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K-α X-Ray Emission Spectra from Highly-Charged Fe Ions in EBIT*

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Abstract A detailed spectral model has been developed for the computer simulation of the 2p→1s K-α X-ray emission from highly-charged Fe ions in the Electron Beam Ion Trap (EBIT). The spectral features of interest occur in the range from 1.84 Å to 1.94 Å. EBIT has enabled the precise investigation of the fundamental radiative emission processes associated with radiationless electron capture or dielectronic recombination, inner-shell electron collisional excitation, and inner-shell electron collisional ionization. Our earlier theoretical investigations had been concerned primarily with the interpretation of spectral observations from high-temperature magnetic-fusion (Tokamak) plasmas. In these plasmas, small or moderate departures from steady-state corona-model charge-state distributions can occur due to ion transport processes, while the assumption of equilibrium (Maxwellian) electron energy distributions is expected to be valid. Our theoretical investigations have now been directed at the identification of spectral features that can serve as diagnostics of extreme non-equilibrium or transient-ionization conditions, and allowance has been made for general (non-Maxwellian) electron energy distributions. In order to investigate the fundamental K-α line-formation processes that can play a dominant role under these extreme conditions, we have simulated the K-α X-ray emission from highly-charged Fe ions in EBIT. For the precise interpretation of the high-resolution X-ray observations, which may involve the analysis of blended spectral features composed of many lines, it has been necessary to take into account the multitude of individual fine-structure components of the K-α radiative transitions in the ions from Fe XVIII to Fe XXV. At electron densities higher than the validity range of the corona-model approximation, collisionally-induced transitions among low-lying excited states can play an important role. A simplified statistical-population model has been adopted for a preliminary determination of the distribution of the initial ions among the different low-lying fine-structure states. The inadequacies of this simple population model can be fundamentally remedied only by a detailed time-dependent collisional-radiative-model description of the dynamic excitation and ionization processes in EBIT. It is found that inner-shell electron excitation and ionization processes involving the complex intermediate ions from Fe XVIII to Fe XXI produce spectral features, in the wavelength range from 1.89 Å to 1.94 Å, which are particularly sensitive to density variations and transient-ionization conditions.

Outline

- Fundamental Radiative-Emission Processes
- Spectral Intensity of Kα Radiative Emission
- Excitation of Autoionizing States in Electron-Ion Collisions
- Determination of the Charge-State Distributions
  - Steady-Sate Ionization-Recombination Balance
  - Non-Equilibrium (Transient-Ionization) Distributions
- Density Dependence of the Spectral Intensity
- Spectral Simulations for Kα Emission
  - Selected 2p → 1s Kα Line Identifications
  - Kα Emission in Tokamak Plasmas
  - Kα Emission in the Electron Beam Ion Trap (EBIT)
- Conclusions and References

Fundamental Radiative-Emission Processes

🟩 Radiationless Electron Capture (Dielectronic Recombination)

$$\mathrm{Fe}^{+(z+1)}(\mathrm{i}) + \mathrm{e}^{-}(\varepsilon_{\mathrm{i}}) \;\Rightarrow\; \mathrm{Fe}^{+z}(\mathrm{j})$$

$$\mathrm{Fe}^{+z}(\mathrm{j}) \;\Rightarrow\; \mathrm{Fe}^{+z}(\mathrm{k}) + \hbar\omega$$

🟦 Inner-Shell Electron Collisional Excitation

$$\mathrm{Fe}^{+z}(\mathrm{i}') + \mathrm{e}^{-}(\varepsilon_{\mathrm{i}'}) \;\Rightarrow\; \mathrm{Fe}^{+z}(\mathrm{j}) + \mathrm{e}^{-}(\varepsilon_{\mathrm{j}})$$

$$\mathrm{Fe}^{+z}(\mathrm{j}) \;\Rightarrow\; \mathrm{Fe}^{+z}(\mathrm{k}) + \hbar\omega$$

🟥 Inner-Shell Electron Collisional Ionization

$$\mathrm{Fe}^{+(z-1)}(\mathrm{i}'') + \mathrm{e}^{-}(\varepsilon_{\mathrm{i}''}) \;\Rightarrow\; \mathrm{Fe}^{+z}(\mathrm{j}) + \mathrm{e}^{-}(\varepsilon_{\mathrm{j}}) + \mathrm{e}^{-}(\varepsilon'_{\mathrm{j}})$$

$$\mathrm{Fe}^{+z}(\mathrm{j}) \;\Rightarrow\; \mathrm{Fe}^{+z}(\mathrm{k}) + \hbar\omega$$

Spectral Intensity of Kα Radiative Emission

At low densities the spectral intensity is simply the sum of individual contributions from the 3 fundamental Kα line-formation mechanisms.

