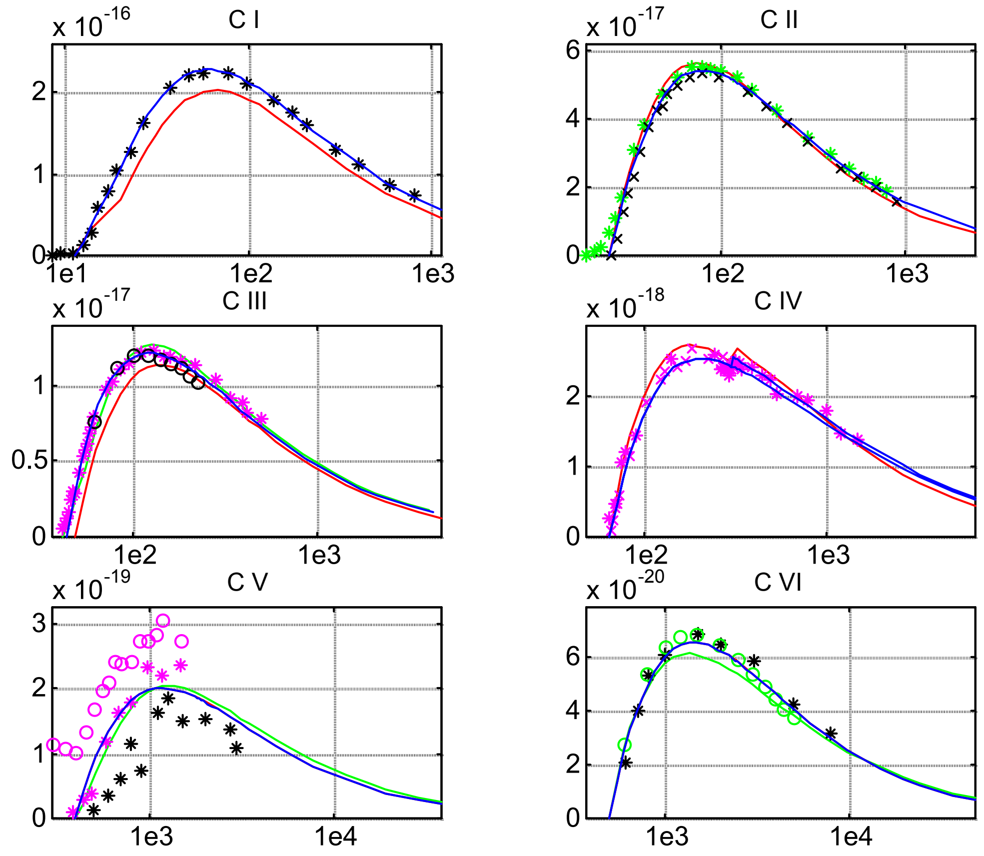


Y: nuclear charge; X: ion charge

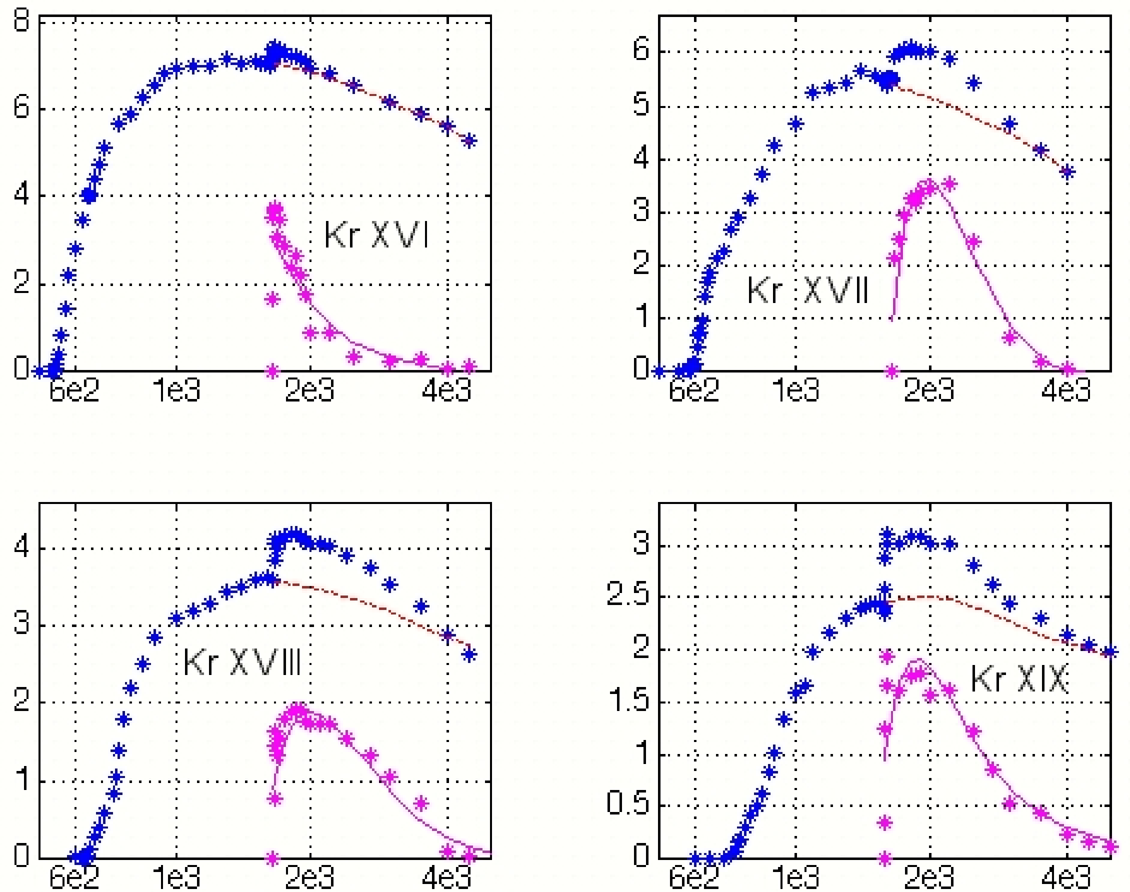
TABLE I: Internet atomic databases for high-temperature plasmas. Keys: CS – cross sections, EL – energy levels, KP – plasma kinetic parameters, LB – line broadening, MSC – miscellaneous spectroscopic and collisional data, RC – rate coefficients, SP – plasma emission spectrum, TP – transition probabilities, WF – wavefunctions, WL – wavelengths.

