Emission Properties of Non-equilibrium Zirconium Plasma in Soft X-ray Region

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Abstract

Zirconium-based plasmas are considered as a source of soft X-ray emission in water window waveband alongside with nitrogen- and bismuth-based radiation plasma sources. Such discharge and laser produced plasmas used in soft X-ray (and EUV) sources are in non-equilibrium state as a rule. This leads to a mismatch between the actual conditions of the plasma and its theoretical/computational estimations because of different effects like non-thermal electron distribution, self-absorption etc. leading to changes in ionization states, state populations, emission intensity and spectrum. In the report the radiance and emission properties of non-equilibrium zirconium plasma is examined and the optimal emission conditions for soft X-ray emission in water window region are explored. Kinetic parameters for non-equilibrium plasma including major inelastic ion interaction processes with non-thermal electrons and radiation, emission and absorption data are obtained in the approach based on Hartree-Fock-Slater (HFS) quantum-statistical model and distorted waves approximation. Modeling of plasma properties and emission is performed by using atomic, kinetic, radiation transport and RMHD Z* code.

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Zirconium XI – XVI Lines

Zirconium Line strengths in Water Window region

4f-3d, 5p-3d transitions in Zr XI – Zr XX intensively emit in water window (WW) region

Line strengths of Zr XI – Zr XVI computed with Flexible atomic code
Zirconium XVII – XXII Lines

Zirconium Line strengths in Water Window region

Most intensive 4p-3d transitions start to contribute into WW region beginning from Zr XV up to Zr XXI

Line strength of Zr XVI – Zr XXII computed with Flexible atomic code
Non-Equilibrium Model

System of Kinetic equations

To calculate spectrum of emission we need to resolve the system of kinetic equations to obtain relative populations $n_\mu$ of levels

$$\frac{dn_\mu}{dt} = \sum_{\nu \neq \mu} n_\nu \alpha_{\nu \rightarrow \mu}(N_i, N_e, T, \rho, F) - n_\mu \sum_{\nu \neq \mu} \alpha_{\mu \rightarrow \nu}(N_i, N_e, T, \rho, F),$$

$$\sum_\mu n_\mu = 1,$$

$\alpha_{v \rightarrow \mu}$ and $\alpha_{\mu \rightarrow v}$ - total rates of the processes leading to increase and decrease of the level $\mu$ population $n_\mu$, $N_i$ and $N_e$ – number of ions and electrons, $T$ – temperature, $\rho$ – density. Total rates include a different set of processes depending of model, kind of modelling etc.

Quasi-neutrality:

$$N_e = Z_0 N_i,$$

$$Z_0 = \sum_\mu z_\mu n_\mu,$$

$z_\mu$ – charge of the ion of level $\mu$, $Z_0$ - average charge
**Zirconium Non-equilibrium Plasma**

### Zirconium Ion populations

**Electron density**

\[ N_e = 10^{19} \text{ 1/ccm} \]

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**Zirconium ion fractions for 1x10**19 **1/ccm electron density**

*Best conditions for emission in water window are expected at \( T > 80 \text{ eV} \) and higher.*
Spectral Efficiency (SE) reaches its maximum (over 40%) at plasma temperature ~90 eV and decreases slightly after: SE = 2%(50eV) – 33%(70eV) – 40%(90eV) – 38%(110eV)
Radiation transfer in plasma

\[ \frac{1}{c} \frac{\partial I_\omega}{\partial t} + (\vec{\Omega} \nabla) I_\omega = j_\omega - k_\omega I_\omega \]

\[ U_\omega = c^{-1} \int I_\omega \, d\vec{\Omega}; \]

\[ \kappa_\omega(n_e, n_i, T_e, U_\omega); \]

\[ j_\omega(n_e, n_i, T_e, U_\omega); \]

\[ I_\omega(r, z, \varphi, \theta) = \int_0^\tau \frac{j_\omega}{\kappa_\omega} e^{\tau - \tau'} \, d\tau; \]

\[ \tau = \tau(x) = \int_0^x \frac{\kappa_\omega(r, z)}{\sin \theta} \, dx; \]

\[ x = \sqrt{r_{out}^2 - r^2 \sin^2 \varphi} + r \cos \varphi \]

\[ z = z_{out} + x \cdot \text{ctg} \theta \]

- Quasi-stationary
- Spectral radiation energy density
- Opacity
- Emissivity
- Intensity
- Cylindrical symmetry
- Optical depth
- Trajectory
Absorption coefficients

Bound-Bound (bb), Bound-Free (bf) & Free-Free (ff) processes

\[ K_\omega = K_{\omega}^{bb} + K_{\omega}^{bf} + K_{\omega}^{ff} \]

\[ K_{\omega}^{bb} = N_i (1 - e^{-\omega / T_e}) \sum_s P_s \sum_{\nu \mu} n_{\nu}^s (1 - n_{\mu}^s) \sigma_{\nu \mu}^{bb} \]

\[ K_{\omega}^{bf} = N_i (1 - e^{-\omega / T_e}) \sum_{\nu} n_{\nu} (1 - f(\varepsilon)) \sigma_{\nu e}^{bf} \]

\[ K_{\omega}^{ff} = N_e (1 - e^{-\omega / T_e}) \int d\varepsilon' f(\varepsilon')(1 - f(\varepsilon)) \sigma_{\varepsilon \varepsilon'}^{ff} \]

\[ f(\varepsilon) = 1 / (1 + \exp((\varepsilon - \mu) / T)) \]
Emissivity

**Emissivity in LTE and nonLTE cases**

**Emissivity ( LTE ):**

\[ j_\omega = \kappa_\omega I_p^{\omega}; \quad I_p^{\omega} = \frac{\omega^3}{e^{\omega/T} - 1} \]

**Emissivity ( general nonLTE )**

\[ j_\omega = j_{\omega}^{bb} + j_{\omega}^{fb} + j_{\omega}^{ff} \]

\[ j_{\omega}^{bb} = N_i \omega^3 \sum_s P_s \sum_{\nu\mu} n_\mu^s (1 - n_\nu^s) \sigma_{\nu\mu}^{bb} \]

\[ j_{\omega}^{fb} = N_i N_e \omega^3 \sum_{\mu} f(\varepsilon') (1 - n_\mu) \sigma_{\nu\varepsilon}^{bf} \]

\[ j_{\omega}^{ff} = N_e N_i \omega^3 \int d\varepsilon f(\varepsilon)(1 - f(\varepsilon')) \sigma_{\varepsilon\varepsilon'}^{ff}, \quad \varepsilon' = \varepsilon + \omega \]
Zirconium target emission

Spectral Modeling for Zirconium spherical target

Zr emission for r=200um spherical target

Emission intensity, a.u.

Wavelength, nm

Electron density

$N_e = 10^{19}$ 1/ccm

Spherical target

$r = 200 \ \mu m$

Temperature raises → Broadening → Power of emission

Efficiency?
Remarks

- Zirconium ions XV – XXI emit intensively in water window region: 4p-3d, 4f-3d and 5p-3d transitions

- Maximum spectral efficiency for emission in water window region is over 40% for plasma at temperature of 80eV and hotter

- For spherical target of 200um radius and $10^{19}$ electron density the spectrum is broadened (absorption broadening)

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