

# Genetic algorithms in spectroscopic diagnostics of hot dense plasmas

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## Abstract

This paper will present a novel genetic-algorithm-based code (GASPED), developed for the analysis of fine features (e.g., satellite structure and line shifts) in X-ray spectra emitted by hot dense plasmas. The problem dependent modification of standard genetic-algorithm concepts allows efficient decomposition of spectra in concrete physical terms, such as resonance and intercombination lines, dielectronic satellites, or prospective nuclear transitions. Two examples of the code application demonstrate the proposed approach. High resolution K-shell spectra emitted from He- and Li-like Al ions immersed in dense, constrained-flow plasma are decomposed into individual pseudo-Voigt components, by using anticipatory theoretical knowledge of the satellite structure simulated by the multilevel collisional-radiative code (MARIA). Line shifts of the He-like resonance and intercombination line are deduced assuming the aggregate plasma-induced shifts of the parent lines and their satellites. The trend in the frequency shifts observed as a function of the variable plasma parameters qualitatively follows the theoretical predictions. The found variations of the exchange energy between the singlet and triplet levels provide a new impact for the line shift theories. The second example concerns the search for low-lying nuclear transitions in hot dense laser-produced plasmas. The spectra of highly ionized Ta are decomposed by combining the GASPED code with results of *ab initio* atomic data calculations performed by the RELAC code. Upper limits for observation of the controversial radiative decay of Ta nuclei at 6.238 eV are estimated.

**Keywords:** Dielectronic satellites; Genetic algorithm; Line shifts; Photo-nuclear excitation; Spectral decomposition; X-ray spectroscopy

## 1. INTRODUCTION

Analysis of X-ray spectra emitted from highly ionized matter is generally one of the most efficient tools for the investigation of phenomena accompanying creation and evolution of hot dense plasmas (Boiko *et al.*, 1985; Griem, 1997). The modern experimental approaches (Renner *et al.*, 2004; Rosmej *et al.*, 2005) are capable of providing detailed, spatially, and temporally resolved spectroscopic data. In order to obtain the maximum information on environmental conditions in extreme states of matter, a diagnostic potential contained in this data—manifesting itself in modification of the spectral line profiles, in particular their intensities, broad-

enings and shifts—should be utilized. Consequently, the development of efficient methods for the analysis and interpretation of complex experimental spectra is of primary importance.

Multi-level collisional radiative approaches and line broadening theories have reached a high accuracy required for many diagnostic purposes. However, there are still very important areas where theory is less predictive but highly demanding, e.g., non-Maxwellian plasmas (Rosmej, 1997), complex satellite spectra (Boiko *et al.*, 1985; Rosmej *et al.*, 2001), and charge exchange driven radiative emission (Rosmej *et al.*, 2002).

We therefore face a situation, where a part of the theory has reached an acceptable accuracy whereas other parts are not well known, but all phenomena, both known and unknown, may considerably contribute to real observations. In such situations, standard decomposition techniques of spectral

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analysis are not very effective and also not very meaningful from the physical point of view (i.e., a good mathematical fit is obtained but the fitting is not well related to physical quantities). It is therefore highly desirable to formulate a problem-dependent spectral decomposition which efficiently interlinks the well established part of the theory with experimental observations, in order to obtain direct information about the not-fully-described-yet phenomena.

Decomposition of measured spectra into individual spectral lines represents an example of a global optimization problem, which cannot be efficiently solved by traditional techniques. The well-known algorithms incorporated into most of the standard spectral analysis packages (based e.g., on Levenberg-Marquardt or downhill-simplex methods) can be successfully used for simple spectra with well-separated peaks and low noise levels. The analysis of complex noisy spectra containing overlapping peaks requires an application of robust optimization methods. Improved optimization tools (albeit frequently used in a traditional manner) often benefit from the genetic-algorithm (GA) approach. The GA solve global optimization problems by examining typically hundreds or thousands of trial solutions encoded into data structures called genomes. The algorithm starts with a set of randomly generated genomes defining the first-generation population. The selective exploration of the search space is performed by randomly combining these solutions (crossover), perturbing them (mutation) and choosing the better ones according to the survival-of-the-fittest philosophy (selection). The principle of working with a large number of solutions at once constitutes the main difference between evolutionary methods and most of the other global optimization methods. The way of encoding the physical problem into genomes as well as the actual methods of crossover, mutation and selection depend on the problem itself. Although there are general concepts of applying the GA to any optimization task, the GAs tailored to the specific problem generally show significantly better performance in terms of stability and convergence.