Institution (Country) Database(s)	Numerical Data	Bibliographic Data	Online Calculations
Harvard-Smithsonian CfA (USA)			
Kelly, Kurucz	EL,WL,TP		
IAEA (Austria)			
AMDIS		MSC	
ALADDIN	CS,RC		
BEXCITE, RATES			CS,KP
IAPCM (China)			
CAMDB	MSC	MSC	
ISAN (Russia)			
BIBL		MSC	
KAERI (Korea)			
AMODS	MSC		EL,WL,TP
LANL (USA)			
LAPC			MSC
NASA (USA)			
TIPTOP	EL,WL,TP,CS,RC		
NIFS (Japan)			
PLAM	CS,RC	MSC	
NIST (USA)			
ASD	EL,WL,TP	TP,LS	SP
Chandra	EL,WL,TP	TP,LS	
ATP		TP	
ASL		LB	
ORNL (USA)			
Bibliography		MSC	
MIRF	CS		
Vanderbilt University (USA)			
MCHF/MCDHF	EL,WL,TP		WF
VNIITF-VNIIFTRI (Russia)			
SPECTR-W[3]	MSC	MSC	

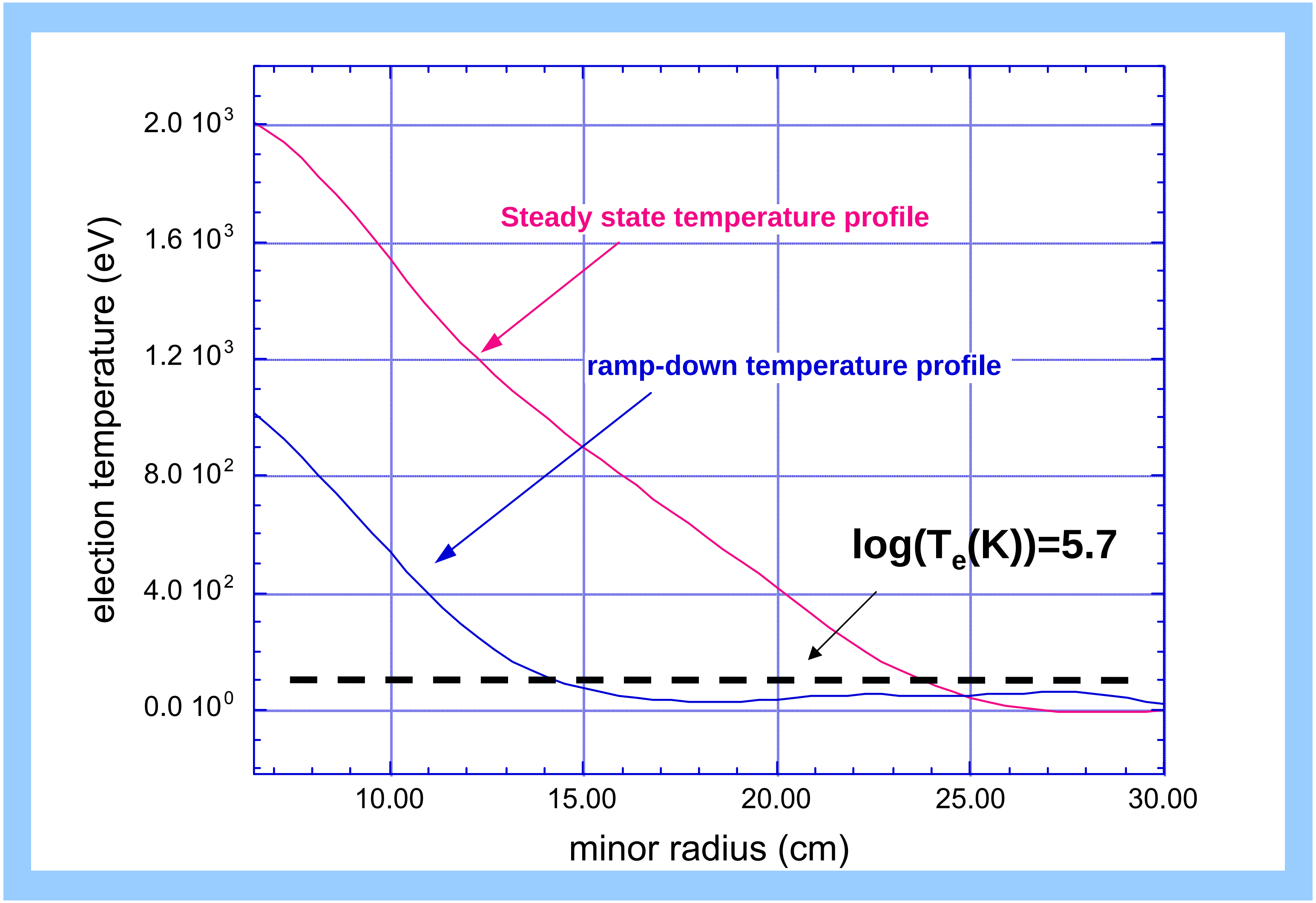
Electron impact ionization rates (ap. Mattioli)



Electron impact ionization rates for Kr (ap. Mattioli)

