

# Methods of charge-state analysis of fast ions inside matter based on their X-ray spectral distribution

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## Abstract

The X-ray spectral distribution of swift heavy Ti and Ni ions (11 MeV/u) observed inside aerogels ( $\rho = 0.1 \text{ g/cm}^3$ ) and dense solids (quartz,  $\rho = 2.23 \text{ g/cm}^3$ ) indicates a strong presence of simultaneous 3–5 charge states with one  $K$ -hole. We show that the theoretical analysis can be split into two tasks: first, the treatment of complex autoionizing states together with the originating spectral distribution, and, second, a charge-state distribution model. Involving the generalized line profile function theory, we discuss attempts to couple charge-state distributions.

**Keywords:** Autoionizing states; Heavy ion beams; Spectroscopy; Stopping power

## 1. INTRODUCTION

In the heavy ion beam driven inertial fusion program, the analysis of the projectile effective charges and the stopping power in various media is of extraordinary interest. In contrast to the projectile charge-state analysis outside the interaction volume (e.g., by means of particle detectors), the information about the projectile mean charge inside matter is required for a direct comparison with theoretical methods. The desired experimental information has to be obtained in an indirect manner, namely from the projectile radiation emission. The request for negligible absorption and observation of several simultaneous charge states leads to the analysis of the X-ray spectral distribution originating from complex autoionizing states (e.g., the  $K_\alpha$ -satellite series  $1s^1 2s^n 2p^m - 1s^2 2s^n 2p^{m-1} + h\nu$ ). A first experimental step was recently put forward at Gesellschaft für Schwerionenforschung–Darmstadt where projectile radiation emission of swift heavy ions inside dense matter was observed (Rosmej *et al.*, 2001; O.N. Rosmej *et al.*, pers. comm.).

Currently, there are no models available to transform the measured projectile spectral distribution into an average

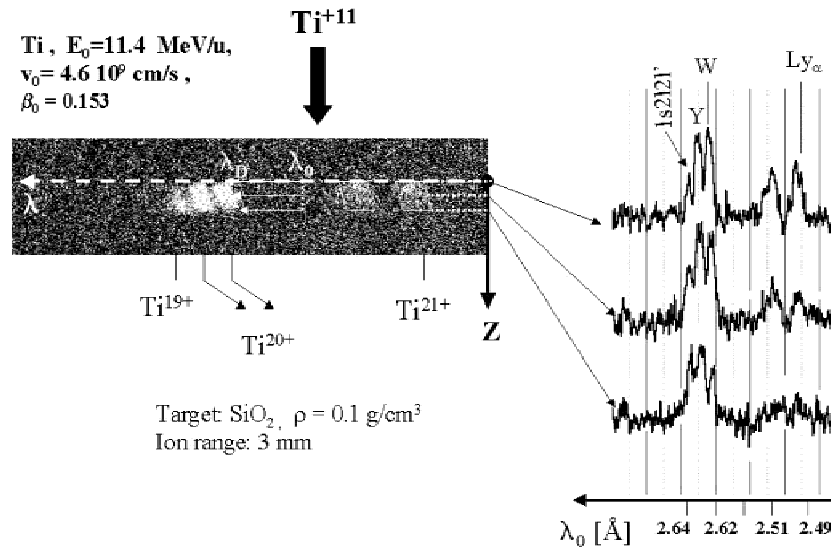
charge state inside matter. The complexity arises from the need for spectroscopic accuracy (in contrast to usual averaged population kinetics), the incorporation of the radiation emission of complex autoionizing states, and the simultaneous treatment of several charge states.

In the present work, we present the first steps toward the development of suitable models to interpret the spectral distribution. The approach is based on the introduction of the generalized line profile function (GLPF) model (Rosmej, 2001) to maintain the full complexity of autoionizing states while reducing population matrixes by orders of magnitude. Spectral distributions containing various charge states are obtained coupling an analytical solution to GLPF to an average atom approach (Rosmej & Moore, 2001). First results of simulations and qualitative discussions with available data are presented.