The GA concepts (Goldberg, 1989) have been used for solving various technological tasks for more than a decade; however, the applications of the GAs in physics are less frequent (Golovkin *et al.*, 1999). Regarding the GA-based diagnosis of hot dense plasmas, pioneering studies were performed by Mancini and his collaborators. Using the GA combined with a case-based memory (Golovkin *et al.*, 2002) and, recently, a multi-objective version of the GA (Welser *et al.*, 2006); the X-ray spectra and monochromatic images of the emitting plasma regions were simultaneously analyzed in terms of determining the dynamic plasma gradients in ICF cores.

In the present work we propose an advanced approach to spectral decomposition combining the GA with spectroscopic information supplied by detailed plasma and atomic physics calculations. Two examples of successful applications of the novel method demonstrate the extraction of line shifts of resonance and intercombination transitions which

are masked by dielectronic satellite contributions and estimating the upper limits for observation of the radiative decay in laser-excited Ta nuclei.

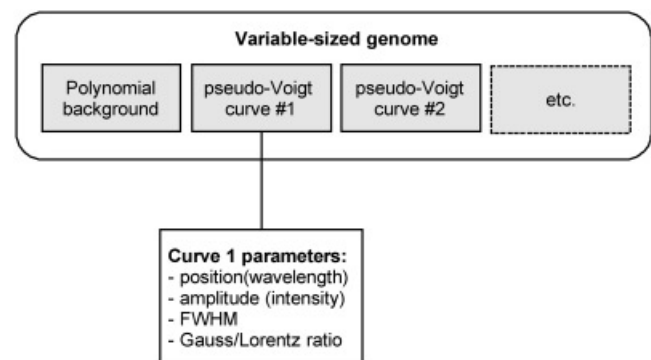
## 2. GASPED CODE

Compared to previous algorithms used for spectral decomposition (McIntosh *et al.*, 1998; Ramirez & Fuentes, 2002; Garcia-Talavera & Ulicny, 2003), our novel fitting code Genetic Algorithm for SPectral Decomposition (GASPED) implements several new features extending the range of the problems solved, improves the convergence rate and provides a graphical user interface for more effective interactive analysis of the resulting fits.

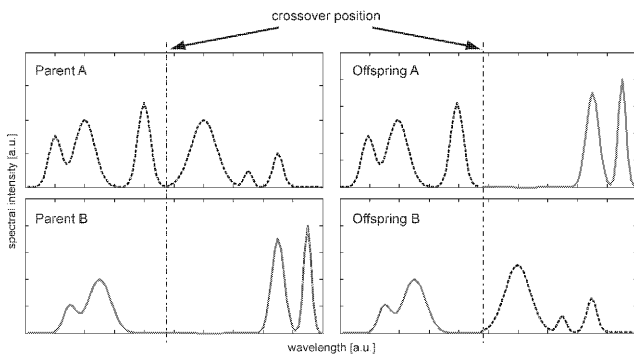
GASPED estimates the quality of a particular decomposition as a  $\chi^2$ -difference between the measured spectrum and its fit consisting of a variable number of pseudo-Voigt curves and polynomial background component. The algorithm searches for fits with the minimum difference from the input data. The problem of the decomposition into individual spectral components is thus reformulated as an optimization of the  $\chi^2$  objective function. With respect to specific problems of spectral decomposition, the code adopted a variable-sized genome (Fig. 1) instead of the common fixed-size concept. This feature allows analysis of the spectra without *a priori* knowledge of the actual number of the lines present.

