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Ka Emission Spectra from Non-Equilibrium Ionizing Plasmas*

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Abstract

Kα X-ray emission spectra from highly charged Fe ions have been theoretically predicted using a detailed and systematic spectral model. Account has been taken of the fundamental atomic radiative-emission processes associated with inner-shell electron collisional excitation and ionization, as well as dielectronic recombination. Particular emphasis has been directed at extreme non-equilibrium or transient-ionization conditions, which can occur in astrophysical and tokamak plasmas. Good agreement has been found in comparisons with spectral observations on the EBIT-II electron beam ion trap at the Lawrence Livermore National Laboratory. We have identified spectral features that can serve as diagnostics of the electron density, the line-formation mechanism, and the charge-state distribution.

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**
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Fundamental Radiative-Emission Processes

🟩 Radiationless Electron Capture (Dielectronic Recombination)

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

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

🟦 Inner-Shell Electron Collisional Excitation

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

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

🟥 Inner-Shell Electron Collisional Ionization

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

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

Spectral Intensity of Kα Radiative Emission

(Low Density Description)

The total spectral intensity is generated by three elementary Kα line-formation mechanisms.

We include the entire arrays of fine-structure radiative transitions 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 autoionizing states 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 functions $L(z, j \to k, \hbar\omega)$ are determined by Doppler broadening and by the autoionization and spontaneous emission rates.

Excitation of Autoionizing States in Electron-Ion Collisions

Rate coefficients C for the three fundamental autoionizing-state 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 ionizing-plasma conditions in the Electron Beam Ion Trap (EBIT), the single-electron velocity 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 s and to the energy-conservation restrictions.

Determination of the Charge-State Distributions

The electron-ion ionization and recombination dynamics, at low densities and ignoring charge-exchange processes:

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

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

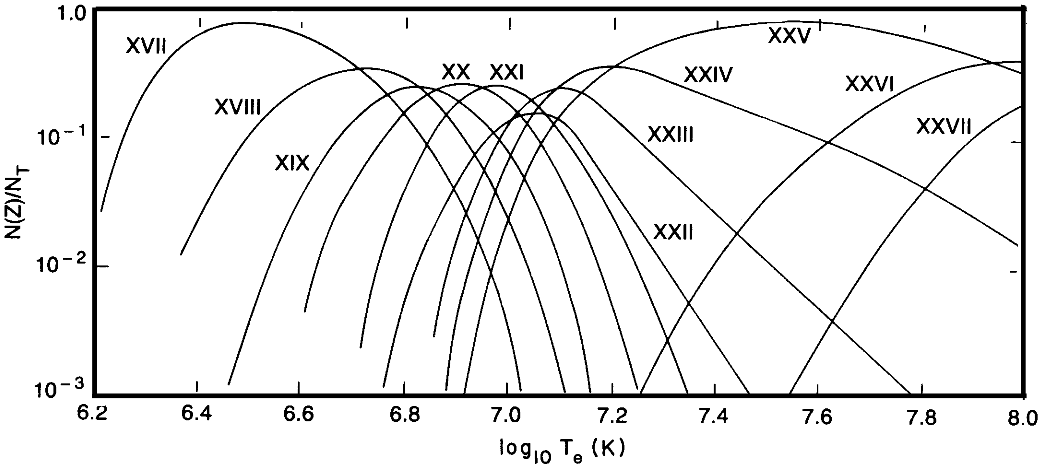
$$\alpha_{rec}(z+1 \rightarrow z) =$$
$$\sum_b [\alpha_{rr}(i \rightarrow b) + \sum_a C_{cap}(i \rightarrow a) Q^{-1}(a,a) A_r(a \rightarrow b)].$$

Steady-State Ionization-Recombination Balance

Equilibrium (Maxwellian) electron velocity distributions: Ionization & recombination rate coefficients S_{ion} and a_{rec} obtained as functions of the local electron temperature T_e

Transport & time-dependent phenomena neglected: Charge-state distributions N(z) determined by the corona-model relations, as functions of the local electron temperature