## 2. OBSERVATION OF X-RAY RADIATION FROM SWIFT HEAVY IONS INSIDE SOLIDS

X-ray radiation emission of swift heavy ions inside matter has been recorded with spherically bent Bragg crystals. The spatial resolution was tuned along the projectile trajectory. More details are described in (Rosmej *et al.*, 2001; O.N. Rosmej *et al.*, pers. comm.). Figure 1 shows the X-ray emission of titanium inside Si aerogel (density  $\rho = 0.1 \text{ g/cm}^3$ );

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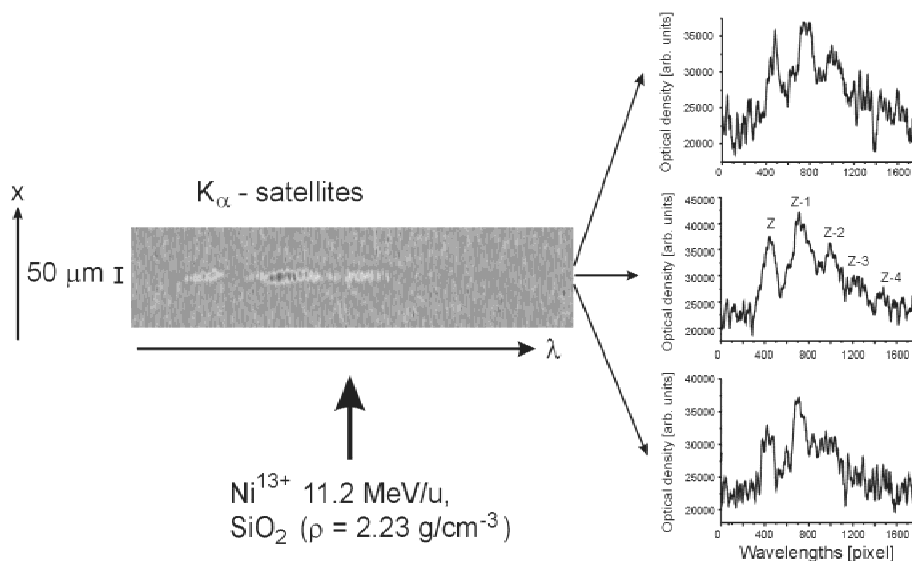
**Fig. 1.** Space-resolved X-ray emission of Ti projectiles along the trajectory (Z-coordinate) inside Si aerogel. The variation of the Doppler shift  $\lambda_D$  is due to the slowing down process of the projectiles.

the  $z$ -axis is the coordinate along the ion trajectory. The Li-like satellite transitions  $1s2l2l' - 1s^22l + h\nu$ , the He-like intercombination line  $Y = 1s2p^3P_1 - 1s^2 + h\nu$ , the He-like resonance line  $W = 1s2p^1P_1 - 1s^2 + h\nu$ , and the H-like Lyman-alpha lines  $Ly_\alpha = 2p - 1s + h\nu$  are well observed. At the entrance (upper spectral trace of Fig. 1) a strong  $Ly_\alpha$ -emission is observed along with strong He-like and Li emission. Near the end (lower trace)  $Ly_\alpha$  is almost absent, whereas the relative intensity of the Li-like satellites has increased relative to the He-like emission. We note that the full range of stopping (about 3 mm) cannot be observed: The slowing down process of the projectile energy near the end of the range is insufficient for  $K$ -shell excitation of Ti.

Figure 2 shows a similar experiment slowing down Ni projectiles in quartz. Due to the high target density, the range is dramatically shortened (to about  $50 \mu\text{m}$ ). The traces show the  $K_\alpha$  satellite series. Essentially emission from 3–5 charge states with one  $K$ -hole (different number of spectator electrons in the  $L$ -shell, i.e., level  $1s^12s^n2p^m$ ) is observed.