Besides the common arithmetic crossover and mutation, the code uses several additional operators tailored to the problem. In *positional crossover* (Fig. 2), the spectral region is randomly divided into two parts. The offspring genomes are then created by combining the curves from the left-hand and right-hand sides of two parental genomes. In contrast to the arithmetic crossover operator, positional crossover takes into account the actual structure of the genome, i.e., manipulates particular curves and background component like integral units, thus producing offspring of higher average quality.

*Intelligent mutation*, following approach originally introduced in evolution strategies (Ramirez & Fuentes, 2002),



**Fig. 1.** Variable-sized genome (tentative solution encoded into a binary string) used in GASPED.

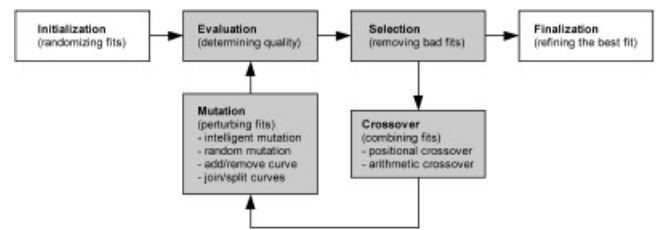


**Fig. 2.** Schematic diagram of a positional crossover. Two parental solutions split and combine in a particular crossover wavelength, thus forming two offspring fits.

adds a new curve to the point of the greatest difference of the solution and the fitted spectrum. In order to keep the total number of curves constant, a randomly chosen curve is removed at the same time, so the operator can be also used for decomposition tasks, where the actual number of fitted curves is initially known and therefore fixed.

Other specific operators, such as curve addition/removal, joining/splitting of curves or adaptive mutation, are designed to search the parameter space more effectively. Premature convergence, a negative phenomenon often occurring in the GAs, is reduced by a pre-initialization of every member of the starting population by a separate GA run with a small population size. The algorithm thus starts with a set of relatively good solutions, which prevents a random strong solution from being copied many times in the selection phase and maintains population diversity.

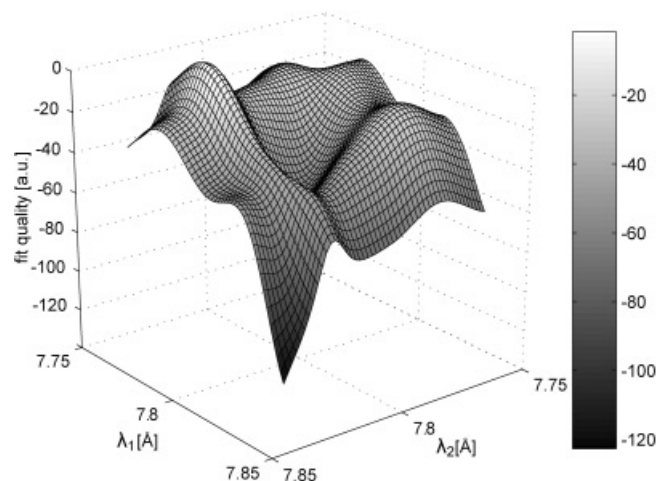
An advanced version of GASPED permits to work with models involving specific constraints. Using the information provided by theoretical spectra, the freedom in choice of the individual parameters relevant for optimization can be defined in more detail—for instance, the number of the spectral lines emerging from spectrum can be fixed, forbidden intervals can be imposed on particular parameters, and several lines can be grouped together by introducing additional common parameters (e.g., the group shifts of the parent transitions and their satellites). Assuming that the theoretical knowledge of the analyzed spectra is limited GASPED is able to operate in an automated mode, where the most of the input parameters are determined by the program itself. We note that the final fit produced in this mode may be perfect from the mathematical standpoint but its physical relevance may be questioned as the solution need not converge to a unique answer and the parameters obtained may lack a deeper physical insight. The fits produced in both GASPED modes can be further refined by a constrained version of the Levenberg-Marquardt method (Marquardt, 1963) which is effective for local optimization near the real optimum. The whole GASPED fitting process is schematically shown in Figure 3. Using the population size of 200 to 1000 genomes in dependence on the number



**Fig. 3.** Overview of the fitting process in GASPED. Gray boxes represent particular steps of the main computation cycle.

of expected curves in the spectrum, a typical number of iterations of the main cycle is 1500.

