Radiative Properties of Krypton Plasma & Emission of Krypton DPP Source in Water-Window Spectral Range

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Abstract

Krypton- and zirconium-based plasmas are considered as possible candidates for 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 self-absorption etc. leading to changes in ionization states, state populations, emission intensity and spectrum. Krypton has a UTA at higher ionization degree than zirconium and thus less preferable but krypton plasma source delivers from debris issues in operation cycle comparing to zirconium and bismuth. Due to wide array of transitions the krypton plasma is less opaque to radiated emission than nitrogen.

In the paper the radiance and emission properties of non-equilibrium krypton plasma is examined and the optimal emission temperature conditions for soft X-ray emission output in water window region are explored. Kinetic parameters for non-equilibrium plasma including major inelastic ion interaction processes, radiation and emission data are obtained in the approach based on Hartree-Fock-Slater (HFS) quantum-statistical model and distorted waves approximation. The emission spectral efficiency for krypton up to 25% is achieved at 130 eV, comparable to the one for zirconium (40% at 90 eV). Results of plasma dynamics modeling in capillary discharge by Z* code are presented. Calculated emission energy up to 300mJ per pulse in water window band corresponds to the conversion efficiency (CE) around 7%.
**Krypton VII – XII Lines**

**Krypton line strengths in water-window region**

Satellite lines for transitions 4f-3d in Kr IX excited ([Ar]3d^94p^1) are in water-window range but their strengths and populations of double excited states shouldn’t be enough for meaningful radiation output.

Line strengths of Kr ions computed with Flexible atomic code.
Krypton XIII – XVIII Lines

Krypton line strengths in water-window region

Resonant transitions 4f-3d in Kr XIV (~4.3nm), Kr XV (~4.1nm), Kr XVI (~3.9nm), Kr XVII (~3.7nm) intensively emit into water-window range
Krypton XIX – XXIII Lines

Krypton line strengths in water-window region

Resonant transitions 4d-3p and 4f-3p in Kr XIX (~2.8nm and ~3.3nm), Kr XX, Kr XXI, Kr XXII and Kr XXIII (~2.5nm and ~2.8nm) contribute in water-window range.
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

\[
\frac{dn_\mu}{dt} = \sum_{\nu \neq \mu} n_\nu \alpha_{\nu \rightarrow \mu}(N_i, N_e, T, \rho, F) - n_\mu \sum_{\nu \neq \mu} \alpha_{\mu \rightarrow \nu}(N_i, N_e, T, \rho, F), \quad \sum_\mu n_\mu = 1,
\]

\( \alpha_{\nu \rightarrow \mu} \) and \( \alpha_{\mu \rightarrow \nu} \) - total rates of the processes leading to increase and decrease the population \( n_\mu \) of level \( \mu \), \( N_i \) 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:

\[
N_e = Z_0 N_i, \quad Z_0 = \sum_\mu z_\mu n_\mu,
\]

\( z_\mu \) – charge of the ion of level \( \mu \), \( Z_0 \) - average charge
Non-Equilibrium Model

Processes included

To process to a correct solution of system of kinetic equations for non-equilibrium plasma the set of impact and radiative processes should be taken into account via rates of the processes.

The processes taken into account leading to increase the population $n_\mu$ of level $\mu$ and to decrease the population $n_\nu$ of level $\nu$ are following:

- Impact recombination and ionization $\nu \rightarrow \mu$,
- Excitation and deexcitation $\nu \rightarrow \mu$,
- Dielectronic capture and autoionization $\nu \rightarrow \mu$,
- Photorecombination and photoionization $\nu \rightarrow \mu$,
- Emission and absorption in lines $\nu \rightarrow \mu$.

In general case the rates are calculated from cross-sections of concordant processes (and for given distribution functions of electrons and spectral functions) in the approach based on Hartree-Fock-Slater (HFS) quantum-statistical model and distorted waves approximation. Complete system of kinetic equations is nonlinear and self-consistent.
Krypton Non-equilibrium Plasma

Krypton ionization

Kr ion fractions for $10^{20}$ 1/ccm electron density

Best conditions for emission in water window range are expected at $T > 90$ eV when Kr XIV - Kr XVII ions are dominant in the plasma composition.

Ion populations simulated by authors kinetic code with rates&cross-sections of impact and radiative processes computed in distorted-wave approach and based on self-consistent Hartree-Fock-Slater quantum-statistical model.
Resonant lines of Kr XIV-Kr KVII start to contribute in WW range at $T > 90\text{eV}$ (average charge $Z_0 \sim 13$) and provide maximum output at $T \sim 130\text{eV}$ ($Z_0 \sim 15.5$): 3.7nm by Kr XVI & 3.9nm by Kr XVII.

Emission spectra modelling done by authors kinetic code with rates & cross-sections of impact and radiative processes computed in distorted-wave approach and based on self-consistent Hartree-Fock-Slater quantum-statistical model.
Spectral Efficiency (SE) for Kr reaches its maximum (~25%) at plasma temperature $T \sim 130$ eV

Maximum SE for Zirconium is ~40% at $T \sim 90$ eV (for $N_e = 10^{19}$)

Emission spectra modelling and SE calculations done by authors kinetic code with rates&cross-sections of impact and radiative processes computed in distorted-wave approach and based on self-consistent Hartree-Fock-Slater quantum-statistical model
Soft X-ray emission DPP Source

**Pulsed power capillary discharge**

- **Pulsed-power**
  - Energy storage line: 5 J
  - Liquid dielectric & coolant
  - Voltage: 25 kV
  - Current: 19 kA
  - Pulse: ~153 ns

- **Capillary dimensions**
  - Ø 1.6 mm
  - L = 18 mm

- Various electrode geometries

- Gas: Kr
  - 0.1 - 2 Torr gradients

**Capillary discharge dynamics & emission features:**
- E-beam, plasma channelling ($\varepsilon >> 1$)
- Volumetric MHD compression (skin depth $>>$ plasma diameter)
- Highly ionized ions (fast electrons)
Krypton Soft X-ray Source: Z* modeling

Capillary discharge: Z* modeling results

Emission energy density
Time integrated

Emission power in WW range

Maximum emission power @ 22 ns
Soft X-ray emission pulse duration ~ 15 ns
Energy emitted in WW range ~ 300 mJ/pulse
Conversion efficiency (CE) ~ 7%

Plasma dynamics and emission are done by Z* code
Krypton Soft X-ray Source: Z* modeling

Capillary discharge: Z* modeling results

Plasma dynamics and emission are done by Z* code

Density distribution @ max emission

Emission power @ max emission

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Conclusion

- Krypton ions XIV - XXII emit intensively in water window range: 4p-3d, 4f-3d and 5p-3d transitions
- Maximum spectral efficiency for emission in water window range reaches over 20% for Kr plasma at temperature of 110eV and hotter
- Compare to Zirconium, Krypton plasma provides less spectral efficiency and needs to be hotter: $SE_{Kr}=25\%@130eV$ versus $SE_{Zr}=40\%@90eV$
- Krypton pulsed-power soft X-ray source based on capillary discharge may produce up to 300 mJ of radiation in water window range and with conversion efficiency $\sim 7\%$

The results were obtained in frame of FP7 FIRE Marie Curie action