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K-line emission profiles with focus on the self-consistent calculation of plasma polarization

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Abstract
The emitted K_α-spectra of moderately ionized titanium radiators in a medium are used to determine plasma temperature and composition in electron heated target regions. A theoretical treatment of spectral line profiles using self-consistent Hartree–Fock and ion sphere model calculations to determine the influence of plasma polarization is applied. We confirm the importance of excited emitter states for line shape modeling.

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(Some figures in this article are in colour only in the electronic version)

1. K-line measurements

In recent years K-line spectra have become the focus of various experiments. Narrow K_α-emission of some keV is an appropriate light source for Thomson scattering on warm dense matter with solid and even over-solid electron density [1]. Moreover, as the K-spectra are often emitted from a warm dense plasma themselves one can infer plasma parameters, i.e. temperature, density and composition, by studying variations of emission energy and line shape [2, 3]. There are a large variety of effects influencing the line profile, for example Doppler-broadening, self-absorption and satellite transitions. Electric and magnetic fields also have a strong impact, thus it is possible to infer field strengths within the plasma via the Stark and Zeeman effect [4]. We will focus here on the influence of plasma polarization effects on the K-line emission.

Typical experiments to create and measure K-line spectra are based on thin foils irradiated by ultra-short high-intensity laser pulses. Laser irradiation of the target creates a hot and dilute plasma on the target surface. The laser pulse cannot penetrate more than the skin depth into the

target. However, hot electrons, accelerated by the laser up to MeV energies, flow through the foil and create a warm dense plasma via impact ionization. X-ray emission and thermalization occur within hundreds of femtoseconds, before any expansion of the sample.

Within the last few years titanium K_α-lines have been analyzed experimentally and theoretically by several groups, see e.g. [3, 5]. In a recent experiment, performed at the 100 TW laser facility at LULI in January 2008, a 10 micron titanium foil was irradiated by a 330 fs laser pulse of an intensity of 9×10^{19} W/cm^2 (single shot). The focal spot size was measured to be 8 micron and the energy was 14 J at the sample surface. A toroidally bent GaAs crystal served as an x-ray spectrometer with a resolution of $E/\Delta E = 15\,000$ and the measurements have 1D spacial resolution of 13 micron. The spectrum analyzed in section 3 was taken at the front side of the sample, at a lateral distance of 105 micron from the point of maximum emission, which is about the x-ray spot radius at half intensity. By choosing a spectrum from the outer part of the sample we avoid integrated measurements over large temperature gradients and observe emission of target regions moderately heated only by electrons. More details are given by Zastrau *et al* in [6]. We calculated titanium K_α-spectra in order to analyze these measurements with respect to the plasma parameters of electron heated target regions.

2. Calculation of plasma polarization

In order to describe the influence of a plasma environment on an emitter, a perturbative ansatz, $H = H^0 + H'$, is chosen. The system's Hamiltonian H is split into a part H^0 describing the isolated emitting particle and a perturbing plasma potential H'. According to the first-order perturbation theory, emission energies are shifted by $\Delta E^{(1)} = \langle\varphi_i|H'|\varphi_i\rangle - \langle\varphi_f|H'|\varphi_f\rangle$, which is given by the difference of the perturbations of the initial one-particle orbital φ_i and the final one-particle orbital φ_f, respectively. The isolated emitter can be described by means of atomic physics. To determine emission and ionization energies of various ionic configurations, we solved the corresponding self-consistent Roothaan–Hartree–Fock equations applying the program package Gaussian 03 (G03) [7]. G03 is a chemical *ab initio* code that allows for a fast and inexpensive calculation. However, due to the Gaussian-like orbital shapes and a strong orbital mixing, G03 calculations prevent straightforward observation of fine-structure splitting. Other atomic physics codes, e.g. FAC [8], overcome this shortcoming but lead to much more expensive calculations.