In order to illustrate the complexity of the search space, let us consider a spectrum composed of five pseudo-Voigt curves and the continuum approximated by a 2nd order polynomial. Each curve is described by four parameters and three additional parameters define the background, i.e., each genome includes 23 parameters. The 23-dimensional GASPED search space is typically explored using  $5 \times 10^5$  evaluations of the  $\chi^2$  objective function (population size  $500 \times 1000$  generations). If only 100 possible values were used for every parameter, the reduction of the computation time compared to a brute-force evaluation of all possible solutions is of the order  $500000/100^{23} \cong 1/10^{40}$ . The topology of the search space is demonstrated in Figure 4. The shown projection of the objective function to two dimensions (in this case, spectral position of two curves) corresponds to the X-ray He $\alpha$  spectrum decomposition discussed in Section 3. Although the actual search space was 25-dimensional, even such projection reveals the complexity of the problem, namely the strongly non-monotonous character and several local extremes of the objective function.



**Fig. 4.** Projection of the 25-dimensional objective function into two dimensions (representing positions of the resonance and intercombination lines in decomposition of the Al He $\alpha$  group emission—see Fig. 5).

### 3. APPLICATIONS IN PLASMA DIAGNOSIS

#### 3.1. Line shifts in hot dense plasmas

The first application concerns the experimental investigation of K-shell line shifts in hot dense plasmas with small transversal gradients. In experiments carried out on the nanosecond laser system LULI at École Polytechnique ( $0.263 \mu\text{m}$ ,  $0.5 \text{ ns}$ ,  $10^{14} \text{ W/cm}^2$ ), the plasma created at thin aluminum foils sandwiched between two plastic substrates was kept in a constrained flow perpendicular to a direction of the spectra observation. The principle diagnostics used in this experiment was a vertical-geometry Johann spectrometer (Renner *et al.*, 1997) fitted with a crystal of quartz (100). The spectra of the Al He $\alpha$  group shown in Figure 5a demonstrate the effects of the varying plasma parameters on the emitted line profiles of the resonance  $w$  ( $1s2p \ ^1P_1 - 1s^2 \ ^1S_0$ ) and the intercombination  $y$  ( $1s2p \ ^3P_1 - 1s^2 \ ^1S_0$ ) lines.