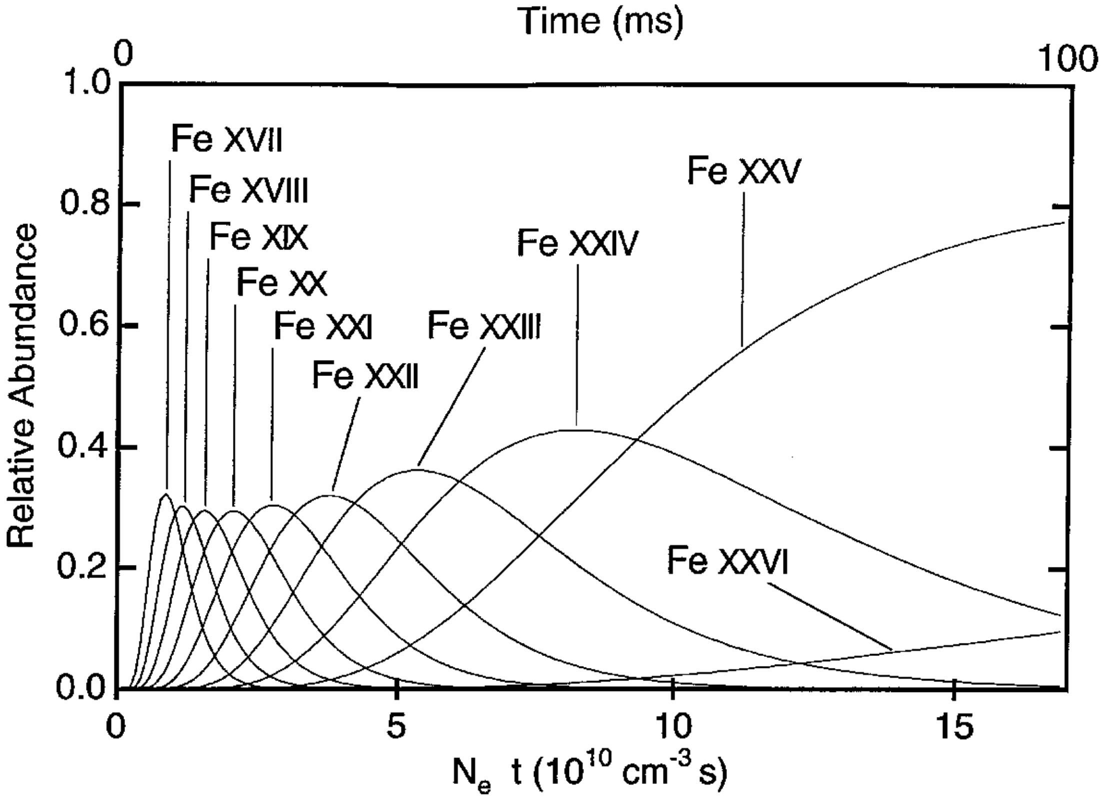
$$N(z)S_{ion}(z \rightarrow z+1) \quad = \quad N(z+1)a_{rec}(z+1 \rightarrow z).$$



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

Non-Equilibrium (Transient-Ionization) Distributions

For the extreme non-equilibrium (transient-ionization) conditions that have been achieved in EBIT, the charge-state distributions N(z) have been 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 very low (corona-model) electron densities ($N_e \leq 10^{10}$ cm^{-3}), the three fundamental Kα excitation processes occur predominantly from ions initially in their ground-state fine-structure levels. All excited states are assumed to undergo de-excitation only by either autoionization or by spontaneous radiative emission processes.
The electron-temperature-dependent 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 of the Kα spectral intensity.