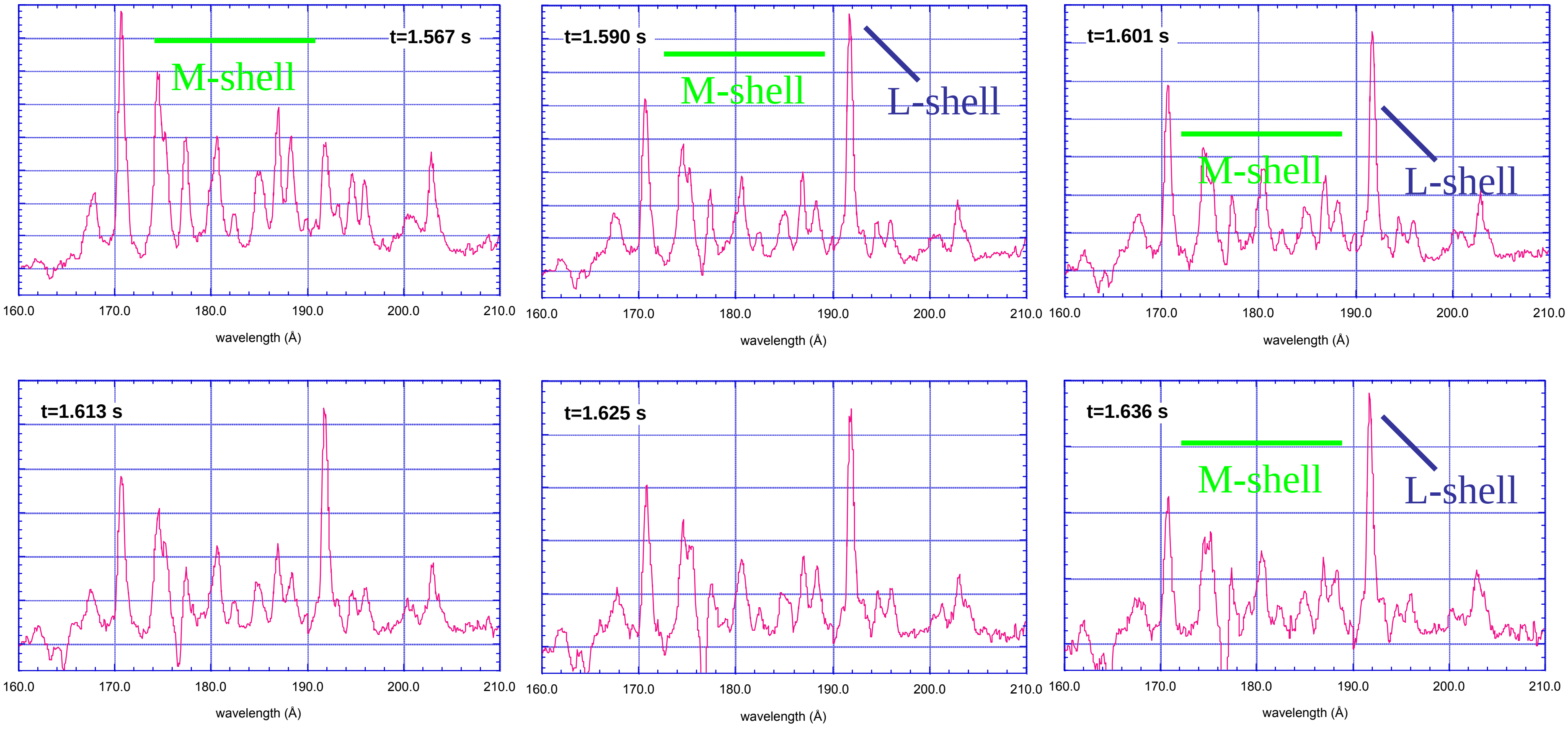


Electron temperature during rampdown is essentially gradient free over large volume



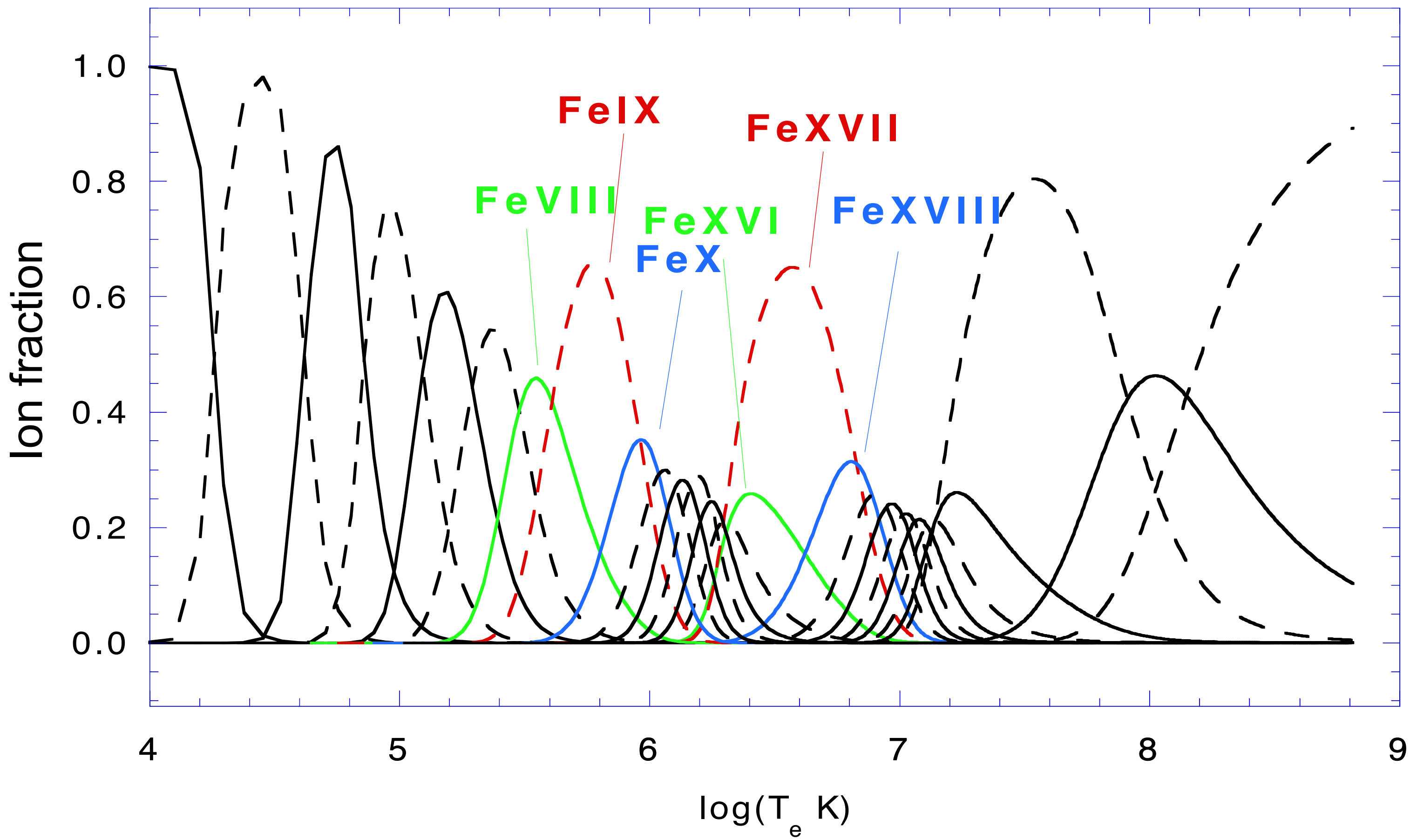
M.J. May, et al., Nucl. Fusion **42**, 1299 (2002)

Background subtracted M-shell iron data from a current ramp-down injection in FTU



