МОДЕЛИРОВАНИЕ АТОМНЫХ ХАРАКТЕРИСТИК МНОГОЭЛЕКТРОННЫХ ИОНОВ И НЕПРОЗРАЧНОСТЕЙ ПЛОТНОЙ ВЫСОКОТЕМПЕРАТУРНОЙ ПЛАЗМЫ И РАЗВИТИЕ БАЗ ДАННЫХ

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CALCULATIONS OF MULTIELECTRON-ION ATOMIC DATA AND OPACITIES OF HOT DENSE PLASMAS AND RELEVANT DATABASE DEVELOPMENTS

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Scope of activities

- **Development of the chemical-picture-based models to consistently simulate EOS & opacities / emissivities of dense multielectron-ion plasmas utilizing both the superconfiguration & detailed description of the LTE ionization balance along with the bound-bound & bound-free spectral distributions.**
- **Atomic-data calculations for multielectron ions.**
- **Development & maintenance of atomic-data & opacity databases.**
- **Application of the developed models and generated atomic data to the modeling of EOS & opacities / emissivities of warm & hot dense matter, targeted at the laboratory-plasma diagnostics, modeling of laser-plasma x-ray sources, etc; filling of the relevant databases.**

Modeling of opacities of multicharged-ion dense plasmas

A variant of STA (Super Transition Arrays) model currently implemented in the SPECTR code to calculate monochromatic opacities

- Superconfigurations comprise occupied atomic shells :

$$\Xi \equiv n_1^{q_1} n_2^{q_2} \ldots n_k^{q_k}$$

- Transition arrays between superconfigurations $\Xi_\alpha \rightarrow \Xi_\beta$ are modeled by effective spectral distributions corresponding to single-electron transitions:

$$n_\alpha l_\alpha j_\alpha \rightarrow n_\beta l_\beta j_\beta$$

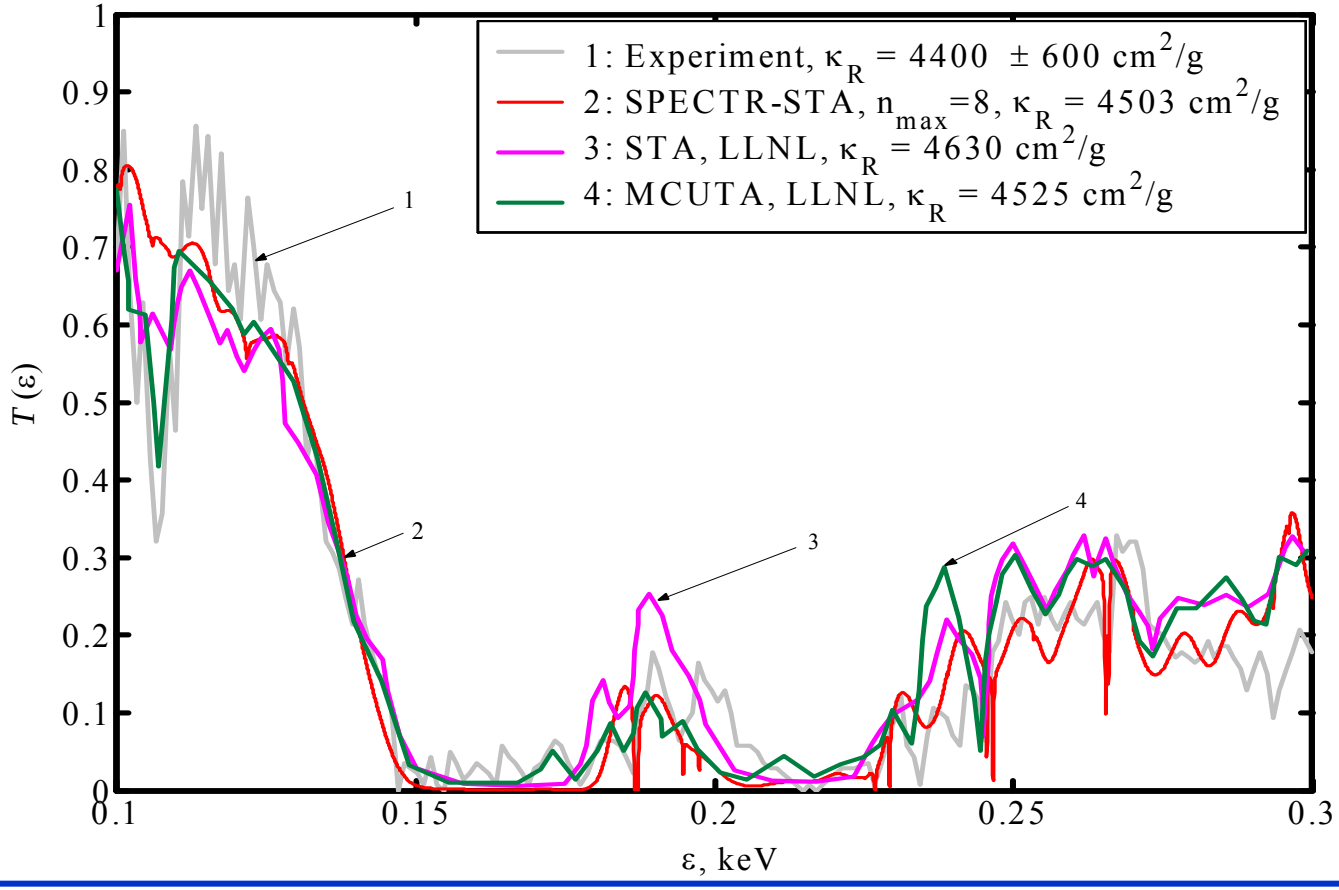
- Ion populations are found from modified Saha equations allowing for plasma-nonideality & electron-degeneracy effects or given by the chemical-picture-based EOS model utilizing the full-scale superconfiguration appoach allowing for plasma-nonideality & electron-degeneracy effects.