We include fine-structure transitions arrays in all abundant Fe ions.

$$I(\hbar\omega) = \sum_z \sum_j \sum_k B_r(z, j \to k) L(z, j \to k, \hbar\omega)$$

$$\Big[\ C_{cap}(z+1, i, \varepsilon_i \to j)\ N(z+1) N_e$$

$$+\ C_{exc}(z, i', \varepsilon_{i'} \to j)\ N(z) N_e$$

$$+\ C_{ion}(z-1, i'', \varepsilon_{i''} \to j) N(z-1) N_e\ \Big].$$

Branching ratio for the radiative transition j ➔ k from the state j:

$$B_r(z, j \to k) = \frac{A_r(z, j \to k)}{\sum_i A_{auto}(z, j \to i, \varepsilon_i) + \sum_{k'} A_r(z, j \to k')}.$$

Spectral-line-shape function $L(z, j \to k, \hbar\omega)$ is determined by Doppler broadening and by the autoionization and spontaneous emission rates.

Excitation of Autoionizing States in Electron-Ion Collisions

Rate coefficients for the 3 fundamental collisional excitation processes:

$$C_{cap}(z+1, i, \varepsilon_i \rightarrow j)$$
$$= \iint d^3v_e\, d\Omega\, |v_e| f_e(v_e)\, \sigma_{cap}(z+1, i, \varepsilon_i \rightarrow j; v_e, \Omega),$$
$$C_{exc}(z, i', \varepsilon_{i'} \rightarrow j)$$
$$= \iint d^3v_e\, d\Omega\, |v_e| f_e(v_e)\, \sigma_{exc}(z, i', \varepsilon_{i'} \rightarrow j; v_e, \Omega),$$
$$C_{ion}(z-1, i'', \varepsilon_{i''} \rightarrow j)$$
$$= \iint d^3v_e\, d\Omega\, |v_e| f_e(v_e)\, \sigma_{ion}(z-1, i'', \varepsilon_{i''} \rightarrow j; v_e, \Omega).$$

For equilibrium conditions, the single-electron velocity (energy) distribution function $f_e(v_e)$ is a Maxwellian.

For the non-equilibrium ionization conditions in the Electron Beam Ion Trap, the single-electron distribution function $f_e(v_e)$ is nearly mono-energetic.

In this case, the emission spectra are more sensitive to the differential electron-ion collision cross sections σ and to the energy-conservation restrictions.

Determination of the Charge-State Distributions

At low densities and ignoring charge-exchange, the dynamical ionization-recombination balance is given by:

$$\frac{\partial N(z)}{\partial t} + \vec{\nabla} \bullet [\vec{V}(z)\, N(z)]$$
$$= N_e N(z-1) S_{ion}(z-1 \rightarrow z) - N_e N(z) S_{ion}(z \rightarrow z+1)$$
$$+ N_e N(z+1) \alpha_{rec}(z+1 \rightarrow z) - N_e N(z) \alpha_{rec}(z \rightarrow z-1).$$

S_{ion} = total ionization rate coefficient for direct electron-impact ionization and autoionization following inner-shell electron-impact excitation:

$$S_{ion}(z \rightarrow z+1) =$$
$$\sum_j [S_{di}(g \rightarrow j) + \sum_a C_{ex}(g \rightarrow a) Q^{-1}(a,a) A_a(a \rightarrow j)] .$$

α_{rec} = total recombination rate coefficient for direct radiation recombination and dielectronic recombination in electron-ion collisions:

$$\alpha_{rec}(z+1 \rightarrow z) =$$
$$\sum_b [\alpha_{rr}(i \rightarrow b) + \sum_a C_{cap}(i \rightarrow a) Q^{-1}(a,a) A_r(a \rightarrow b)].$$