We see the evolution of the iron charge state distribution during the injection

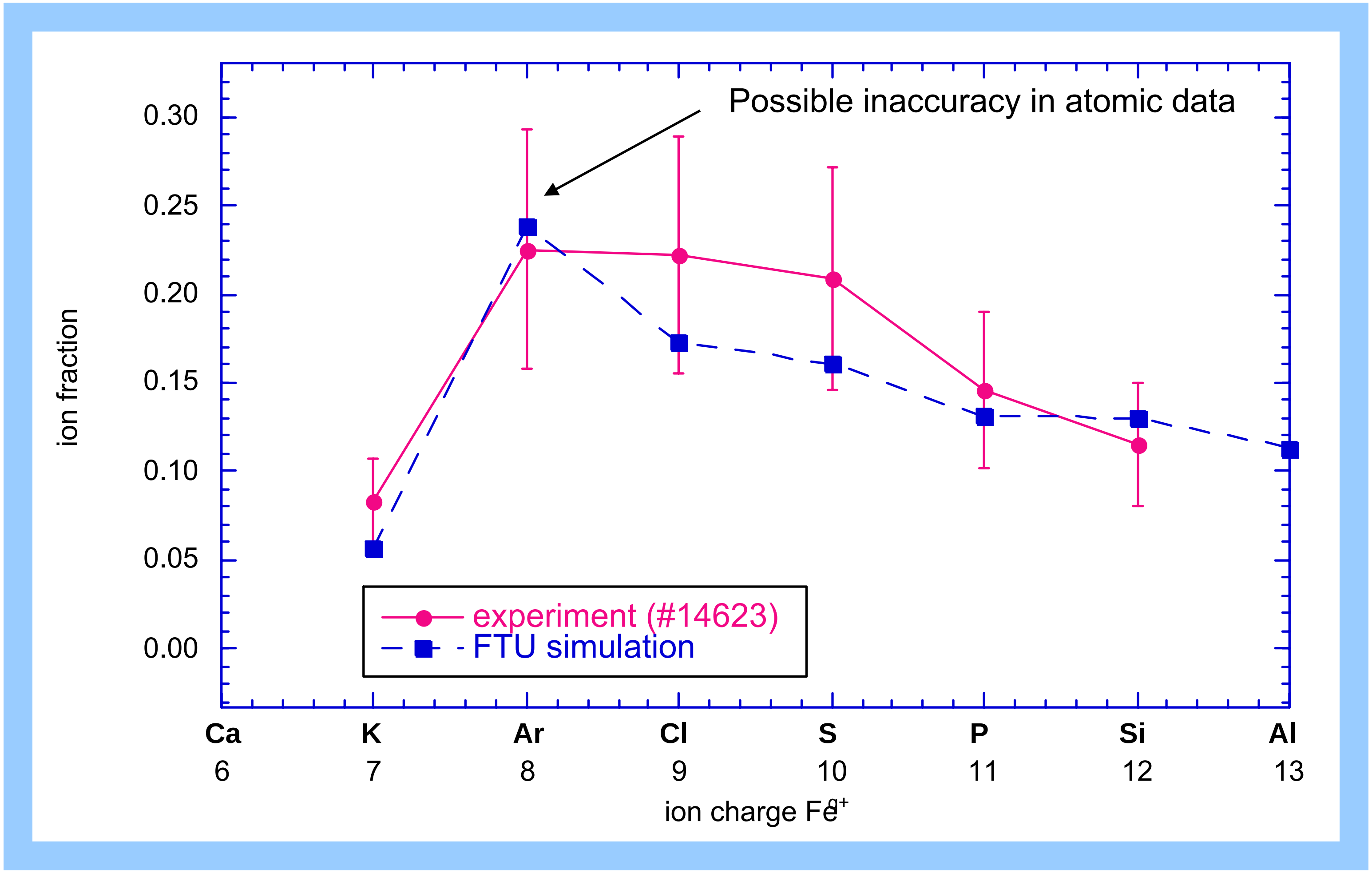
Ionization equilibrium calculations are essential for interpreting spectroscopic data



Calculations must include multi-step processes (EA and DR)