The SPECTR-STA model to calculate monochromatic opacities

- **Gaussian or Voigt effective line shapes for transition arrays include statistical energy dispersion and Doppler broadening or Doppler + homogeneous (radiative + electron-collisional) broadening.**
- **Single- & two- electron atomic data, as well as configuration properties are calculated by using RCN36 program being the principal constituent of the well-known Cowan's suite of atomic codes (to be replaced by the FAC-code data in a new full-scale version of SPECTR-STA).**

Comparison of the LTE iron-transmission spectra

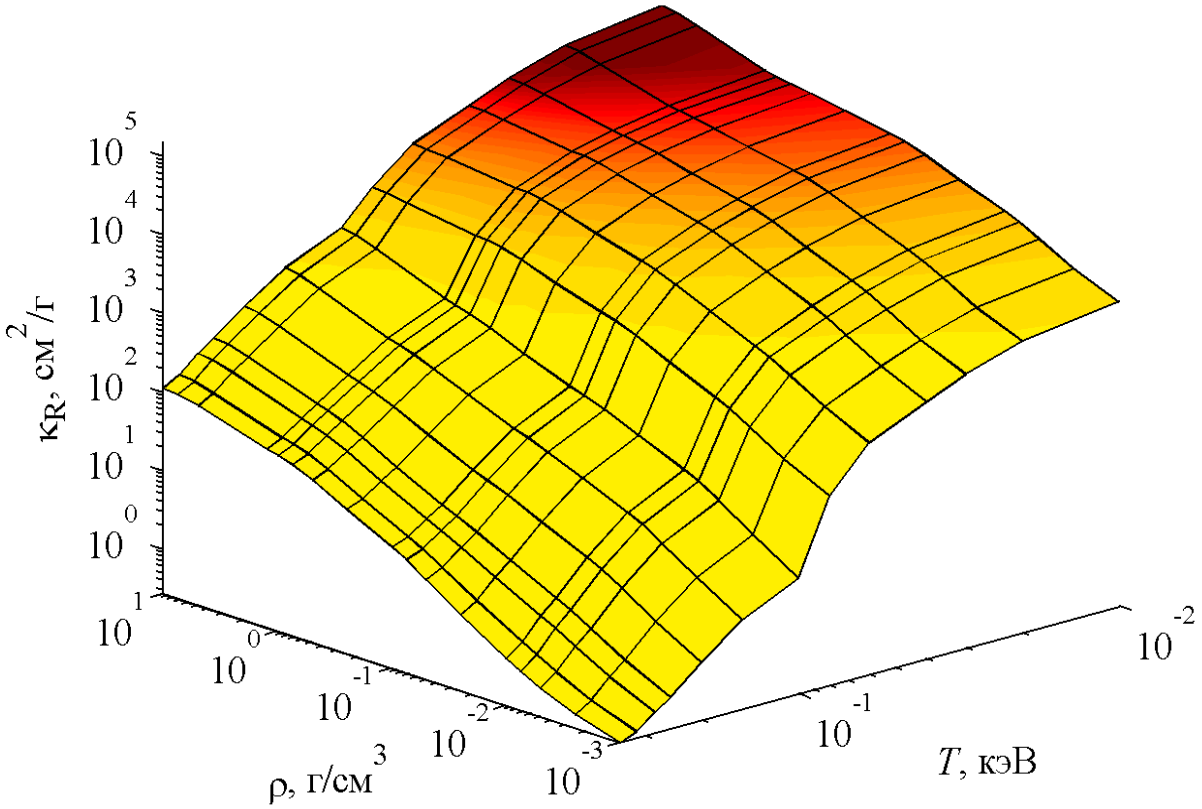
LTE-transmission spectra $T(\varepsilon) \equiv I_{trans} \big/ I_0 = \exp\left[-\kappa(\varepsilon) L\right]$ of the Fe-component in the 300 μm-long plasma layer of Fe:NaF mixture at a density $\rho = 0.0113$ g/cm^3 and temperature $T = 59$ eV compared to experimental and calculated (STA, MCUTA) spectra of P.T. Springer et. al (PRL 69, 3735--3738 (1992))