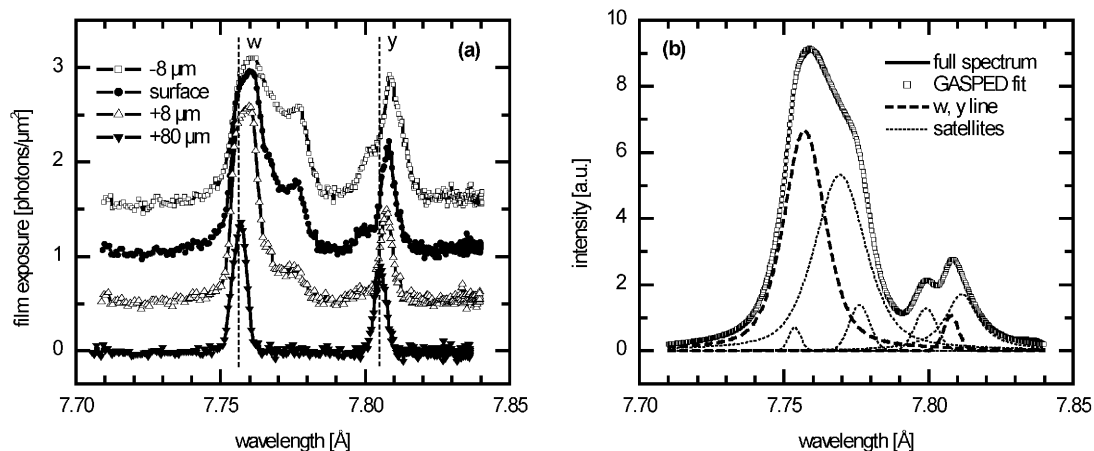
Line shift phenomena are most pronounced and most interesting (from the theoretical point of view) in low temperature and high density plasmas. However, under such conditions, resonance lines are strongly masked by dielectronic satellite lines. The spectral distribution of the satellite emission has been obtained from the multilevel collisional-radiative code MARIA (Rosmej, 1997) for different plasma conditions. The simulations indicate that due to a strong satellite emission overlapping the parent lines, the distinct red shifts of the observed profiles cannot be directly identified as frequency shifts of the  $w$  and  $y$  transitions.

In order to obtain physically meaningful results, we applied the approach combining the theoretical knowledge of the satellite structure with an assumption of the aggregate plasma-induced shift of the parent lines and their satellites. First, we used GASPED to analyze the synthetic satellite spectrum from the Figure 5b. As indicated in the figure, the complex

satellite structure containing more than 300 of  $n = 2, 3$ , and 4 satellites can be well fitted by five pseudo-Voigt profiles. This knowledge represented a starting point for subsequent analysis of the experimental data.

The individual spectral traces were decomposed using several models differentiated by the constraints imposed on appearance and grouping of  $w$ ,  $y$ , and satellite lines (Renner *et al.*, 2006). An example of the spectra fitting obtained with the “relaxed” GASPED version (i.e., small relative shifts and an introduction of additional satellites were permitted) is shown in Figure 6. With respect to the VJS characteristics, both symmetric parts of the experimental spectra should be identical; observed discrepancies are ascribed to the sensitivity of the spectral profiles to the parameters of the dense and relatively cold plasma at the target surface. Despite these discrepancies resulting in an appearance of different number of line components, the error in determining the  $w$  and  $y$  line positions introduced by the spectra decomposition is estimated at  $\sim 0.4 \text{ m}\text{\AA}$ .

The repeated GASPED runs pointed out that the found positions of the dominant spectral lines are relatively insensitive to the electron plasma density and temperature used for the satellite modeling. This is demonstrated in Figure 7a where the shifts of the  $y$  line deduced by using two different sets of plasma parameters ( $3 \times 10^{22} \text{ cm}^{-3}$ ,  $300 \text{ eV}$ , and  $4.5 \times 10^{22} \text{ cm}^{-3}$ ,  $100 \text{ eV}$ , respectively) are shown. The found positions of the Al He $\alpha$   $w$  and  $y$  lines shift to red with the decreasing distance from the irradiated target surface, i.e., with the increasing electron density and the decreasing temperature of the plasma. Theoretical models (Junkel *et al.*, 2000) relate the existence of the frequency shifts to an excess of the free plasma electrons around the ionic radiator. The bound electron levels and wavefunctions are perturbed, the emitted X-ray lines are broadened and their wavelengths are shifted to the red. The trends observed in the behavior of the  $w$  and  $y$  spectral lines agree with the predictions of the



**Fig. 5.** Spatially resolved spectra of the Al He $\alpha$  group observed close to the surface of the laser-irradiated sandwiched Al target (a). Simulations performed by the MARIA code (b) demonstrate a strong spectra modification due to the presence of the  $n = 2, 3, 4$  satellites.

