Plasma Diagnostics and Atomic Astrophysics for the International X-ray Observatory

Nancy S. Brickhouse*

Harvard-Smithsonian Center for Astrophysics

ABSTRACT. The International X-ray Observatory will observe a wealth of spectral diagnostics to measure the physical properties of highly ionized plasmas and to study their time-dependent and dynamical processes. We give examples of diagnostics for both collisionally and photoionized plasmas, with new applications. We also discuss the laboratory astrophysics program needed to realize the potential of the mission.

*On behalf of the former Constellation-X Facility Sciences Team panel on Plasma Diagnostics and Atomic Astrophysics, Greg Brown, Li Ji, Vinay Kashyap, Masao Sako, Daniel Savin, Dave Schultz, Wayne Waldron, and Brad Wargelin.

A Laboratory Astrophysics Program for X-ray Astronomy

International X-ray Observatory (*IXO*) spectra will contain a wealth of line and continuum diagnostics to measure the physical properties of highly ionized astrophysical plasmas and to study their time-dependent and dynamic physical processes. The spectral band contains strong lines from elements between carbon and zinc which can be used to determine temperatures, opacities, electron densities, velocities, and elemental abundances. Highly ionized gas also emits a broad continuum spectrum that often traces time variability. With the spectral resolution of *IXO*, direct measurement of the electron temperature (T_e) will become routine, using emission lines or radiative recombination features. Comparison of the so-called "line ratio T_e" with that derived from the overall charge state distribution is extremely useful for determining if a plasma is in ionization equilibrium. *IXO* will also measure absorption along the line of sight at all scales from line and broadband effects. *IXO* will determine velocities from line centroid measurements, and for the hottest ions, from broad line profiles, allowing tests of electron-ion thermal equilibration.

X-ray astrophysics has long relied on publicly available spectral modeling codes for the analysis of data at low spectral resolution. Collaboration for more than two decades among modelers, atomic physics theorists, and experimentalists has contributed to the production of fundamental atomic, molecular and solid state data, experimental tests of these data, and public databases containing critically evaluated data, all supporting models accessible to observers through standardized software packages. This "laboratory astrophysics" community has focused efforts to improve the accuracy of popular diagnostics. By maintaining this critical infrastructure, with a healthy balance between theoretical and experimental work, we can expect to develop the models needed for *IXO*.

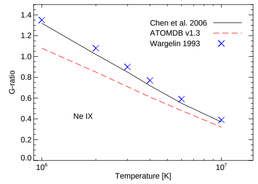


Figure 1. He-like Ne IX "G-ratio," showing agreement to within 7% between new theoretical calculations and EBIT measurements (Chen et al. 2006, Phys Rev A, 74, 042709).

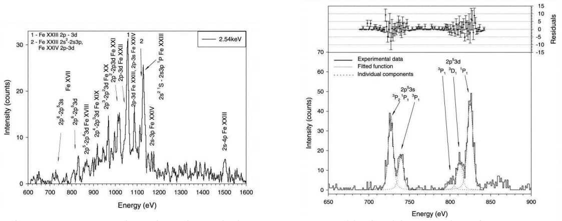


Figure 2. *Left* Section of a microcalorimeter spectrum of ionized iron produced at an EBIT with beam energy of 2.54 keV. *Right* Strong diagnostic lines of Fe XVII from an EBIT with a beam energy of 900 eV. (From Laming et al. 2000, ApJ, 545, L161).

Plasma spectral models require vast amounts of atomic data for radiative and collisional processes, including transition wavelengths and probabilities, oscillator strengths, and rates for photoionization and radiative recombination, collisional ionization and excitation, dielectronic recombination, and charge exchange. Theoretical calculations for some processes can now in principle achieve accuracies of 5 to 10%, comparable to the measurement uncertainties (Fig. 1); however, most rates in the literature are only accurate to 20 to 30% and many are known only to factors of two. Achieving high accuracy for a single process requires large computational effort and months if not years of research effort. Large, but less accurate models of weak lines are also needed to avoid incorrect assignment of their flux to other lines or continuum. Focused programs to calculate accurate and complete data need to continue.