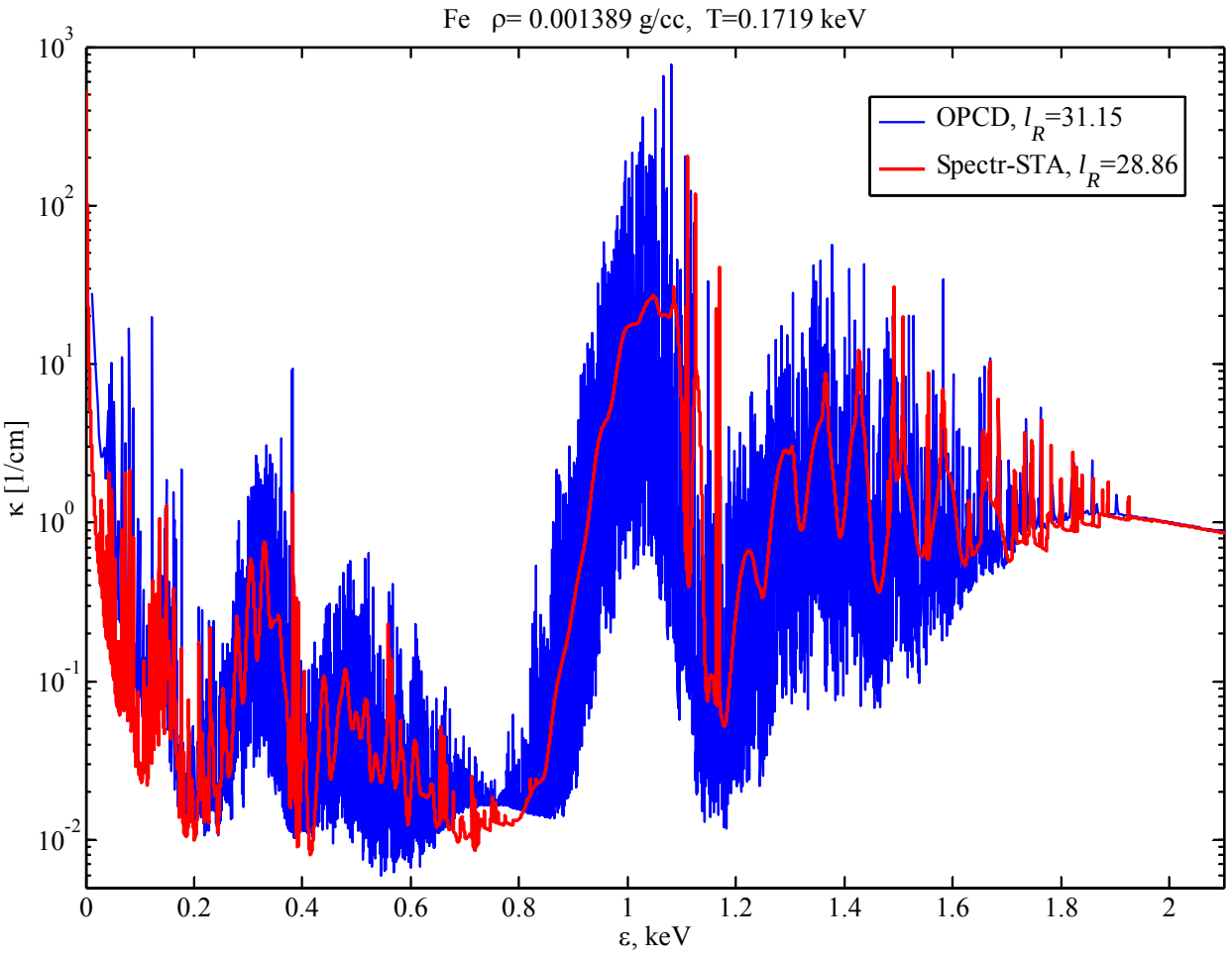
Rosseland means of the Be(99.1%):Cu(0.9%) mixture

Promising targets for ISKRA-6: N.G. Karlykhanov et al. JETP Lett., 79, 25--27 (2004)