In order to provide an 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 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 very high (laser-produced plasma) 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 (EBIT)}
Dominant Kα Line Excitation Processes	Radiationless Electron Capture (Dielectronic Recombination) Inner-Shell Electron Excitation	Radiationless Electron Capture (Only for 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

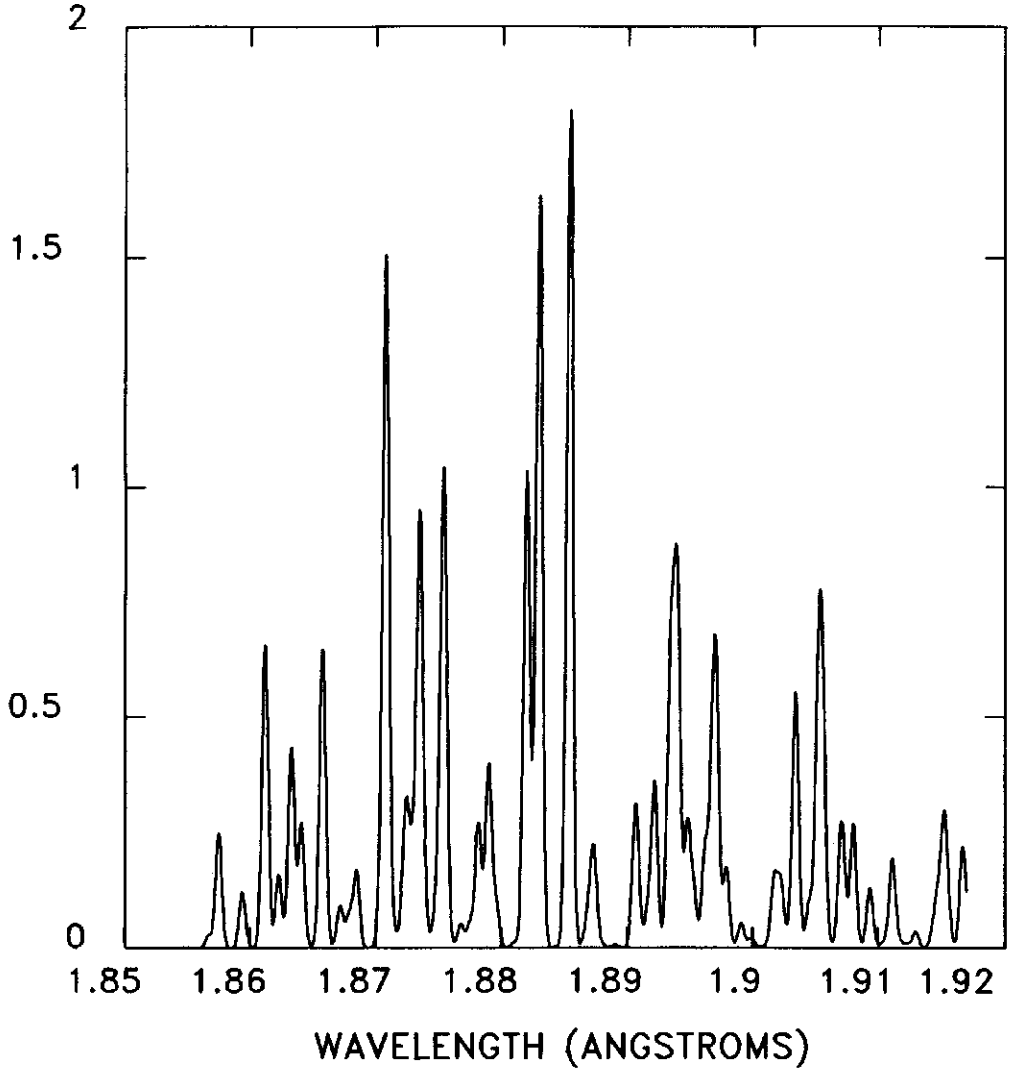
Label	Ion	Transition	Wavelength*
C8*	FeXXI	${}^3P_2 \rightarrow {}^1D_2$	1.89455
C9*	FeXXI	${}^3D_1 \rightarrow {}^3P_0$	1.89475
C10*	FeXXI	${}^3S_1 \rightarrow {}^3P_2$	1.89535
N7	FeXX	${}^2D_{3/2} \rightarrow {}^2D_{3/2}$	1.90595
N11	FeXX	${}^4P_{5/2} \rightarrow {}^4S_{3/2}$	1.90845
O4	FeXIX	${}^3P_2 \rightarrow {}^3P_2$	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).