### 3. MODELS FOR CHARGE-STATE ANALYSIS

The interpretation of the spectral distribution of swift heavy ions inside matter (e.g., for the purposes of charge-state analysis) is one of the most important but also very difficult tasks in the projectile spectroscopy. The extraordinary difficulties arise from the following circumstances:



**Fig. 2.** Space-resolved X-ray emission of Ni projectiles inside quartz.

1. The necessary spectral distribution involves radiation emission from complex autoionizing states, giving rise to a number of LSJ-split levels, about  $N = 10^3\text{--}10^6$ . As the population matrix is of dimension  $N^2$ , it is obvious that population kinetic approaches are almost hopeless.
2. Known reduction schemes (e.g., super-configurations (Bar-Shalom *et al.*, 1989)) reduce the necessary spectroscopic accuracy of autoionizing states (Rosmej, 2001) and are therefore not useful.
3. Cross sections for heavy particle collisions, in particular those involving multielectron processes, are still not well known.
4. Charge-state distribution models taking account of hollow ions are not available.

In the following we make the first attempts toward a spectroscopic theory for the interpretation of the X-ray spectral distribution. Let us begin with issues 1 and 2. In most general terms, the spectral distribution can be written as

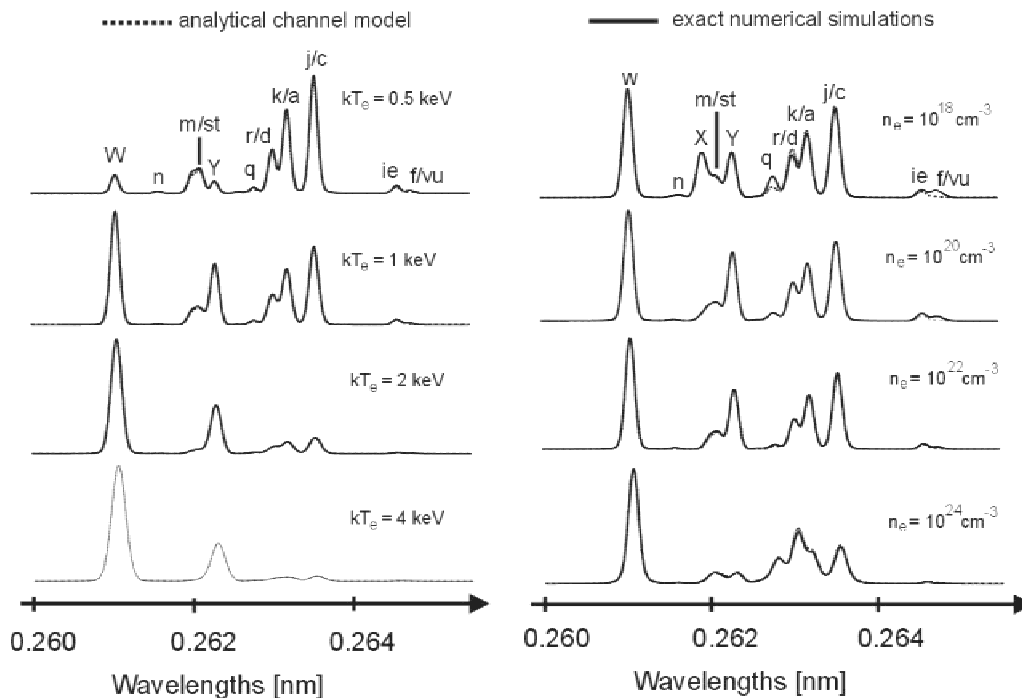
$$I(\omega) = \sum_{k=0}^{Z_n} \sum_{j=1}^{N_k} \sum_{i=1}^{N_k} \hbar \omega_{k,ji} A_{k,ji} n_{k,j} \Phi_{k,ji}(\omega), \quad (1)$$

where  $\omega$  is the transition frequency,  $A$  is the spontaneous transition probability,  $n$  is the population density of the upper state,  $\Phi$  is the line profile,  $k$  indicates the charge state, and the bound-bound transition is indicated by the indices  $i\text{--}j$ . The summation has to be carried out over all transitions and charge states. Known reduction schemes (e.g., super-configurations) (Bar-Shalom *et al.*, 1989) reduce the num-