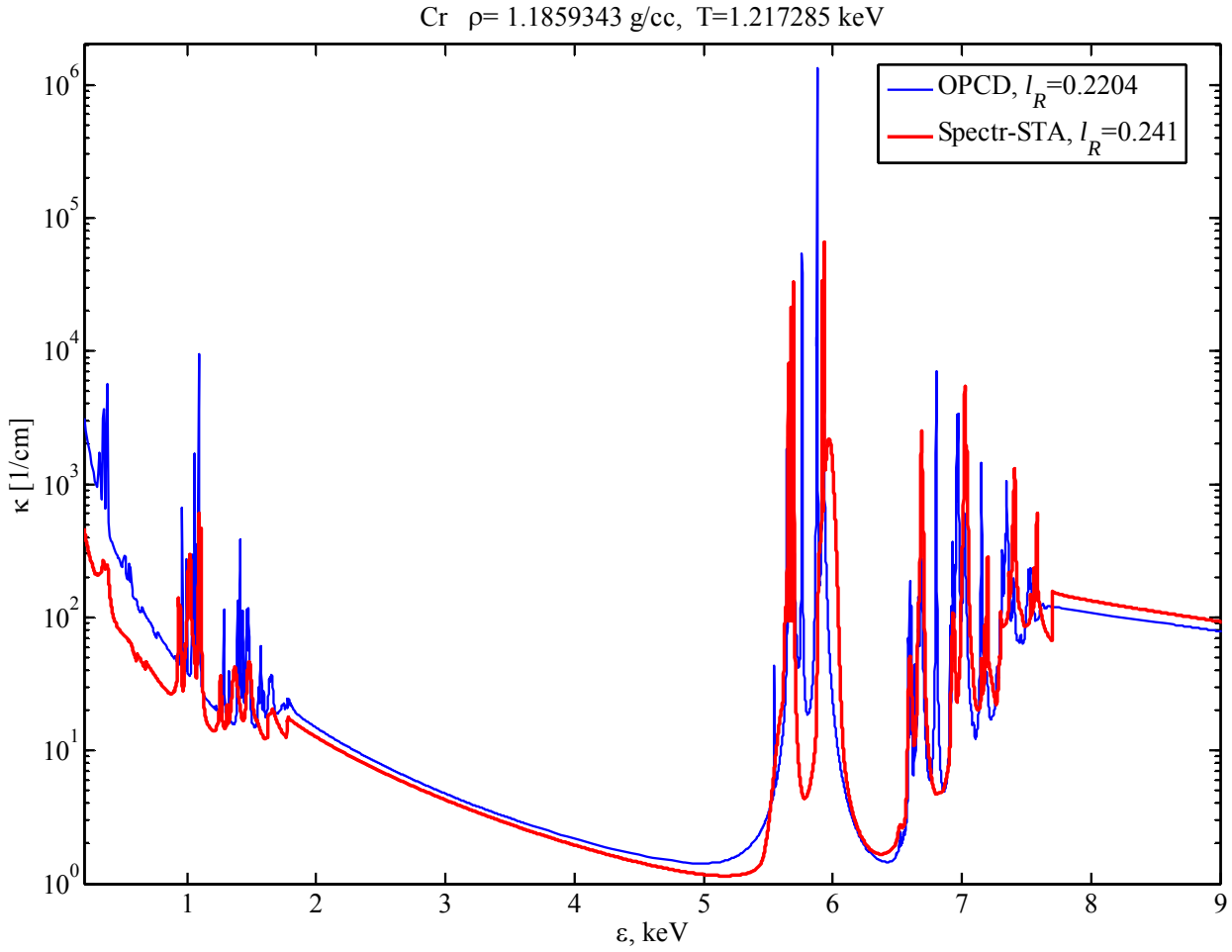
SPECTR-STA opacities: P.A. Loboda et. al, J. Phys. A., 39, 4781--4786 (2006)



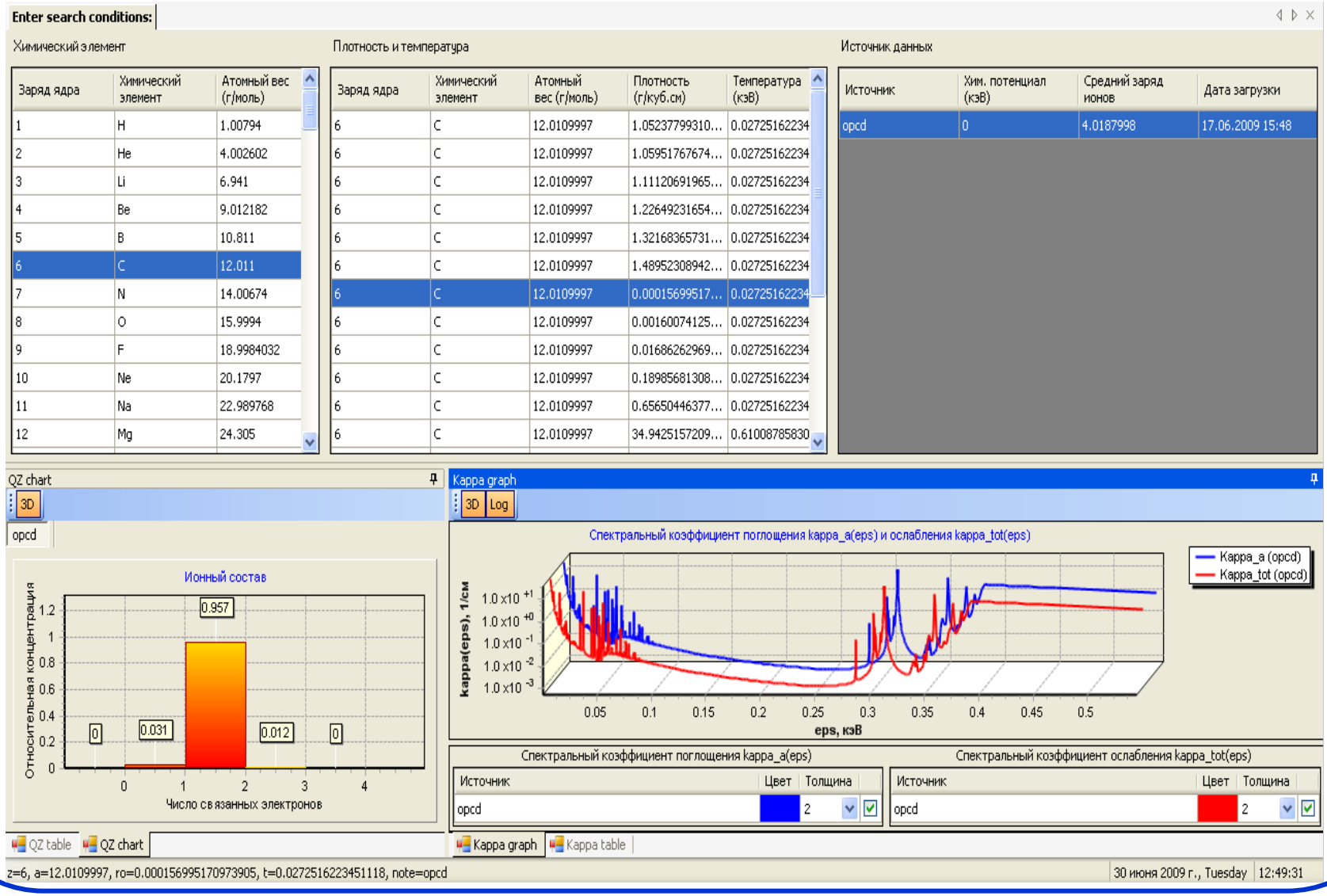
SPECTR-STA monochromatic partial opacities for heavy-element fractions of Solar mixture