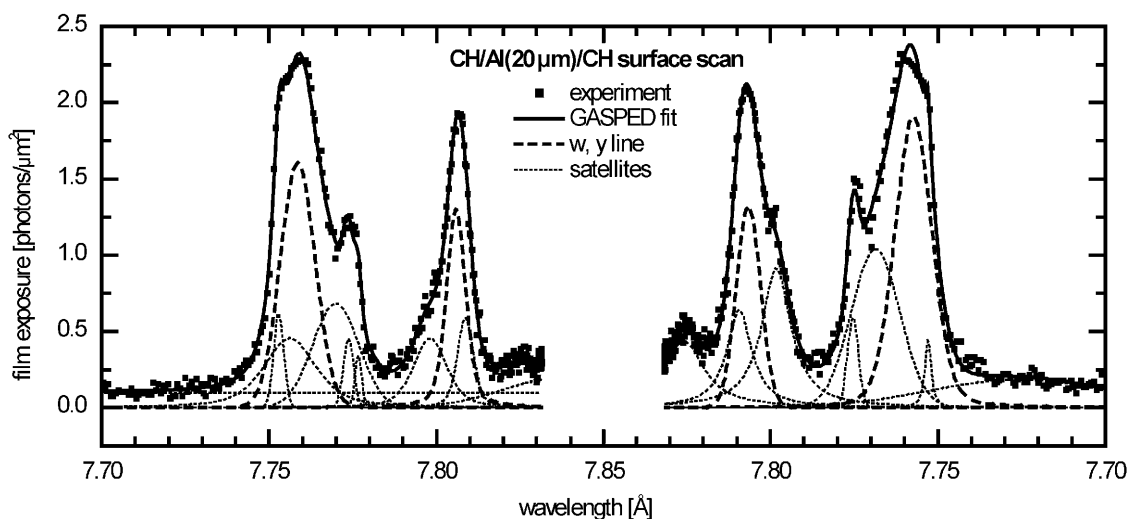


Fig. 6. GASPED decomposition of the Al He $\alpha$  group emitted from the laser-irradiated foil.

quantum mechanical impact theory and self-consistent-field calculations of the energy levels of He-like ions immersed in hot dense plasmas (Koenig *et al.*, 1988).

As follows from Figure 7b, different shifts of these lines result in small variations of the exchange energy (EE) defining the separation between the singlet and triplet energy levels. The observed values of the EE are slightly smaller than those stated in different databases (Boiko *et al.*, 1988; Ralchenko *et al.*, 2006; Kelly, 2006). Combined with the found density-dependent decline of the EE, this data provide a new impact for the line shift theories. The stability and reproducibility of the found solutions corroborate the feasibility of the accurate decomposition of the complex spectra and support the conjecture that the shifts and widths of the K $\alpha$  lines are very useful for diagnostics (Chung *et al.*, 2005).

### 3.2. Search for nuclear transitions in complex spectra emitted from Ta targets

The second application of the GASPED code concerns the analysis of the complex X-ray spectrum emitted from the laser-irradiated Ta target. The interest in these spectra bears on efforts to demonstrate excitation and decay of low-lying nuclear states in the dense laser-produced plasmas. Within the last decade, the studies of photo-nuclear reactions induced by high-power lasers have become one of the most intensively developing disciplines of the contemporary high-energy-density physics (Ledingham *et al.*, 2003). The laser-matter interaction at intensities above the relativistic limit  $I\lambda^2 \approx 10^{18} \text{ Wcm}^{-2} \mu\text{m}^2$  results in acceleration of electrons to MeV energies (Malka & Fritzler, 2004; Koyama *et al.*,