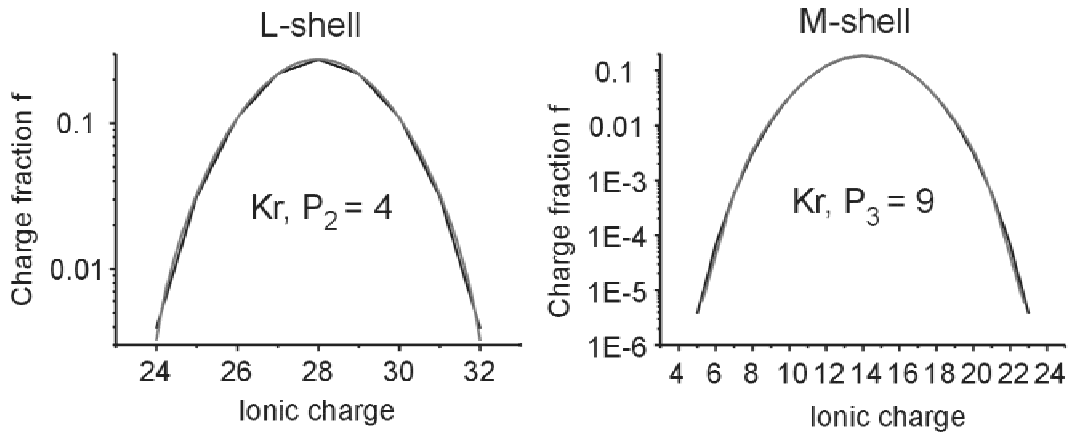
ber of levels  $N$ ; however, at the same time, the bound-bound transitions are inherently reduced resulting also in a reduced (and therefore not useful) spectral distribution. The GLPF, however, permits order of magnitude reduction without loss of spectral details (Rosmej, 2001). In the GLPF theory, a Layzer complex is shown to have a general spectral distribution for each atomic excitation channel. A “virtual” kinetics with total line shapes (composed from all LSJ-split transitions of a Layzer complex) mixes the channels to obtain the final distribution. As the theory is shown to have an analytical solution even when reducing the total Layzer complex by one “super-level,” the approach leads to many orders of magnitude reductions. This opens up the field for the analysis of spectral distributions originating from hollow ions. The spectral distribution in the GLPF theory is given by (Rosmej, 2001)

$$I(\omega) = \frac{n_a}{g_a} \sum_{i=1}^{N_i} \sum_{j=1}^{N_j} \hbar \omega_{ij} A_{ij} \Phi_{ij}^{tot}(\omega). \quad (2)$$

$n_a$  is the “super-level,”  $g_a$  is its statistical weight, and  $\Phi$  is the generalized line profile function. Although the huge number of levels  $N$  is reduced to one level, the summation is carried out over all LSJ-split transitions and the final distribution in non-LTE due to the “virtual” line shape kinetics involved in  $\Phi$ . Figure 3 shows the comparison between GLPF and full LSJ-split population kinetics for the configurations  $1s2l2l'$ . The density interval chosen ranges from gaseous targets to solids, the temperature range from dom-



**Fig. 3.** Comparison of the analytical channel model with exact numerical calculations for titanium projectiles. Excellent overall agreement is seen for extremely wide ranges of temperature and density.



**Fig. 4.** Charge state distribution of Kr projectiles for different average occupation numbers of the *L*- and *M*-shell. The respective widths of the charge state distribution are  $\text{FWHM}(L\text{-shell}, P_2 = 4) = 3.5$ ,  $\text{FWHM}(M\text{-shell}, P_3 = 9) = 5.1$ .

inating hollow ion emission to negligible ones. In all cases, an excellent overall agreement is seen, providing confidence that issues 1 and 2 listed above can be considered as essentially solved.