SPECTR-STA monochromatic partial opacities for heavy- element fractions of Solar mixture



Monochromatic partial opacities for heavy- element fractions of Solar-mixture: Sunbase



Numerical modeling of radiative properties of multicharged-ion plasmas using DTA-approach

A numerical model Spectr-DTA based on detailed description of bound-bound and bound-free radiation / absorption spectra (Detailed Term Accounting: DTA-approach) is developed to calculate radiative properties (spectral emissivities & opacities) of multicharged-ion plasmas

- **to analyze & model radiation/absorption spectra of dense plasmas being measured in laser-plasma experiments;**
- **to benchmark approximate statistic methods for simulating radiative properties of dense plasmas.**

Spectr-DTA model to calculate spectral opacities

- **Ionization balance & ion-state populations are found from**
  - **superconfiguration ionization balance models + Boltzmann distribution over detailed terms (LTE);**
  - **calculations with other collisional-radiative models (NLTE).**
- **Spectr-DTA uses pre-calculated atomic data for bound-bound (atomic-state properties, multipole transition matrix elements) & bound-free radiative transitions (photoionization cross-sections for ground + excited levels, if necessary) contributing to the spectral range of interest.**
- **Voigt lineshapes for transitions include Doppler and homogeneous (autoionization, radiative, & electron-collisional) broadening.**
- **Detailed Stark-broadened lineshapes may also be employed, if necessary & reasonable (more expensive).**

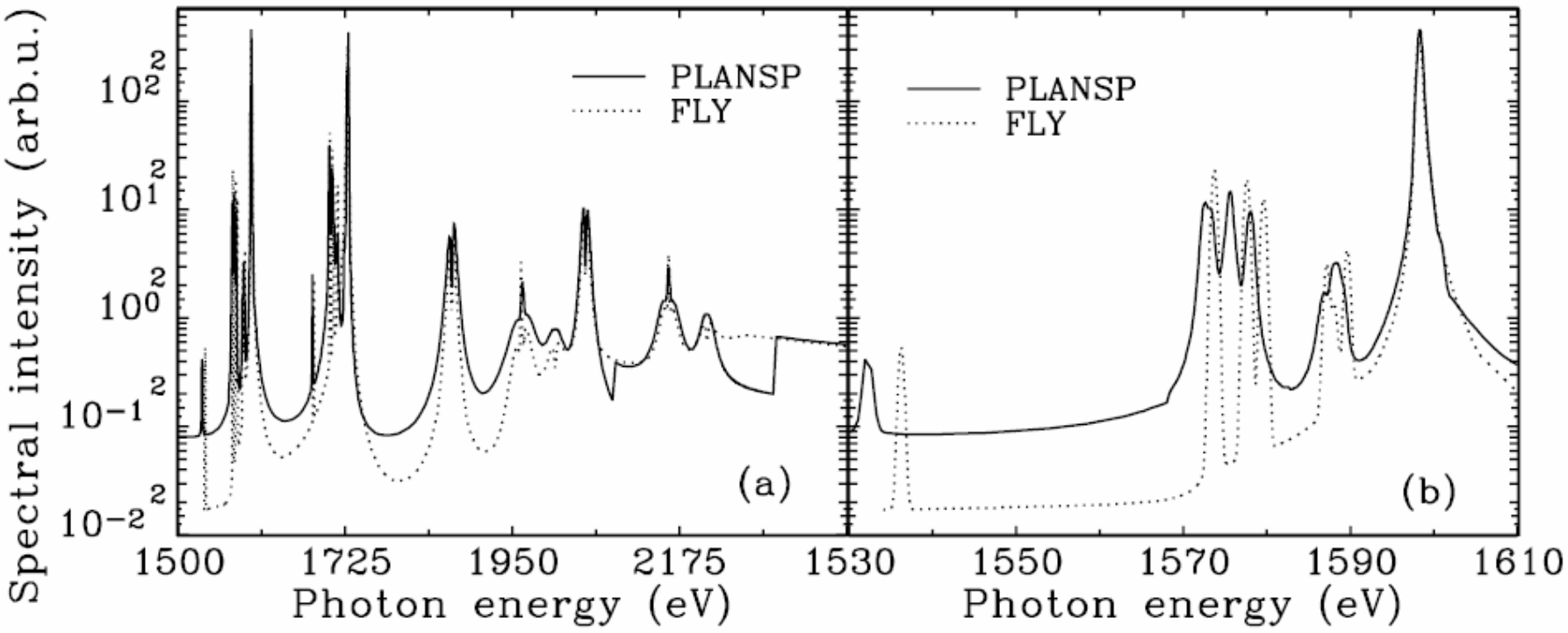
Spectr-DTA model to calculate spectral opacities