Experimental measurements are essential tests of the atomic theory. It is also important to note the synergism between experiments and instrumentation: today microcalorimeters like the ones to be flown on *IXO* are measuring the fundamental properties of highly charged ions in electron beam ion trap (EBIT) experiments (Fig. 2). Very few absolute cross sections are available in the literature for highly charged ions, yet these data are invaluable for pushing the theoretical calculations beyond their current solutions. Meanwhile, systematic spectral surveys of ions produced in plasma experiments such as EBITs or tokamaks are additional useful benchmarks of the theory, for example testing line ratios from a particular ion. For the more complex ions, wavelength measurements are more accurate than theory and are used in the atomic databases.

Development of New Plasma Diagnostics

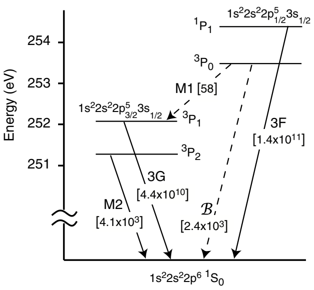
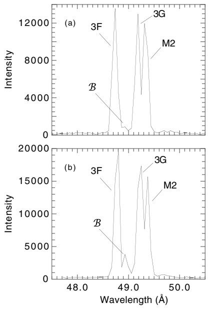
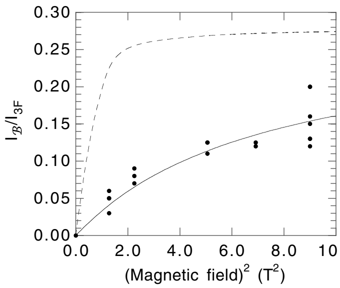


Figure 3. Energy level diagram for Ne-like argon.

In addition to improving existing models, new observations will undoubtedly inspire new ideas and demand new models. The X-ray laboratory astrophysics community has responded quickly to unexpected needs from observations, providing calculations of inner-shell absorption lines observed in AGN warm absorbers (Behar et al. 2001, see below), new theory and experimental measurements of charge exchange rates (e.g. Kharchenko 2005, AIP Conf Proc 774, 271; Wargelin et al. 2008, Can J Phys, 86, 151), and low temperature dielectronic recombination (e.g. Savin et al. 2006, ApJ, 642, 1275). Entirely new diagnostics useful to *IXO* may also be developed (Fig. 3, 4).

Figure 4 (*right*). Beiersdorfer et al. (2003, PRL, 90, 235003) have identified a new emission line diagnostic for magnetic fields in Ne-like systems (Fig. 3). The line labeled $\mathcal{B}$ is a strictly forbidden line except in the presence of a magnetic field. The magnetic field breaks the degeneracy of the magnetic sublevels and allows mixing. The figure to the *immediate right* shows the spectrum measured at the LLNL EBIT at 11 kGauss (*upper*) and 30 kGauss (*lower*). The figure to the *far right* shows the dependence of the line ratio on magnetic field in Tesla from measured points and fit (*solid*) at 7×10^{10} cm^{-3} and the zero-density limit (*dashed*). Note that Ne-like iron is a good candidate for *IXO* and is sensitive near 30 kGauss.





Key Science: Abundances in Type Ia Supernova Remnants

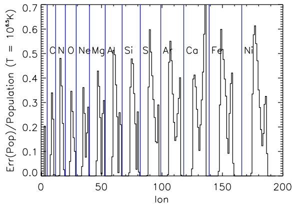


Figure 5. Simulation propagating the estimated errors in ionization and recombination rate coefficients. Errors in the ion population fraction range between 10 and 70%, implying errors of this order in the elemental abundance. Errors in the line excitation rates contribute to the accuracy of the elemental abundances as well, so that it is believed today that relative abundances in SNR can only be determined to a factor of ∼2.

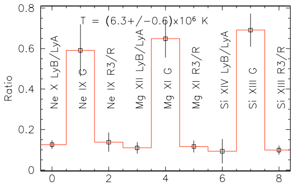


Figure 6. Simulation showing that T_e can be determined to about ±10% from line ratios of H- and He-like ions (not relying on the Fe-group elements of interest for abundances), and can be further tested by the T_e-dependent shape of the bremsstrahlung continuum. With T_e determined independently, the Fe-group emission lines of direct interest depend only on the fundamental atomic data. EBIT experiments are needed to benchmark these data.