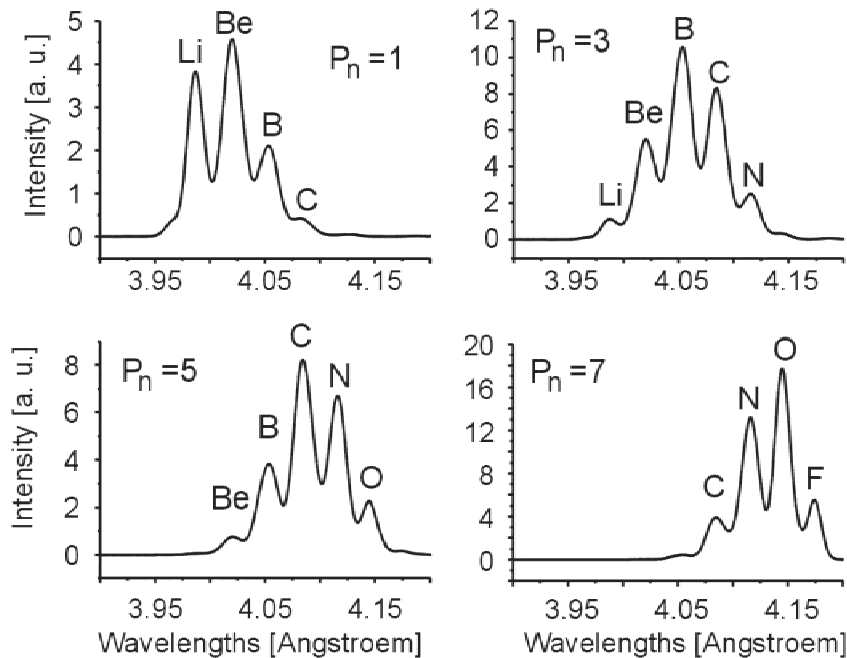
The next issue concerns the distribution of charge states. In this respect it should be noted that the identification of the line transition automatically identifies the charge state; however, this is a charge state of an excited state which does not necessarily coincide with the majority of ions in the same charge state having no excited state. This is even more important, as it has long been well known (e.g., Beyer *et al.*, 1982) that ion–ion collisions lead to multiple-electron ionization with cross sections as large as those for single-electron ionization.

To generate a spectral distribution involving several charge states, we choose

$$f(k_n) = \left(\frac{P_n}{2n^2}\right)^{k_n} \left(1 - \frac{P_n}{2n^2}\right)^{2n^2 - k_n} \frac{2n^2!}{(2n^2 - k_n)! k_n!} \quad (3)$$

$f(k_n)$  is the probability to find  $k$  electrons in shell  $n$  if the average noninteger population is  $P_n$ . Figure 4 shows the corresponding charge-state distribution for krypton for *L*-shell and *M*-shell occupation. The respective FWHM of the charge state distribution is about 3–5.

The charge state distribution model, Eq. (3), can be combined with Eqs. (1) and (2), resulting in a final spectral distribution given by



**Fig. 5.** Spectral distribution of Ar projectile X-ray emission for different numbers of average *L*-shell population  $P_{n=2}$ .

$$I(\omega) = \sum_{k_n} \sum_{i,j} h\omega_{k_n,j,i} A_{k_n,ji} f(k_n) \Phi_{k_n,i,j}(\omega). \quad (4)$$

Figure 5 shows the distribution of argon projectiles with different  $L$ -shell average population  $P_2$ . It can be seen that emission from three charge states are dominating and a further two charge states are still visible. This is in qualitative agreement with the limited experimental results available so far. However, it should be noted that despite this qualitative agreement, a satisfying charge-state distribution model is not available and even its principle nature of construction is rather unclear up to now.

#### 4. CONCLUSION

The X-ray spectral distribution of swift heavy ions *inside* dense matter has been analyzed experimentally and theoretically. A new approach for the interpretation based on a “virtual” line shape kinetics has been introduced. Attempts

for charge state analysis have been made and qualitative agreement with first experimental results are obtained.

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