Generalized theoretical model LineDM for calculating local line radiation/ absorption spectra for arbitrary multielectron ions in plasmas [P.A. Loboda et al. LPB 18, 275 (2000)]:

- **consistent implementation of the density-matrix approach;**
- **arbitrary bound-bound transitions;**
- **most important line-broadening mechanisms: ion quasi-static & electron Stark broadening, natural, autoionization, and Doppler broadening;**
- **enables to describe the effects of plasma microfield and radiation field on the population kinetics of ionic states (individual calculations).**

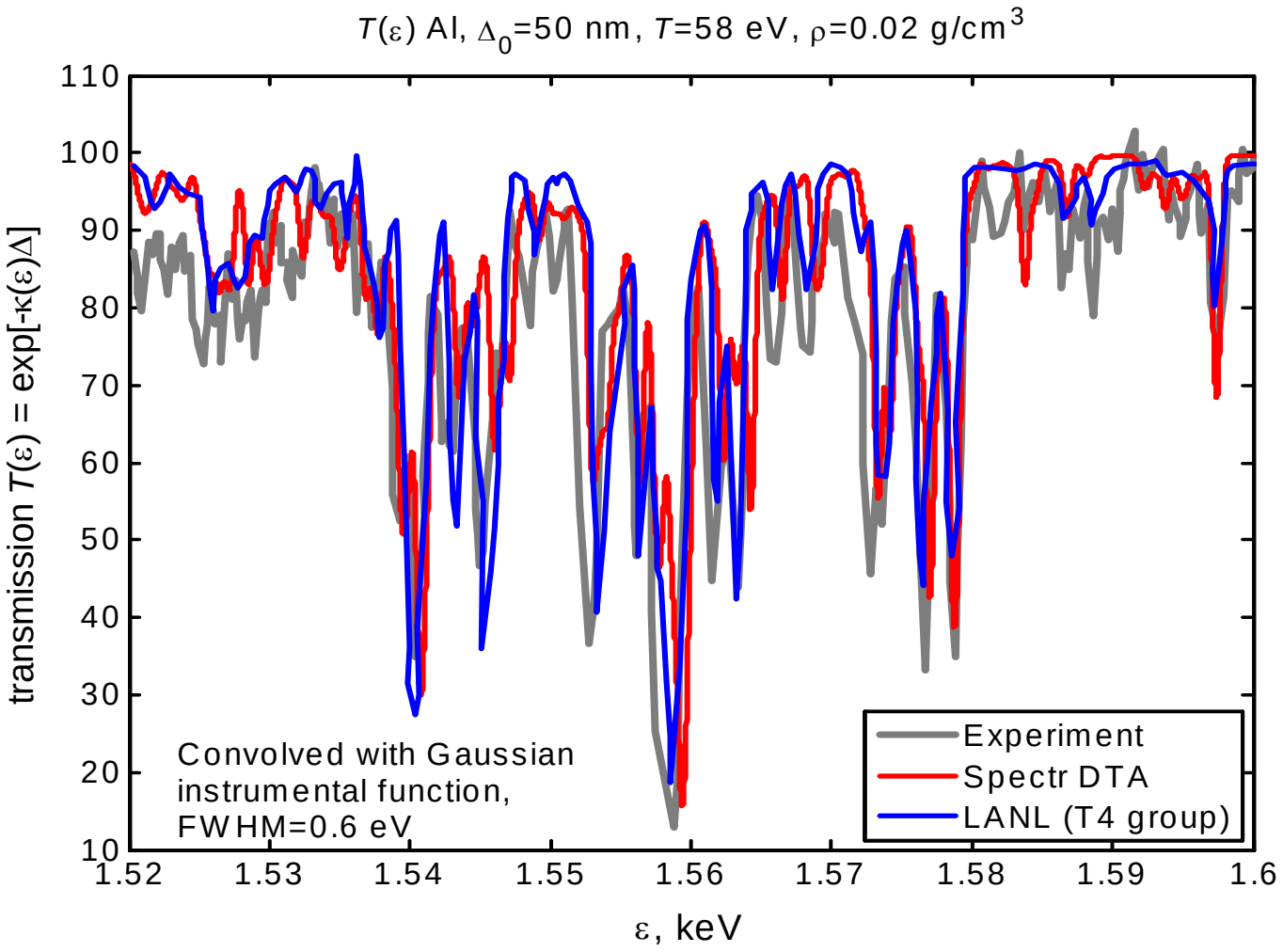
K-shell emission spectra of simple Al ions to model short-pulse sources of narrowband x-ray radiation