M. Arnaud and J. Raymond, ApJ, **398**, 394 (1992)

Measured iron M-shell CSD and best simulation using updated atomic physics

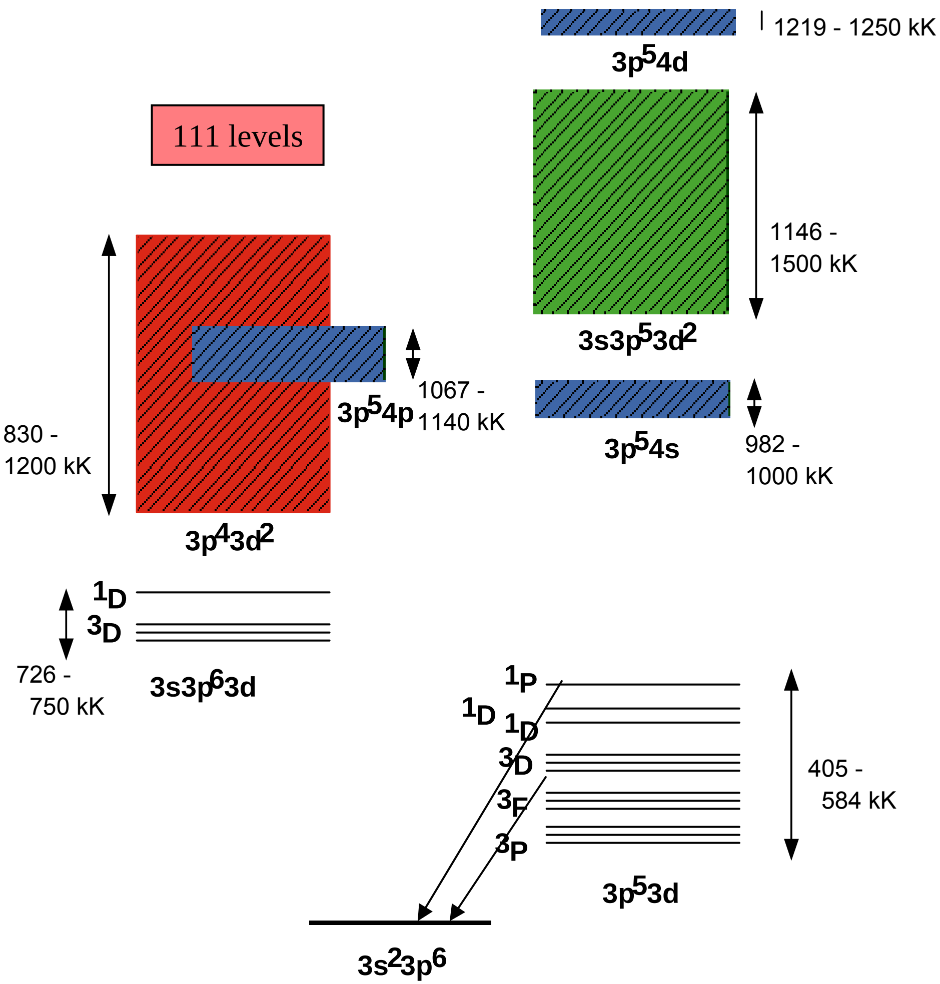


These observations confirm modeling codes used to compute emission measures

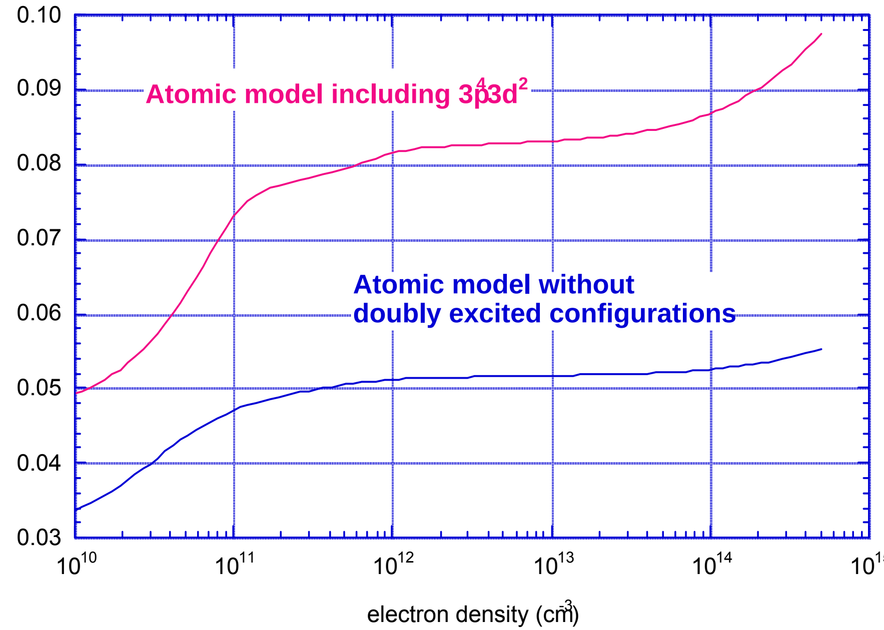
K.B. Fournier, et al., ApJ **550**, L117 (2001)

FeIX line emission is sensitive to population flux from highly excited configurations

Some configurations in FeIX



FeIX Ratio (217Å/171Å)



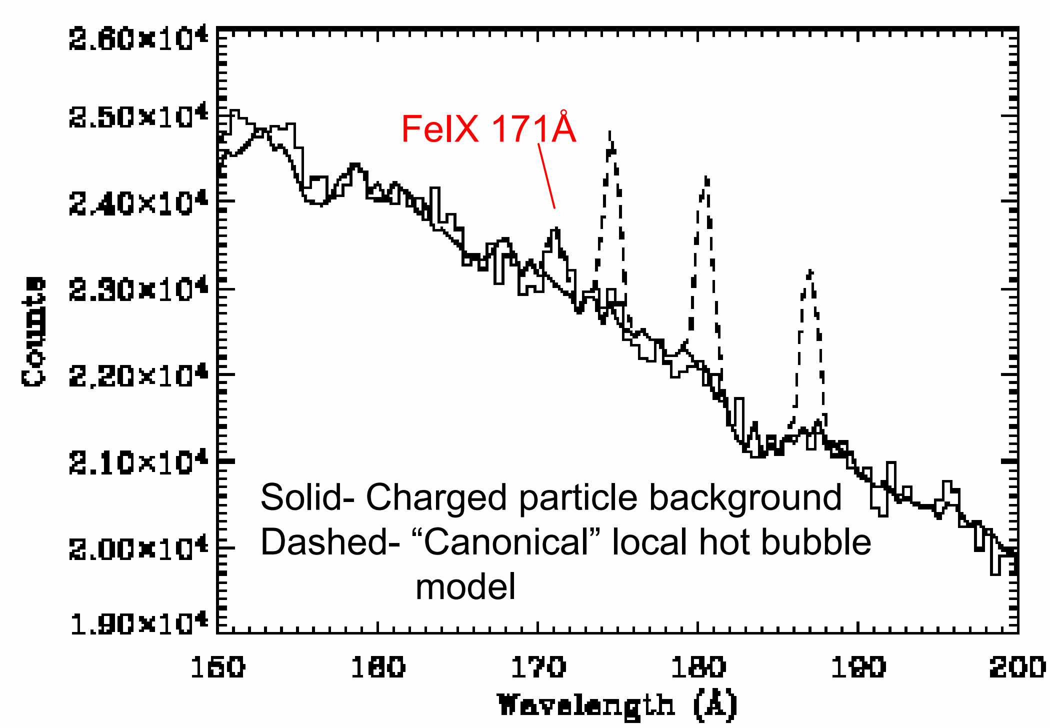
Including $3p^4 3d^2$ in the FeIX model results in a ≥ 50% enhancement of the $^3D_1$ - ^1S / ^1P - ^1S ratio

D.A. Liedah., *Atomic Data Needs for X-ray Astronomy*, NASA/CP-2000-209968

Recent CHIPS observations of FeIX soft x-ray emission indicate local ISM is out of equilibrium