Steady-State Ionization-Recombination Balance

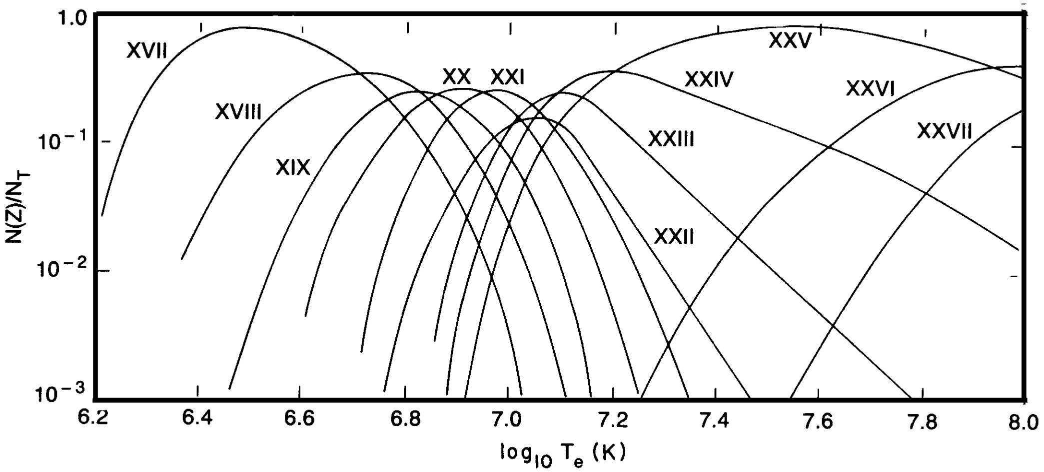
Equilibrium (Maxwellian) electron distributions:

The ionization and recombination rate coefficients S_{ion} and α_{rec} are functions of the local electron temperature T_e.

Transport & time-dependent phenomena neglected:

The charge-state distributions N(z) are determined as functions of the local electron temperature T_e.

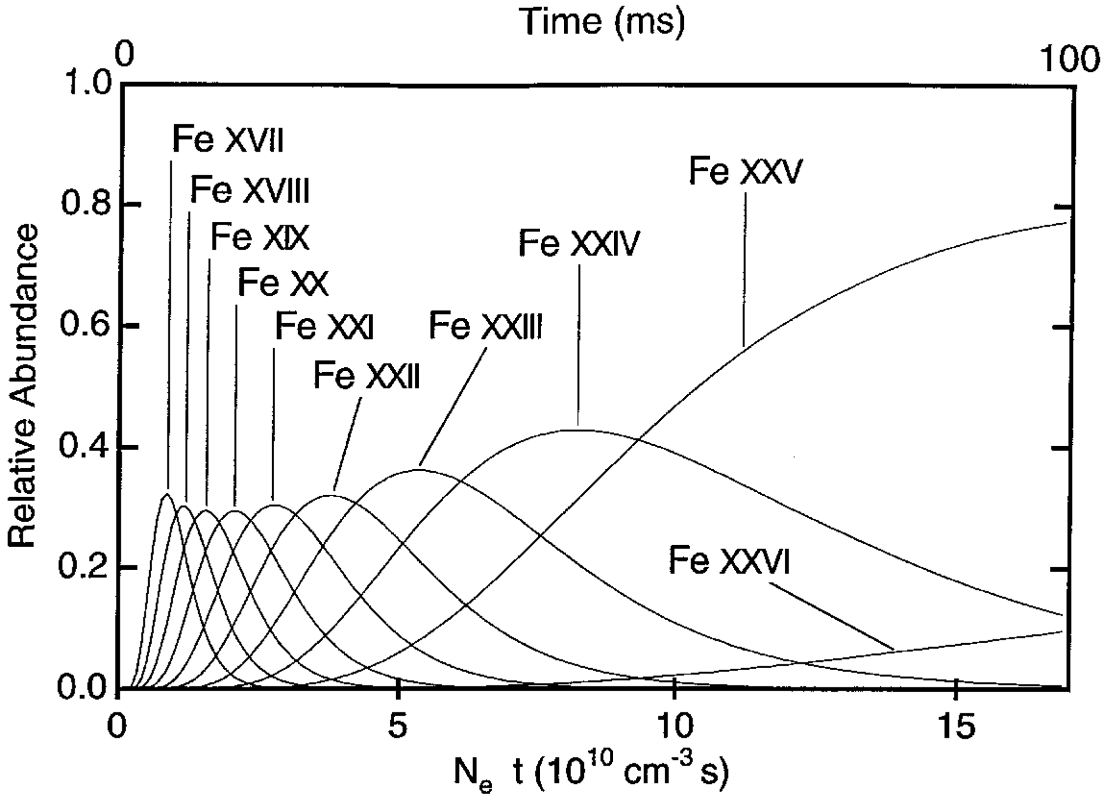
$N(z)S_{ion}(z \rightarrow z+1) = N(z+1)\alpha_{rec}(z+1 \rightarrow z)$. **(Corona-Model Relations)**