J. Limpouch et al. Proc. SPIE, 5228, 584--593 (2003)



Al: $N_e = 10^{23}$ cm^{-3}, $T_e = 600$ eV

LLNL experimental data for near-LTE Al transmission at T=58±4 eV, ρ = 0.02±0.007 g/cm^3 vs. DTA-model calculations



Δ_0 = 0.05 μm

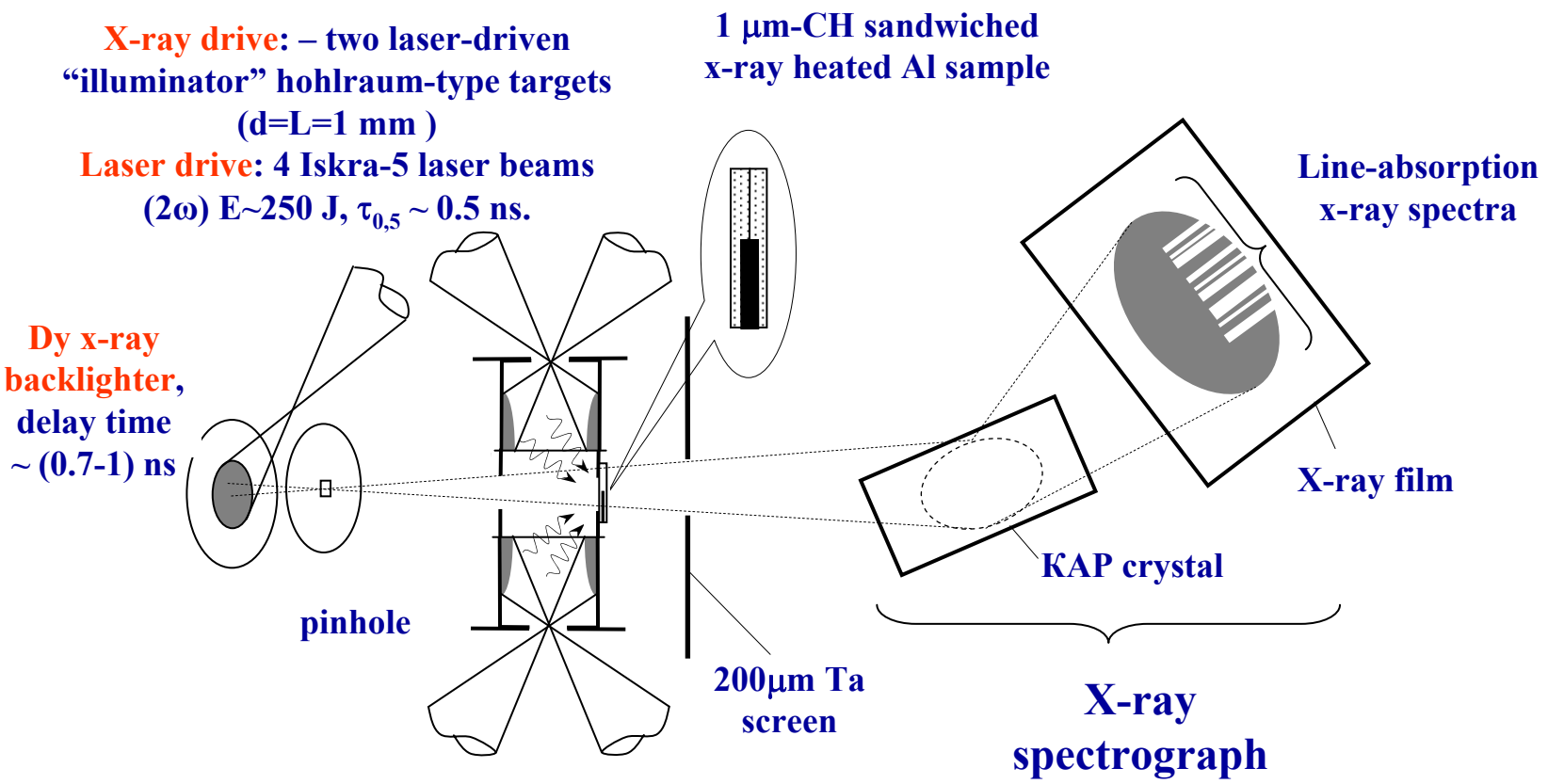
$\Delta = \Delta_0 \cdot \rho_0/\rho$=67.5 μm

Ion	Fraction	Lines
[Li]	12%	470
[Be]	16%	10646
[B]	42%	58558
[C]	31%	141911
[N]	8%	115144