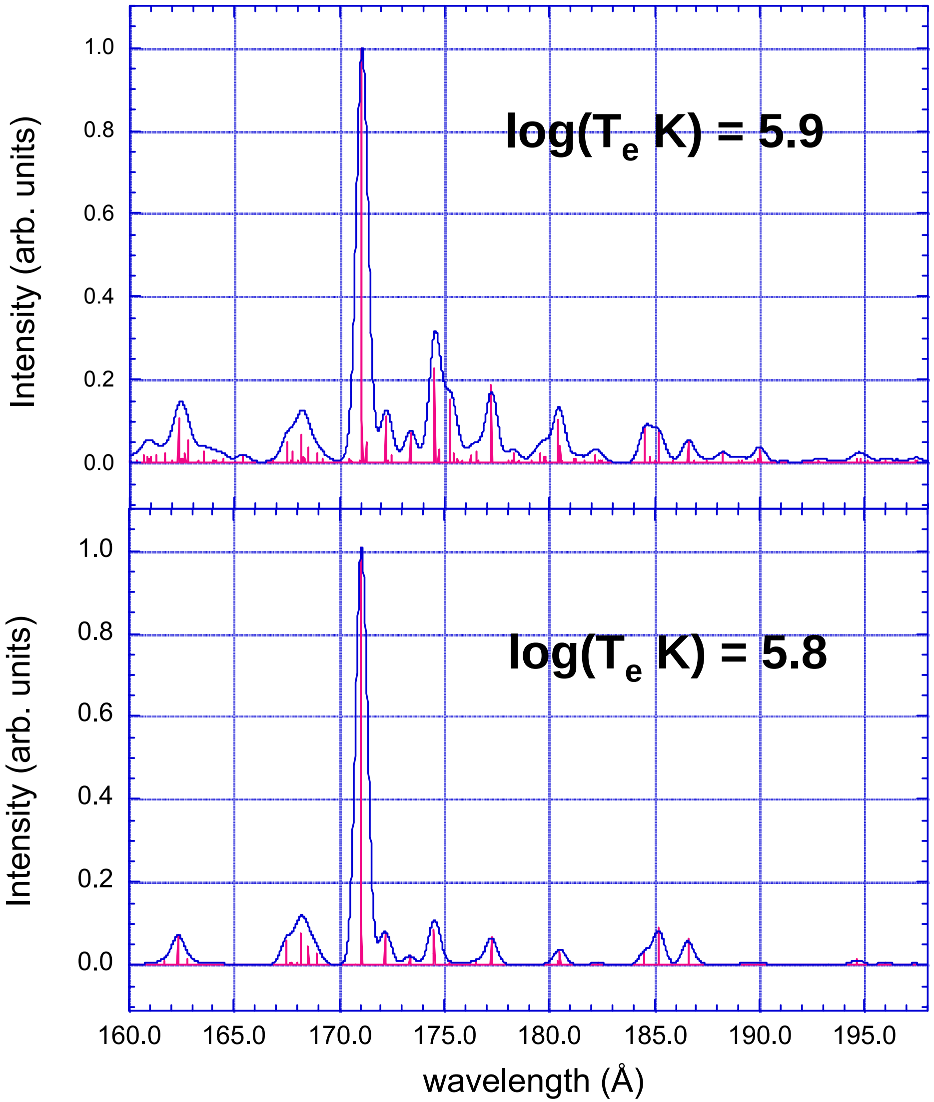
Recent work of Hurwitz, Sasseen and Sirk:

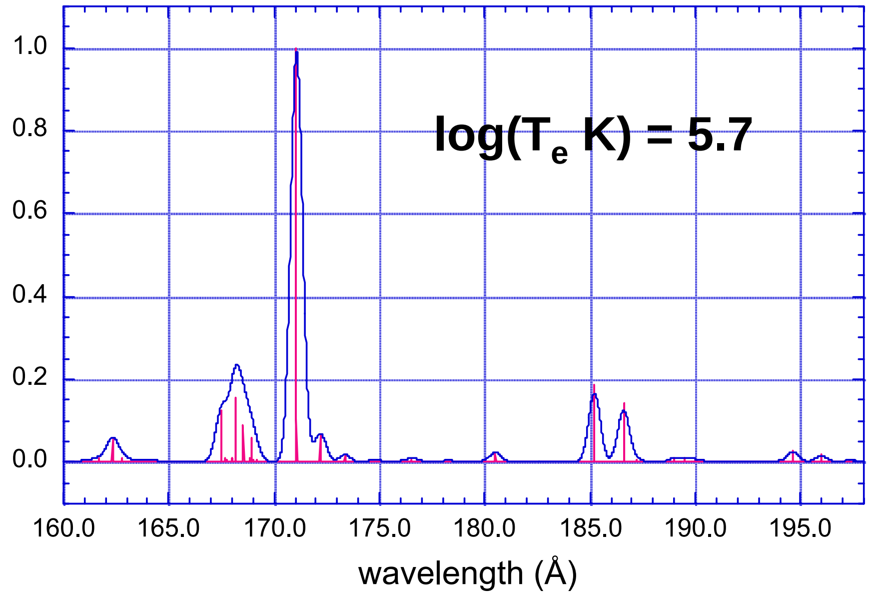
- Substantial counts above the background in the bins covering FeX - FeXII emission should be seen to be in agreement with the canonical models of the local bubble as a CIE gas.
- Diffuse x-ray emission supports this picture.
- Our results indicate a lower temperature of the emitting gas

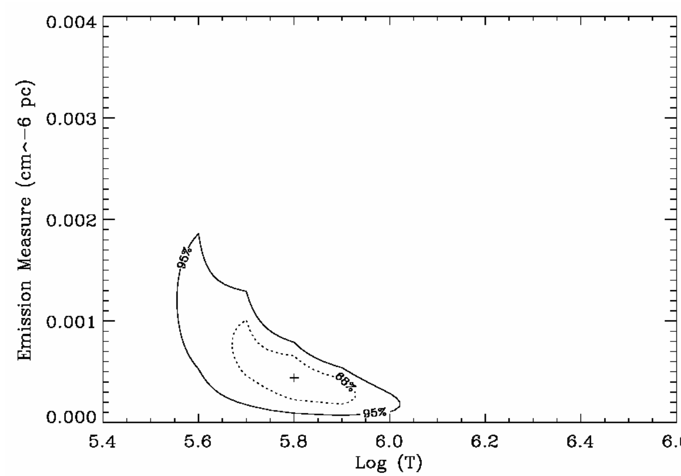


ApJ Letter preprint at http://chips.ssl.berkeley.edu/AAS1.pdf

M-shell simulations support CHIPS local ISM observations of log(Te)~XXY component