Suzaku observations of the Tycho SNR show Kα lines of Cr and Mn, in addition to the strong lines of Fe Kα and Kβ (Tamagawa et al. 2008,). "Inner shell" K lines from ionization states with more than 2 electrons are too close in energy to resolve with current instruments in space, but will be resolved with *IXO* and, will be measured with better statistics and high spectral resolution for a number of SNR. Badenes et al. (2008, ApJ, 680, L33) propose using the Cr/Mn elemental abundance ratio to determine the progenitor metallicity, and this ratio is also useful for understanding the detonation mechanism. Here we explore what atomic data are needed to obtain an accurate elemental abundance ratio of Cr to Mn from the supernova ejecta. In addition to the relative elemental abundances, two parameters control the emission spectra of the ejecta, the fluence ($n_e\ t$) and the electron temperature (T_e). Today, the best we can do is to fit collisionally ionizing plasma models to the spectra and determine the best fit $n_e\ t$ and T_e. The fits to both of these parameters are dominated by the charge state distribution as manifested in the spectrum by the emission lines (Fig. 5).

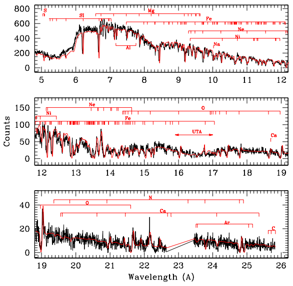
IXO observations coupled with reduced modeling errors should significantly improve our ability to determine abundances (Fig. 6). Experiments on the LLNL EBIT have already demonstrated the production of Kα spectra of multiple charge states during ionization from neutral iron (Decaux et al. 1995, ApJ, 443, 464; 1997, ApJ, 482, 1076). A systematic program of spectral measurements as functions of time (for fixed n_e) and beam energy can (almost) provide a set of simulations for direct comparison of astrophysical observations. We need the qualifier "almost" because the experimental conditions are not a perfect match to the astrophysical conditions (narrow Gaussian beam vs Maxwellian electron energy distribution, differences in n_e, etc.), and thus models are still needed to predict spectra from both types of plasmas. We expect to reduce the systematic uncertainties in relative abundances to about 10% with a dedicated program targeting *IXO* science.

Key Science: Feedback from Outflows in Active Galactic Nuclei

A few high signal-to-noise, high resolution X-ray spectra have given us a wealth of new information on the physical conditions and location[s] of AGN winds. For example, Figure 7 shows numerous discrete, but heavily blended features attributable to highly ionized plasma outflowing from the AGN. Before the launch of Chandra the absorption was generally attributed to recombination edges. With improvements to the fundamental spectroscopy over the last five years, models of NGC 3783 now do a good job of matching the spectral features.

The Fe M-shell unresolved transition array (UTA), observed near 16 Å, responds sensitively to changes in the flux of the ionizing continuum (see Krongold et al. 2005, ApJ, 622, 842). Fe M-shell absorption is consistent with the gas being close to photoionization equilibrium; for Fe L-shell the gas does not have time to reach equilibrium. Time constraints from these data imply limits on the density of the gas ($> 10^4$ cm^{-3}) and its location ($<$ 6 pc from the central source). Limits set for NGC 4051 from variability including both equilibrium and non-equilibrium cases show that, for this AGN, the ionized wind is not important to IGM-Galaxy feedback; however, the question is still open for systems with higher mass accretion rates. Additional diagnostics will be available with *IXO*. For example, line ratios within the M-shell are likely to provide directy density diagnostics, but no calculations have been performed to date.

Figure 7 (*near right*). Chandra spectrum and model fit to the absorption spectrum of NGC 3783 (from Krongold et al. 2003, ApJ, 597, 832).



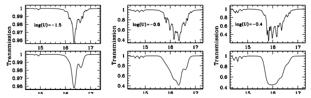


Figure 8 (*above*). Calculations of the UTA for Fe X-XIII (*upper*) using HULLAC without abbreviation, compared with Behar et al. (*lower*). Calculations in the literature by Behar et al. (2001, ApJ, 563, 497) were only published in abbreviated form, and thus are not available for detailed comparison with spectra. More work is needed on these systems.