Corona-Model Charge-State Distributions (Predicted for Fe Ions)

Non-Equilibrium (Transient-Ionization) Distributions

The EBIT charge-state distributions are predicted as functions of time, taking into account direct ionization, radiative recombination, and charge exchange.



Charge-State Distributions for Fe Ions in EBIT
(Predicted for an Electron Beam Energy of 12 KeV)

Density Dependence of the Spectral Intensity

At low electron densities ($N_e \leq 10^{10}$ cm^{-3}), the 3 fundamental Kα excitation processes occur predominantly from ions in the fine-structure levels of the ground-state configuration (or a metastable-state configuration). All excited states are assumed to undergo de-excitation only by either autoionization or by spontaneous radiative emission.

The electron-temperature-dependent Kα spectral intensity varies as N_e^2.

For intermediate charge states of Fe ions (Fe XVIII to Fe XXI) in a Tokamak plasma or in EBIT ($10^{12} \leq N_e \leq 10^{14}$ cm^{-3}), collisional transitions among the fine-structure states of the ground-state electronic configuration can produce a substantially more complicated electron-density dependence.

In order to provide a preliminary (and approximate) description of this electron-density dependence, which can be accurately predicted only by means of a detailed time-dependent collisional-radiative model, we have adopted a hierarchy of simple statistical-population models for the distribution of the initial ions among the fine-structure levels:

$$\frac{N(z,i)}{N(z)} \approx \frac{g(z,i)}{\sum_{i'} g(z,i')}, \quad g(z,i) = 2J_i + 1.$$

At high densities ($N_e \geq 10^{24}$ cm^{-3}), collisional transitions among autoionizing states are important.

The spectral intensity can become a strong function of the local electron density.

Spectral Simulations for Kα Emission

Plasma Conditions	Near Equilibrium (Tokamak Plasmas, Solar Corona)	Transient Ionization (Electron Beam Ion Trap)
Dominant Kα Line Excitation Processes	Radiationless Electron Capture (Dielectronic Recombination) Inner-Shell Electron Excitation	Radiationless Electron Capture (Resonant Beam Energies) Inner-Shell Electron Excitation Inner-Shell Electron Ionization
Processes Determining the Charge-State Distributions	Direct Ionization Autoionization Following Inner-Shell Electron Excitation Radiative Recombination Dielectronic Recombination Ion Transport	Direct Ionization Autoionization Following Inner-Shell Electron Excitation? Radiative Recombination Charge Exchange