We calculated (isolated) emission energies of various ionization stages with the outermost shell in the ground-state configuration and found a blue shift with increasing ionic charge which is caused by a stronger Coulomb interaction within the emitter when electrons are removed. Furthermore, we considered states with one of the M-shell electrons excited. Whether the electron is brought to an upper level or completely removed from the emitter, makes only a small difference for the K_α emission energy because in both cases the electron's contribution to the screening of the nucleus tends to zero. In particular, exciting the outermost electron to an unoccupied 3d or 4s level leads to emission energies comparable to the line position of the next ionization stage. The perturbing plasma potential H' is determined within an ion sphere model (ISM) calculation [2]. For this, we solve the Poisson equation within a Wigner–Seitz sphere self-consistently with respect to the free electron density, which is taken in the non-degenerate Maxwell–Boltzmann limit.

Calculations of the K-line shift as a function of the plasma temperature ($T = 10$–100 eV) and free electron density ($n_e = 10^{22}$–10^{24} cm^{-3}) were performed for various ionic configurations of mid-Z materials, such as Ti, Cl and Si. We found a red shift of the K_α emission energies of several eV due to the formation of a polarization cloud of free electrons around

the emitter's nucleus (plasma polarization shift). The free electrons screen the interaction between core and bound electrons, resulting in smaller binding energies and narrowing the energy gaps between the orbitals. This shift decreases with increasing temperature since the polarization cloud is spatially extended and thus the screening is reduced. The shift increases with increasing density of free electrons because the amount of electrons within the polarization cloud and thus the screening rises.

3. Line profiles

We now want to construct experimentally relevant line profiles using the single emission energies and their shifts determined so far. For this, it is necessary to know the composition of emitters within the plasma. We calculate this composition self-consistently via coupled Saha equations under the assumption of a local thermal equilibrium. Continuum lowering due to free electrons is taken into account also applying the ISM. Hence, the composition is not only temperature- but also density-dependent.

Since bulk titanium is a metal, delocalized quasi-free electrons have to be taken into account. Averaging the Hall coefficients, see e.g. Scovil [9], over the angle between the c-axis of the hexagonal Ti crystal and the magnetic field one can obtain an effective Hall coefficient of $R_H = -2.9 \times 10^{-11}\ \mathrm{m^3\,C^{-1}}$. According to $n_e = (eR_H)^{-1}$, the density of free or quasi-free electrons within the metal can be estimated at $n_e(\mathrm{cold}) \approx 2.1 \times 10^{23}\ \mathrm{cm^{-3}}$. In relation to the titanium bulk density of $n_{\mathrm{bulk}} = 5.66 \times 10^{22}\ \mathrm{cm^{-3}}$, the average (cold) ionic state of the emitter can be assumed to be fourfold ionized. Thus, to determine titanium K_α-spectra the iterative ISM calculations start at $n_e = n_e(\mathrm{cold})$. Moreover, we take into account six ionization stages starting at Ti^{4+}, i.e. configurations from Ar- to Al-like titanium.

As mentioned before, emission energies of excited emitters are close to the emission energies of the next ionized ground-state emitter. However, to excite an electron needs several 10 eV less energy than to ionize it. In conclusion contributions to the line shapes of excited state emitters look like contributions of the next ionized ground states, but appear at lower temperatures. To take this effect into account, we introduce electronic configurations with one electron excited to a 3d or 4s level to the partition function. To avoid discontinuities when these states vanish into the continuum, the partition function is taken in Planck–Larkin renormalization [10].

Due to the fact that fine splitting is not accessible by G03, the two components of the K_α-line corresponding to the $P_{1/2}$ and $P_{3/2}$ initial states are constructed semi-empirically by using the measured line distance of $\Delta E = 6.26$ eV as given by the experiments [6].

Each (shifted) emission energy is assigned a Lorentzian line profile. Their heights are given by the fraction of emitters in the particular state. For all their widths we took one variable value that appears as an additional parameter within our calculations. Furthermore, a convolution with a 0.3 eV wide Gaussian profile is performed to account for the rather small instrumental broadening. Figure 1 shows a comparison of such calculated line profiles and experimental data of the recent measurements. The dashed curves depict spectra measured at the outer part of the emission region. The solid curves depict the calculated Ti K_α-spectra. The left-hand side shows a spectrum with no excited states of the outer shell accounted for. By fitting the calculated spectra to the central line feature, plasma parameters can be inferred. For the particular experiment we find a plasma temperature of $T = 29$ eV and free electron density of $n_e = 2.90 \times 10^{23}\ \mathrm{cm^{-3}}$. However, it is known that excited states are of large relevance for K-line emissions if M-shell electrons are present [11]. Thus, we allowed occupation of states with one of the outer electrons excited to a 3d or 4s level unless the states vanish due to