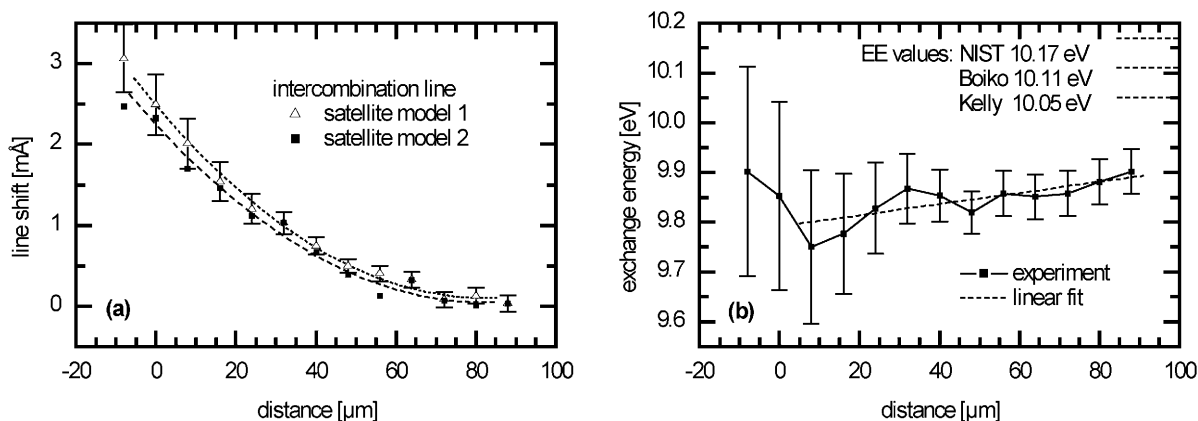


Fig. 7. Plasma-induced shifts of the Al He $\alpha$  intercombination line as a function of the distance above the surface of the laser-irradiated Al foil sandwiched between plastic substrates. Discrepancies in line positions introduced by alternate satellite structures calculated for different plasma parameters (a) partly smear small variations of the exchange energy (b).

2006; Lifschitz *et al.*, 2006) capable of initiating (directly or indirectly, via their conversion to  $\gamma$ -rays or energetic heavy ions) photo-nuclear processes. Subrelativistic plasmas produced at intensities  $10^{16}$ – $10^{17}$  Wcm $^{-2}$  provide much lower electron temperatures, typically 2–10 keV. However, even these electron energies are sufficient to activate the low-lying nuclear levels which subsequently decay in radiative or non-radiative processes.

The first isomeric state of  $^{181}\text{Ta}$  with the excitation energy of 6.238 keV and a lifetime of 6.8  $\mu\text{s}$  represents a challenging test bed for such research. The only positive results hitherto published (Andreev *et al.*, 2000) report X-ray measurements of the Ta decay kinetics by using two different pulse-duration lasers; however, recent experiments trying to verify these results (Fedosejevs *et al.*, 2005; Hannachi *et al.*, 2006) were not successful. The purpose of our analysis is to evaluate the feasibility of experiments directed to nuclear studies at subrelativistic intensities.

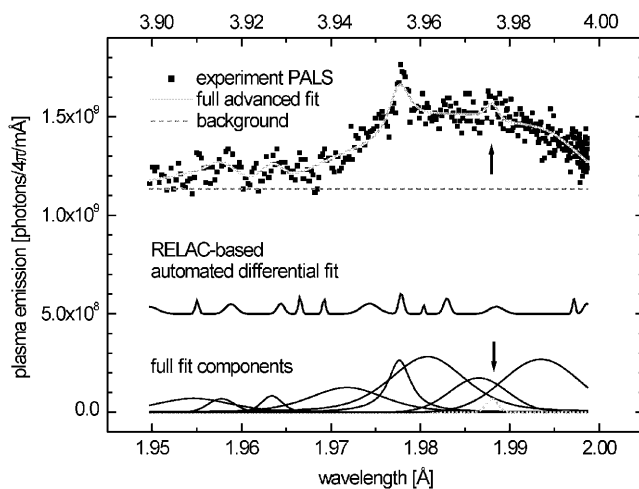
Experiments have been carried out with the iodine laser system PALS (Jungwirth *et al.*, 2001; Jungwirth, 2005). A single laser beam (156 J, 1.315  $\mu\text{m}$ , 0.25 ns) was focused to a diameter of 80  $\mu\text{m}$ , yielding a maximum intensity of  $1.2 \times 10^{16}$  W/cm $^2$ . The radiation was incident normally onto a massive Ta target. The plasma emission was analyzed using the VJS equipped with the crystal of quartz (220). The spectra were observed at an angle of 14° to the target surface, recorded on absolutely calibrated X-ray film Kodak Industrex CX, digitized and recalculated to the linear wavelength scale by using a previously described algorithm (Renner *et al.*, 1997). The absolutely calibrated experimental spectra are shown as points in the upper part of Figure 8.

