Computer simulation and experimental studies of the N I $3p^2S_{1/2} \rightarrow 3d^2P_{1/2}$ spectral line Stark broadening

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Abstract. A computer simulation method, dedicated to lines, which energy levels are influenced only by the quadratic Stark effect, is introduced and tested in this paper. The simulated profiles of the well isolated N I line $3p^2S_{1/2} \rightarrow 3d^2P_{1/2}$ are compared with experimental ones.

1. Introduction
The computer simulation method (CSM) [1] is successfully used for calculation of the Stark broadening of the plasma spectral lines mainly for hydrogen, hydrogen-like and helium lines, e.g. [2]. Profiles obtained in this way, are characterized by high reliability. Whereas in the case of the line profiles of non-hydrogen atoms, the so-called $j(x)$ profile [3] is commonly applied in computation. The impact approximation for electrons, the quasi-static approximation for ions and the separation of the strong and the weak collisions are basic assumptions lying on the basis of the $j(x)$ model. The CSM do not require such simplifications. In this paper the CSM for non-hydrogen lines is presented and delivered by this method results are compared with other ones. The required in semi-empirical calculation atomic data (line strengths) have been taken from NIST [4].

2. Simulation method
The model of the plasma is essentially the same as in commonly used by computer simulation method (CSM) [1]. Ions and electrons, the charged components of plasma, are treated as classical particles, which move along straight-line trajectories independently from each other and from the emitter. The shape of simulated volume is a sphere, with the electrically neutral emitter resting at its center. The Schrödinger equation describes an evolution of a quantum state of the emitter caused by varying in time electric fields produced by ions and electrons. The starting point of this consideration is the relation between the spectral line profile and the average of the dipole autocorrelation function $C(t)$, which can be written in the following way:

$$I(\Delta \omega) = \lim_{t_f \to \infty} \pi^{-1} \int_0^{t_f} C(t) e^{i \Delta \omega t} dt, \quad C(t) = \text{Tr} \left\{ \tilde{d} \cdot U_{f f'}(t, 0) \tilde{d}_{f' i} U_{i i'}(t, 0) \rho_{i i'} \right\}_{av}, \quad (1)$$

where $\tilde{d}$ is the dipole operator for the emitter, while $i$, $i'$ and $f$, $f'$ indicate the sublevels of the initial ($E_i$) and final ($E_f$) states of the unperturbed atom, respectively. The frequency separation
from the line center is given by $\Delta \omega = \omega - (E_i - E_f) / h$, whereas $U(t,0)$ is the operator of the time development of the emitter in the presence of the electric field produced by electrons and ions. The averaging $\langle \cdots \rangle$ is taken over all initial simulated field strengths and possible time histories. The time-evolution operators $U_{ii'}(t,0)$ and $U_{ff'}(t,0)$ (corresponding to the initial and final states, respectively) satisfy the following Schrödinger equation:

$$i\hbar \dot{U}(t,0) = [H_0 + V(t)]U(t,0),$$

where $H_0$ is the Hamiltonian of the isolated emitter and $V(t) = -\vec{d} \cdot \vec{F}(t)$ is the emitter-plasma interaction potential. The Strang symmetrical splitting formula [5], was applied to solve the Schrödinger equation of evolution, leads to unitary evolution of time:

$$U(t + \Delta t, t) \equiv \exp \left( i\hbar F_x \Delta t/2h \right) \exp \left( i\hbar F_y \Delta t/2h \right) \exp \left( i\hbar F_z \Delta t/2h \right) \exp \left( -i\hbar H_0 \Delta t/h \right) \exp \left( i\hbar F_x \Delta t/2h \right) \exp \left( i\hbar F_y \Delta t/2h \right) \exp \left( i\hbar F_z \Delta t/2h \right).$$

### 3. Comparison of the simulation and experimental results

Line shape measurements were performed using a wall-stabilized arc, operated at atmospheric pressure. The radiation of the plasma, emitted from homogeneous plasma layers in end-on direction, was measured using a grating-spectrometer with a two-dimensional CCD detector. In this way the spectrum corresponding to the N I $3p^2 S_{1/2} - 3d^2 P_{1/2}$ spectral line have been measured. In Figure 1 the comparison of the simulated profile with the pure experimental one is shown.

![Figure 1](image_url)

**Figure 1.** The simulated profile (solid line) of the spectral line N I $3p^2 S_{1/2} - 3d^2 P_{1/2}$ is presented and compared with experimental result (circles). Doppler and instrumental broadening are included. As can be seen, the experimental profile is more asymmetric than the simulated one. Real and imaginary parts of the autocorrelation function are shown in the inset.

Experimental values of Stark broadening parameters have been obtained from the best fit procedures applying the Griem-like profile $j(x)$ [3], convoluted with the corresponding Doppler and apparatus profile. Profile $j(x)$ has three parameters: electron impact width $w_e$, electron impact shift $d_e$ and ion asymmetry parameter $A$. We may regard all three parameters of the spectral line as free, or restrict the number of free parameters to two, using relation between $w_e$ and $A$: $A = (w_{e0}/w_{e0})^{3/4} (N_e/10^{16})^{1/4}$, where the constant $w_{e0}$ is related to the quadratic Stark splitting in the normal electric field $F_0$. This new approach to determination of the asymmetry parameter is described in detail in [6]. The results of the fitting procedure with two different $w_{e0}$ parameters are shown in Figure 2.

In Figure 3 the electron impact width obtained from the fitting procedure for the simulated and measured profiles are compared. The results of the calculation performed according to the impact and quasi-static theory are also shown.
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