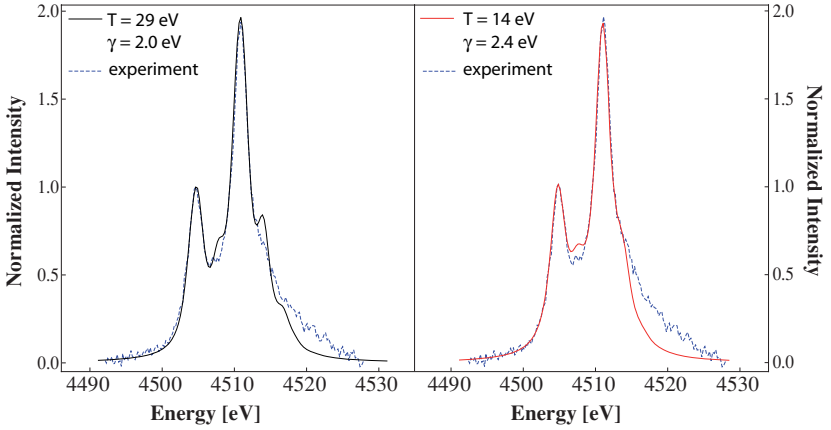

Figure 1. Comparison of measured (dashed) and calculated (solid) Ti K_α-line profiles. (Left) without excited states, (right) with excited states.

continuum lowering, resulting in a spectrum shown on the right-hand side of figure 1. We infer $T = 14\,\mathrm{eV}$, $n_e = 2.34 \times 10^{23}\,\mathrm{cm}^{-3}$ and $\bar{Z} = 4.11$. Since the excitation energies are much less than the ionization energies, there is a large drop in the determined temperature. This confirms the importance of including the close to continuum-excited states, they have a significant contribution to the line profiles. Since the experimental spectrum is taken far from the point of maximum emission, we assume a single temperature for all radiators. However, integrating over the whole sample length incorporates radiation from various plasma conditions, which may cause the deviation of the blue wings in figure 1. Our results may serve as average plasma conditions at a distance of about 0.1 mm from the center of emission.

It should be noted that, to fit the spectra as shown in figure 1 the Lorentzian line width had to be set to $\gamma = 2.4$ eV. This rather large width may be caused by a variety of possible broadening mechanisms. For example, we restricted the calculations here to three components per ionization stage, i.e. ground state and spectator in 3d or 4s, respectively. By inclusion of more detailed multiplet-structure, we find overlapping lines, which cause an effective broadening. Moreover, self-absorption may play an important role and electro-magnetic fields can cause significant Stark and Zeeman broadening. Currently, work on identifying the relevant broadening processes is in progress, see Stambulchik *et al* [12] for more details.

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References

[1] Glenzer S H *et al* 2003 *Phys. Plasmas* **10** 2433
[2] Sengebusch A *et al* 2007 *Contrib. Plasma Phys.* **47** 309
[3] Hansen S B *et al* 2005 *Phys. Rev.* E **72** 036408
[4] Davara G *et al* 1998 *Phys. Plasma* **5** 1068
[5] Chen S N *et al* 2007 *Phys. Plasmas* **14** 102701

[6] Zastrau U *et al* 2009 at press
[7] Frisch M J *et al* 2004 *Gaussian 03* (revision c.02) (Wallingford, CT: Gaussian Inc.)
[8] Gu. M F 2003 *Astrophys. J.* **582** 1241
[9] Scovil G W 1966 *Appl. Phys. Lett.* **9** 247
[10] Rogers F J 1986 *Astrophys. J.* **310** 723
[11] MacFarlane J J *et al* 1993 *Phys. Rev.* E **47** 2748
[12] Stambulchik E *et al* 2009 *J. Phys. A: Math. Theor.* **42** 214056