The identification of individual spectral components emitted by high-Z multicharged ions is generally burdened with

a lack of reliable wavelength databases for resonance lines and with the presence of many unresolved transitions arrays associated with these lines. In our experiment, the spectra reconstruction was further complicated by presence of two overlapped diffraction orders—quartz diffraction (110) and (220) has comparable integrated reflectivities. Thus the application of the robust code for the line decomposition was of a key importance for analysis of the spectra. With respect to the VJS alignment uncertainty of 1.4 mÅ, the wavelength scale was refined using a tabulated Ni-like Ta transition at 3.956 Å (Tragin *et al.*, 1988). The contributions of the Cu-, Ni-, and Co-like Ta ions to the overall X-ray emission around the energy range of interest were estimated by means of the *ab initio* detailed calculations performed with the RELAC code (Bar-Shalom *et al.*, 2001). These synthetic spectra were analyzed using the GASPED code, a set of wavelengths found for their dominant components (completed by another pseudo-Voigt profile in a position of the anticipated Ta nuclear emission, i.e., at 1.988 Å) was used as a fixed input information for advanced decomposition of the experimental data. On the other hand, the amplitudes of individual spectral components were not constrained.

A typical result of several GASPED fits based on fixed positions of all these lines is shown as a solid line in the upper part of Figure 8, the positions and amplitudes of individual components are shown in the lower graph. The area under the component corresponding to the prospective nuclear transition (arrows in the upper and lower graphs) estimates its emission to  $1.1 \times 10^8$  photons/ $4\pi$ . With respect to uncertainties in the energy of the sought nuclear transition, we have performed a complementary GASPED fit where the presence of the nuclear emission was not anticipated. Differences between this RELAC-based fit and the experimental data were again analyzed by the GASPED code; the resulting differential profile composed of several peaks (middle graph in Fig. 8) indicates alternate positions for the nuclear transition. The existence of these peaks may be alternatively explained by a statistics of the spectra detection or by a presence of Ta O- or even H-like transitions (albeit according to calculations, these lines should not be observable). Importantly, the source emission corresponding to any of these peaks does not exceed the value of  $1.2 \times 10^8$  photons/ $4\pi$ .

This value can be compared with simple theoretical estimates of the excited Ta nuclei population in the whole plasma volume. Various models give the values in the interval  $10^5$ – $10^7$  excited nuclei per laser shot. The validity of these estimates is conditioned by the complexity of the models used. Detailed dynamic simulations are expected to give values closer to the lower end of this interval (Andreev *et al.*, 2002), on the other hand the uncertainties connected with the nuclear level broadening in the plasma, internal electron conversion etc. result in more optimistic estimations. In this sense, the found values represent the upper limit for the prospective X-ray emission accompanying the decay of the excited nuclear states of  $^{181}\text{Ta}$ .



**Fig. 8.** GASPED analysis of X-ray emission from the laser-irradiated Ta target. The full fit includes dominant spectral components identified using the RELAC code and an anticipated nuclear transition (arrows in the upper and lower graphs) which was not included into theoretical model used for the differential fit.

#### 4. CONCLUSIONS

We have demonstrated that a problem dependent genetic algorithm is capable to employ results of established theories to extract physical quantities (e.g., line shifts) of not well known theories from experimental data. The GASPED code was developed for applications in plasma spectroscopy. This approach was shown to be stable and robust even in a poorly understood search space. Although still being developed, the current code version is available upon request.

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