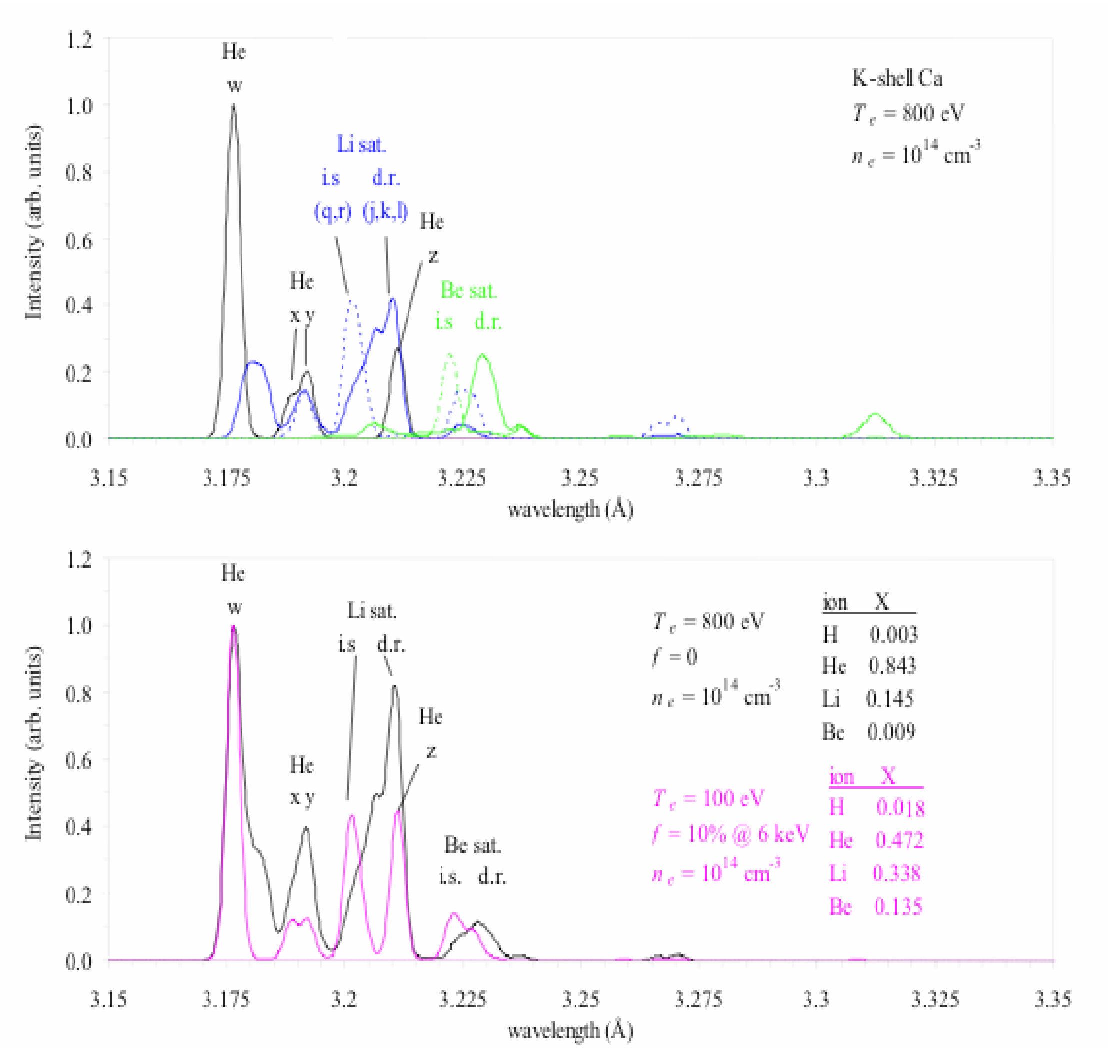


Conclusions

- General and obvious: both communities, astrophysical and fusion, need data in all the domains, atomic structure, collisional and photo-excitation, ionization and recombination
- General and not-obvious: how do we get all these in a more efficient manner
- ICAMDATA conferences offer a very good environment for these kind of discussions!

EXTRA SLIDES

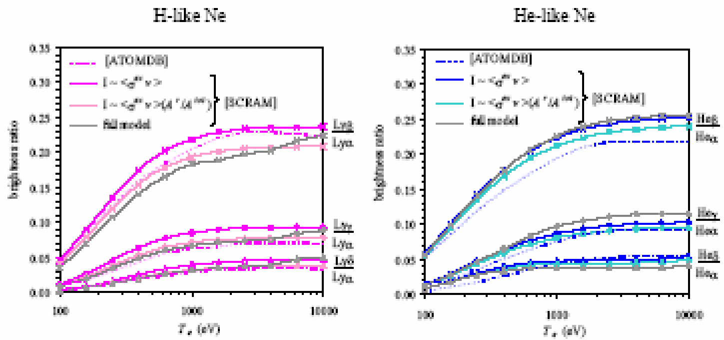
Non-thermal plasma effects can be studied with appropriate heating schemes



Hot electrons broaden charge-state distributions and enhance inner-shell lines

Calculations with the FAC code of M.F. Gu and SCRAM
S.B. Hansen and A.S. Shlyaptseva, PRE **70**, 036402 (2004).

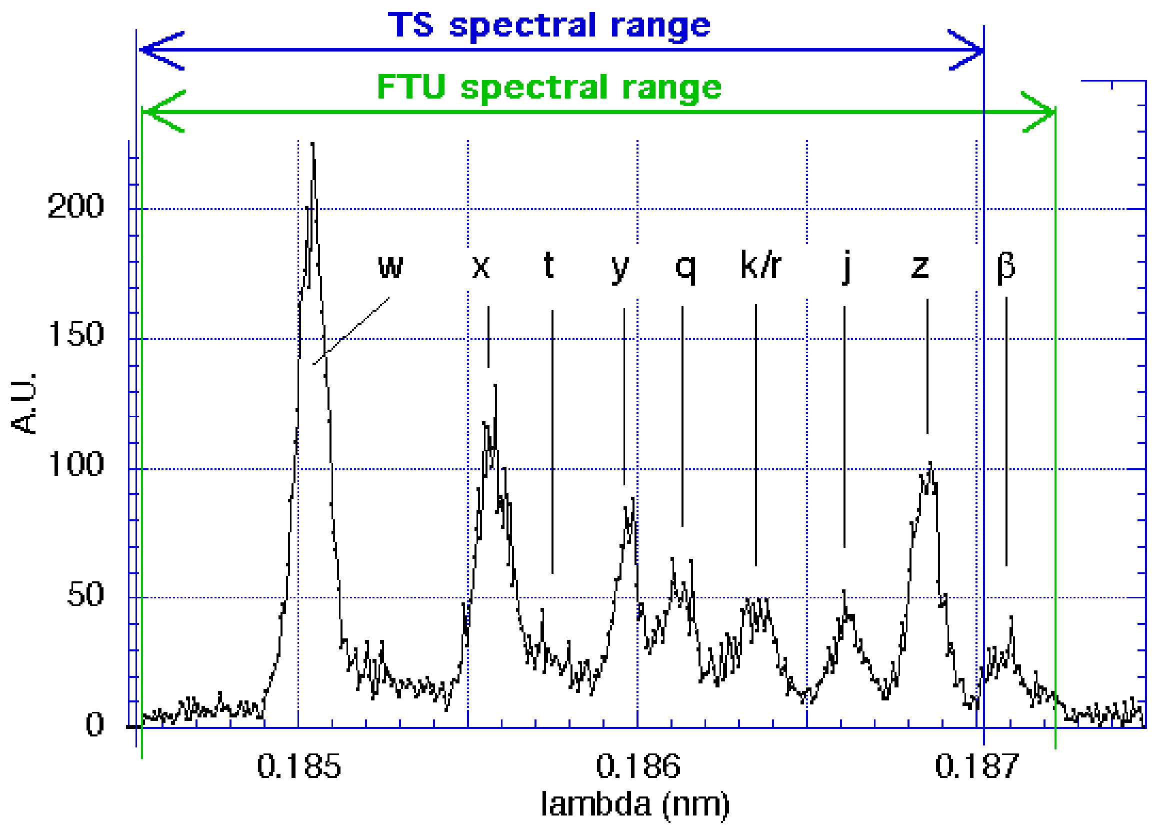
Model dependence of $(np - 1s)/(2p - 1s)$ ratios



In the coronal approximation (Intensity ~ $\langle \sigma^{ex} v \rangle$), intensities are limited by collisional excitation rates. Branching ratios A^r/A^{tot}, kinetic effects (cascades, recombination…), and the underlying model structure also affect line intensities.