Selected 2p → 1s Kα Line Identifications

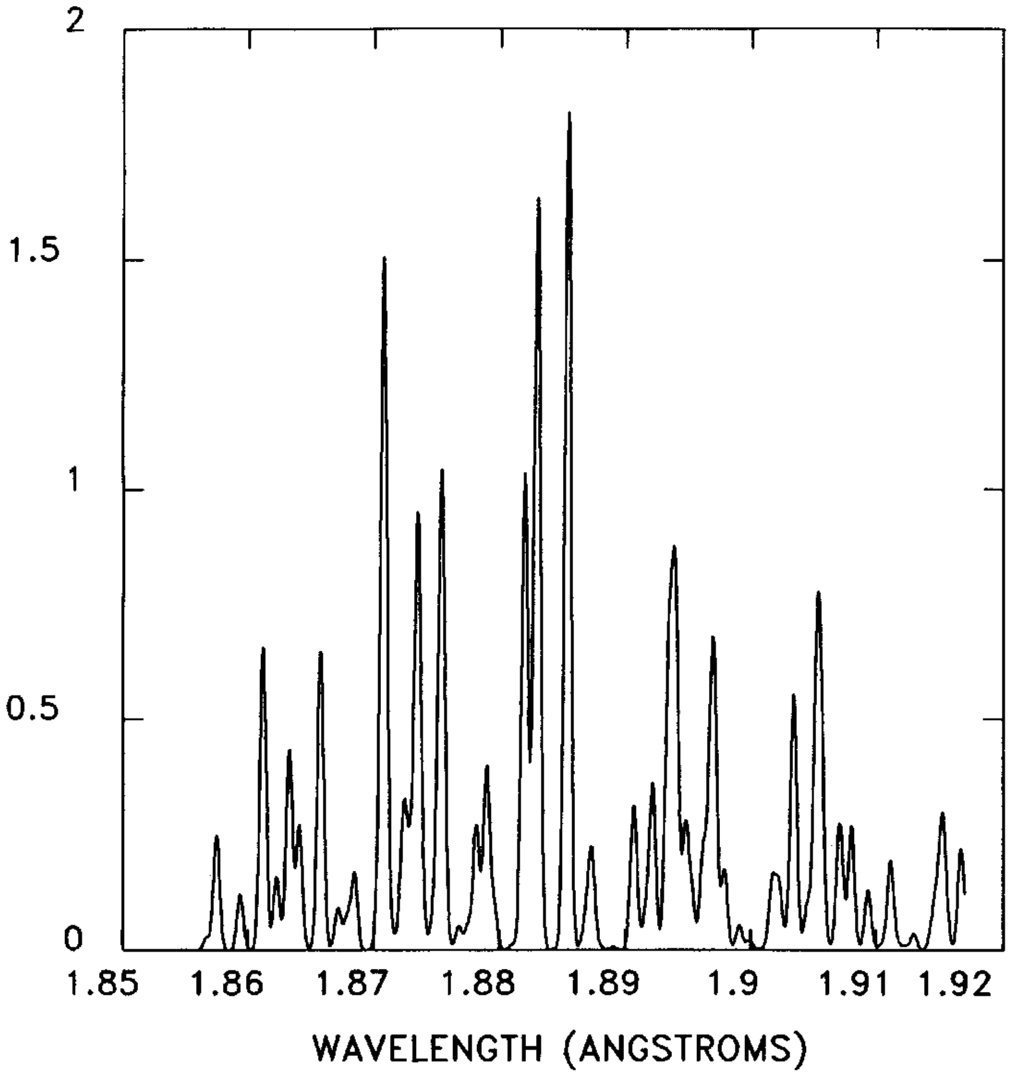
Label	Ion	Transition	Wavelength*
C8*	FeXXI	${}^3P_2 \rightarrow {}^1D_2$	1.89455
C9*	FeXXI	${}^3D_1 \rightarrow {}^3P_0$	1.89475
C10*	FeXXI	${}^3S_1 \rightarrow {}^3P_2$	1.89535
N7	FeXX	${}^2D_{3/2} \rightarrow {}^2D_{3/2}$	1.90595
N11	FeXX	${}^4P_{5/2} \rightarrow {}^4S_{3/2}$	1.90845
O4	FeXIX	${}^3P_2 \rightarrow {}^3P_2$	1.91765
O7	FeXIX	${}^3P_2 \rightarrow {}^3P_1$	1.92085
F1*	FeXVIII	${}^2S_{1/2} \rightarrow {}^2P_{3/2}$	1.92145
F2*	FeXVIII	${}^2S_{1/2} \rightarrow {}^2P_{1/2}$	1.93125

* Seely, Feldman, and Safronova, Ap. J. 304, 838 (1986).