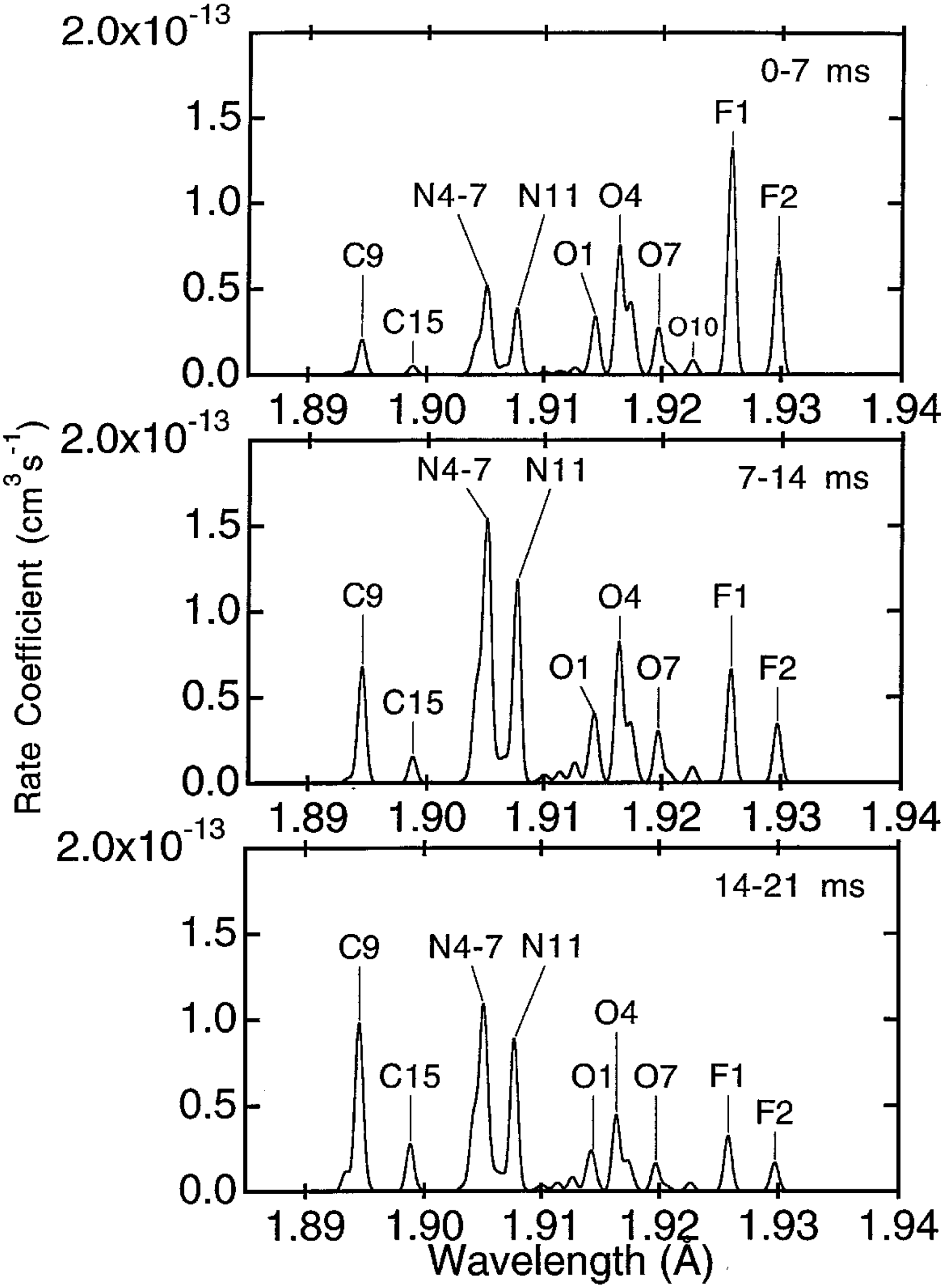
* Particularly sensitive to electron-density variations

* Particularly sensitive to transient-ionization conditions

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



Kα Emission in the Electron Beam Ion Trap (EBIT)
(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. Consequently, 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, involving 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) 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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