Thermal plasmas can be used to study Fe K-shell ionization balance and spectral line strengths

Data courtesy of M. Leigheb, http://efrw01.frascati.enea.it/Documents/TaskForcesFTU/Spectroscopy/CEAENEA



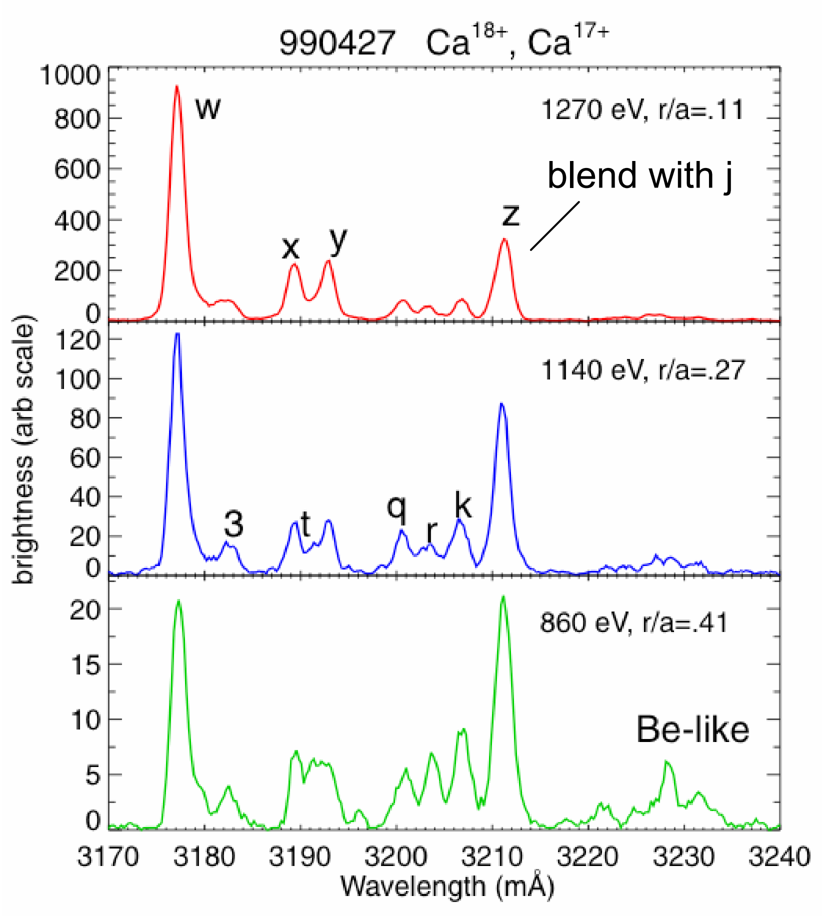
Bent crystal spectrometer:
Spectral resolution ≥ 10000
time resolution = 140 ms
possible to select among eight different wavelenght ranges

T_i = 12.8MK
T_e = 25.5MK
$n_H:n_{He}:n_{Li}$ ::
0.02:1.0:0.6

Fe K-shell lines will be discussed at length by others at this meeting (from titles alone):
Palmeri, Beiersdorfer, Liedahl, Jacobs, Rozanska

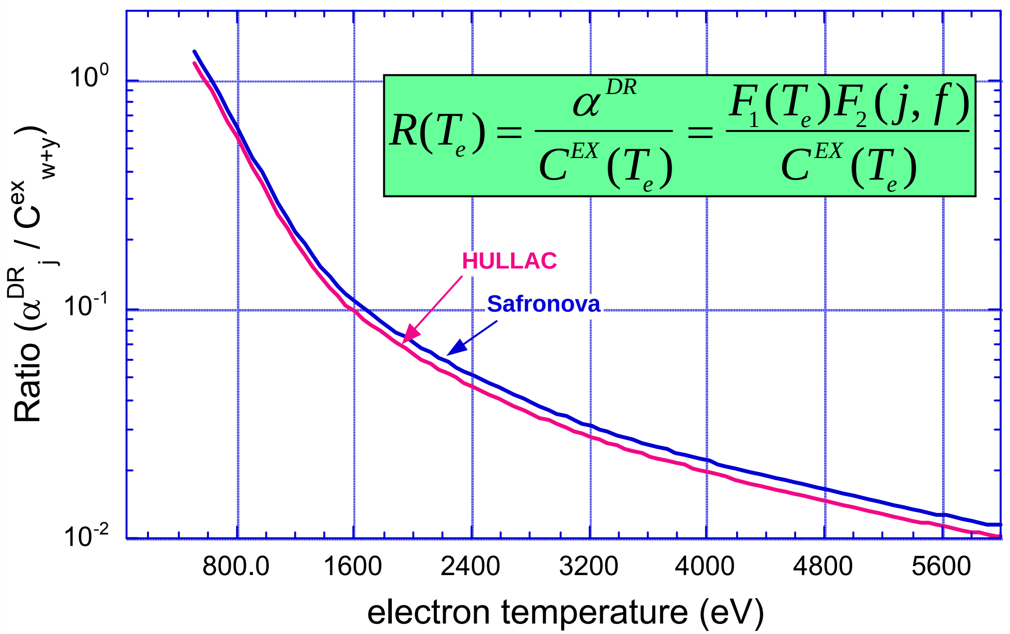
K-shell diagnostic line ratios can be benchmarked in thermal plasmas

Ca injection in Alcator C-Mod



Data from J.E. Rice, MIT, see
J. Rice, et al., Phys. Plasmas **7**, 1825 (2000)

DR to CX rate coefficients for Ca



$$R(T_e) = \frac{\alpha^{DR}}{C^{EX}(T_e)} = \frac{F_1(T_e)F_2(j,f)}{C^{EX}(T_e)}$$

The usual (j+k)/W ratio used to diagnose T_e is compromised here by blending of Z and j