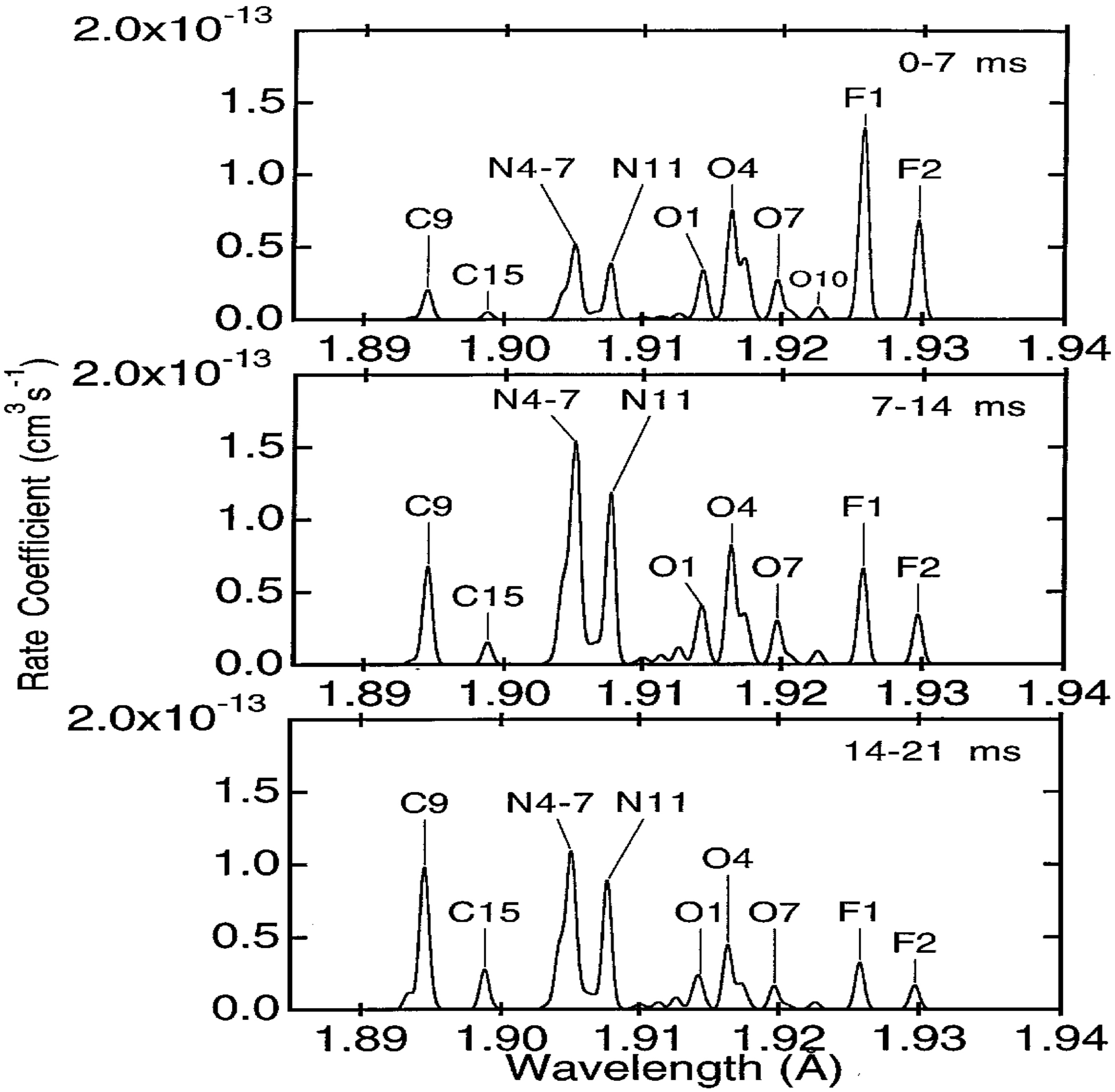
* Particularly sensitive to electron-density variations

* Particularly sensitive to transient-ionization conditions

Kα Emission in Tokamak Plasmas (Predicted for an Electron Temperature of 10^7 K)



Kα Emission in the Electron Beam Ion Trap (Predicted for an Electron Beam Energy of 12 KeV)



Conclusions

In equilibrium plasmas, the Kα emission lines are produced predominantly by the processes of radiationless electron capture (dielectronic recombination) and inner-shell electron excitation.

In the Electron Beam Ion Trap (EBIT), radiationless electron capture processes can occur only for resonant electron beam energies. For non-resonant energies, the observed Kα emission is produced by the processes of inner-shell electron excitation and inner-shell electron ionization.

Inner-shell electron excitation and ionization processes in EBIT, which occur in the complex intermediate ions from Fe XVIII to Fe XXI, produce spectral features, which are particularly sensitive to electron-density variations and transient-ionization conditions.

For a fundamental treatment of the electron-density dependence of the Kα line emission, it will be necessary to develop a detailed and systematic time-dependent collisional-radiative-model description of the dynamic (fine-structure resolved) excitation and ionization processes.

For a precise description of the Kα line emission produced by directed-electron interactions, it will be necessary to incorporate into the simulation program a treatment of the angular distribution and polarization of the emitted photons, using a density-matrix approach.

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