On the Stark broadening of some Cr II spectral lines in a plasma

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Outline

– Introduction: Atomic structure of the Cr II ion
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  Plasma constituents
  Line profile-width and shift of a spectral line
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  SE approach
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**Introduction:** Atomic structure of the Cr II ion

Singly ionized chromium Cr II is important for technology applications. It is also important for investigation in plasma physics, fusion research and plasma technologies.

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$$[\text{Ar}]\ 3d^5$$

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$3d^4 4p\; ^2F_{5/2} \quad E = 74436.10\text{cm}^{-1}$

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Introduction: Atomic structure of the Cr II ion

\[ 3d^4 4p \quad x^2 F_{5/2} \quad E = 74436.10 \text{cm}^{-1} \]

\[ 3d^4 4p \quad y^2 F_{5/2} \quad E = 70584.39 \text{cm}^{-1} \]

\[ 3d^4 4p \quad z^2 F_{5/2} \quad E = 68583.31 \text{cm}^{-1} \]

Seniority number
Stark broadening of spectral lines in plasma:

Plasma constituents
Stark broadening of spectral lines in plasma:

Line profile-width and shift of a spectral line
Stark broadening of spectral lines in plasma:

Line broadening

Spectral Line Broadening in Plasma

- Natural width
- Doppler width
- Collisional width

\[ L(x) = \frac{1}{\pi^{\frac{3}{2}}} \frac{\gamma_L^2}{(x^2 + \gamma_L^2)} \]

\[ j_{A,R}(x) = \frac{1}{\pi^{\frac{3}{2}}} \frac{W_R(\beta)}{1 + \left( x - A^{\frac{3}{2}} \beta^2 \right)^2} \, d\beta \]

\[ G(x) = \sqrt[\ln(2)]{\pi \frac{-\ln(2) \left[ \frac{x}{\gamma_G} \right]^2}{\gamma_G}} \]
Stark broadening of spectral lines in plasma:
General expression for the width of an isolated ion line

According to the impact approximation (Baranger, 1958), the full half-width (FWHM) of an isolated ion line is given by:

\[
W = N \left\{ v \left[ \sum_{i'} \sigma_{j'\bar{i}} + \sum_{f'} \sigma_{f'\bar{f}} \right] \right\}_{av} + W_{el}
\]

where \(N\) is the electron density, \(\sigma_{j'\bar{j}}\) the inelastic cross sections for collisional transitions, \(\{.\}_{av}\) is the average over the electron velocity \(v\) distribution and \(W_{el}\) is the line width induced by elastic collisions.

Stark broadening of spectral lines in plasma:
SCP approach

According to the semiclassical perturbation approach (SSB 1969 and SSB et al. 2014):

\[ W = N \int v f(v) \left( \sum_{i' \neq i} \sigma_{i'i}(v) + \sum_{f' \neq f} \sigma_{f'f}(v) + \sigma_{el} \right) \]

where \( f(v) \) is the Maxwellian velocity distribution function for electrons,

\[ \sum_{j' \neq j} \sigma_{j'j}(v) = \frac{1}{2} R_1^2 + \int_{R_1}^{R_D} 2\pi \rho d\rho \sum_{j'j} P_{jj'}(\rho, v) \]

is the inelastic cross section and the elastic cross section is given by:

\[ \sigma_{el} = 2\pi R_2^2 + \int_{R_2}^{R_D} 2\pi \rho d\rho \sin^2 \delta + \sigma_r \]


According to the semiempirical approach (Griem, 1968), the full half-width (FWHM) of an isolated ion line is given by:

\[
W = N \frac{8\pi}{3} \frac{\hbar^2}{m^2} \left( \frac{2m}{\pi kT} \right)^{1/2} \frac{\pi}{\sqrt{3}} \left[ \sum_{i'} R_{i'i}^2 g \left( \frac{E}{\Delta E_{i'i}} \right) + \sum_{f'} R_{f'f}^2 g \left( \frac{E}{\Delta E_{f'f}} \right) \right]
\]

where \( E = \frac{3kT}{2} \) is the energy of the perturbing electron, \( \Delta E_{j'j} = |E_{j'} - E_j| \) is the energy difference between levels \( j' \) and \( j \), \( R_{j'j}^2 \) is the square of the coordinate operator matrix element and \( g(x) \) the Gaunt factor function for width.

Stark broadening of spectral lines in plasma: 
MSE approach

According to the modified semiempirical approach (Dimitrijević and Konjević, 1980), the full half-width (FWHM) of an isolated ion line is given by:

\[
W = N \frac{8 \pi}{3} \frac{h^2}{m^2} \left( \frac{2m}{\pi kT} \right)^{1/2} \frac{\pi}{\sqrt{3}} \left[ R^2_{l_i,l_i+1} \tilde{g} \left( \frac{E}{\Delta E_{l_i,l_i+1}} \right) + R^2_{l_i,l_i-1} \tilde{g} \left( \frac{E}{\Delta E_{l_i,l_i-1}} \right) + R^2_{l_f,l_f+1} \tilde{g} \left( \frac{E}{\Delta E_{l_f,l_f+1}} \right) + R^2_{l_f,l_f-1} \tilde{g} \left( \frac{E}{\Delta E_{l_f,l_f-1}} \right) + \sum_{i'j'} (R^2_{ii'}) \Delta n \neq 0 g \left( \frac{3kTn_i^3}{4Z^2E_H} \right) + \sum_{f'f} (R^2_{ff'}) \Delta n \neq 0 g \left( \frac{3kTn_f^3}{4Z^2E_H} \right) \right]
\]

\(E = \frac{3kT}{2}\) is the energy of the perturbing electron, \(\Delta E_{j',j} = |E_{j'} - E_j|\) is the energy difference between levels \(j'\) and \(j\), \(R^2_{j',j}\) is the square of the coordinate operator matrix element, \(\tilde{g}(x) = 7 - \frac{1}{Z} + g(x)\) and \(g(x)\) are the Gaunt factor functions for width.

Stark broadening of Cr II spectral lines:

Precedent calculations (Dimitrijević et al. 2007 & Simić et al. 2013)


Stark broadening of Cr II spectral lines: 
Recent experimental work (Aguilera et al. 2014)

Table 1. Stark widths (FWHM) $w$ (pm) and shifts $d$ (pm) at electron density 10$^{17}$ cm$^{-3}$ of Cr II spectral lines, compared to experimental and theoretical values reported in the literature. The temperature range is 12 000–16 300 K. The relative error of $w$ is 15 per cent. The relative error of $d$ is 11 per cent, with a minimum absolute error of 0.1 pm.

<table>
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Stark broadening of Cr II spectral lines:
Recent experimental work (Aguilera et al. 2014)

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<sup>a</sup>Rathore et al. (1984). Temperature 13 700 K.
<sup>b</sup>Dimitrijević et al. (2007). Data interpolated to a temperature of 14 000 K.
<sup>c</sup>Simić et al. (2013). Data interpolated to a temperature of 14 000 K.
Stark broadening of Cr II spectral lines:
Present calculations

Cr II: 4s $a^4D - 4p z^4F^\circ$
$\lambda=3127.92 \, \text{Å}$

$log(W(\text{Å})) = 1.56305 - 0.74906 \log(T(K)) + 0.03043 (\log(T(K)))^2$

Aguilera et al. Experimental values (2014)

$W(\text{MSE}) = 1.4 \, W(\text{Ag})$
$W(\text{Ag}) = 260 \, W(\text{D})$

$log(W(\text{Å})) = 0.33379 - 1.48039 \log(T(K)) + 0.12909 (\log(T(K)))^2$
Stark broadening of Cr II spectral lines: Present calculations

Cr II: 4s b^4P - 4p y^4D°
λ=2942.89 Å

log[W(Å)] = 2.00848 - 1.00029log[T(K)] + 0.06125(log[T(K)])^2

Aguilera et al. Experimental values (2014)
Conclusion

In this work, we calculate the spectral line widths of some Cr II lines at an electron density of $10^{17}$ cm$^{-3}$ and electron temperatures from 5000 K to 80000K using the modified semi-empirical (MSE) approach. The needed atomic data are taken from NIST database.

The obtained widths are compared to Dimitrijević et al. (2007), Simić et al. (2013) and Aguilera et al. (2014) values.
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