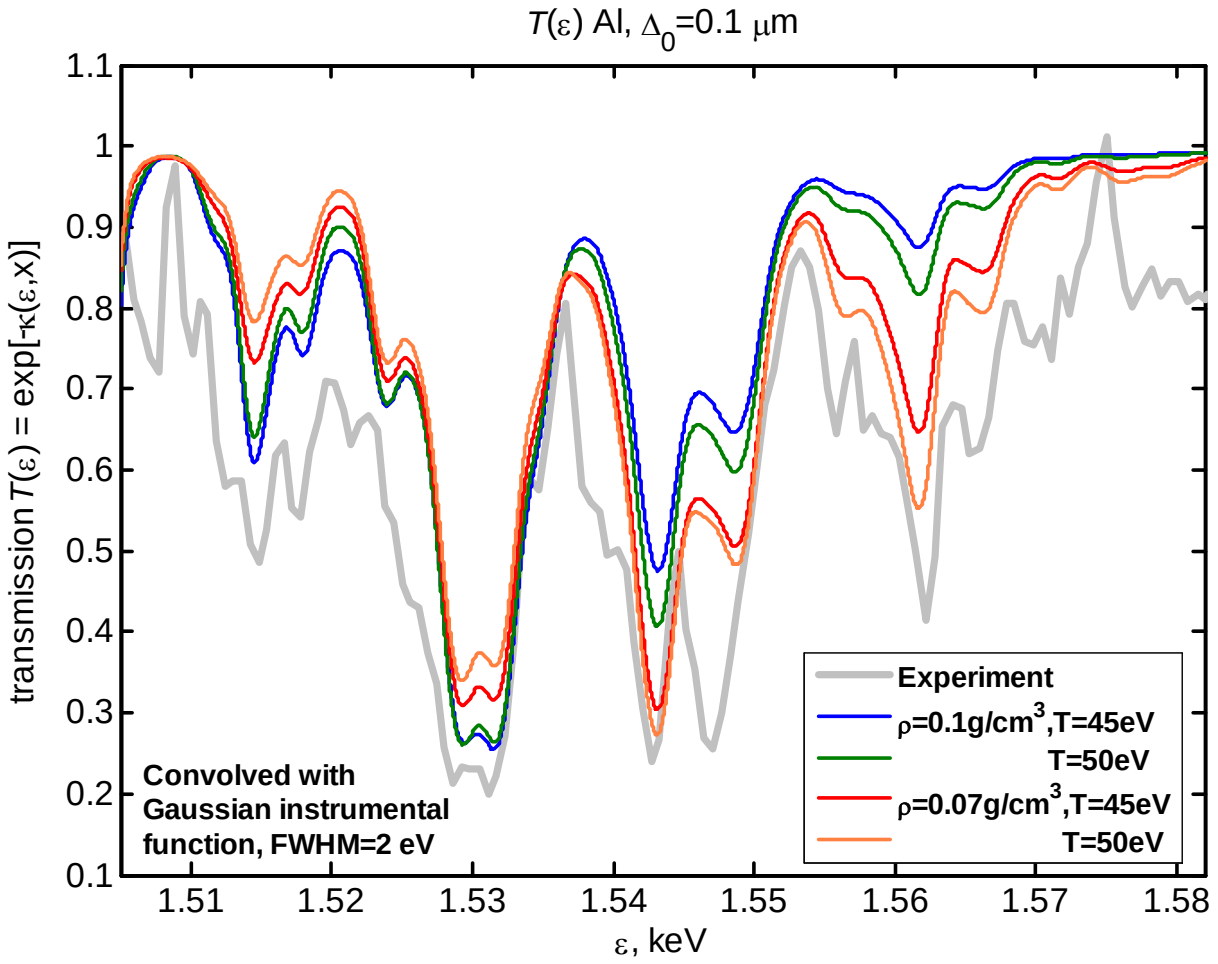
T.S. Perry, et al. Phys. Rev. Lett., **67**, 3784-3787 (1991)

Iskra-5 experiments for near-LTE Al transmission at RFNC-VNIIEF

One-sided x-ray irradiation experiments with Al samples Δ_0=0.9 & 0.1 μm



Measured near-LTE transmission of Al radiatively heated by laser-driven "illuminator" hohlraum-type targets in 4-beam Iskra-5 experiment (April, 2007) vs. Spectr-DTA calculations



"Thin" sample

$\Delta_0 = 0.1$ μm

$\Delta = \Delta_0 \cdot \rho_0 / \rho$

Ion	Fraction	Lines
[Be]	4%	10646
[B]	24%	58558
[C]	43%	141911
[N]	24%	115144
[O]	5%	17136

Presented @ ECLIM-2008

Input atomic data for Spectr-DTA

- **Spectroscopic data are calculated for detailed radiative transitions between relativistic ionic terms with**
  - **an improved version of the GRASP^2 package (up to 2500 detailed terms and 3x10^6 transitions in a single GRASP^2 run)**
  - **parametric-potential relativistic Flexible Atomic Code (FAC) (somewhat less accurate than GRASP^2, but easier to run)**
- **Autoionization widths, photoionization cross-sections are calculated using the distorted-wave approach with the FAC code (if necessary).**
- **A pilot version of the relevant database to accumulate and maintain detailed atomic data is developed and being filled now with consistent spectroscopic data for multielectron ions.**

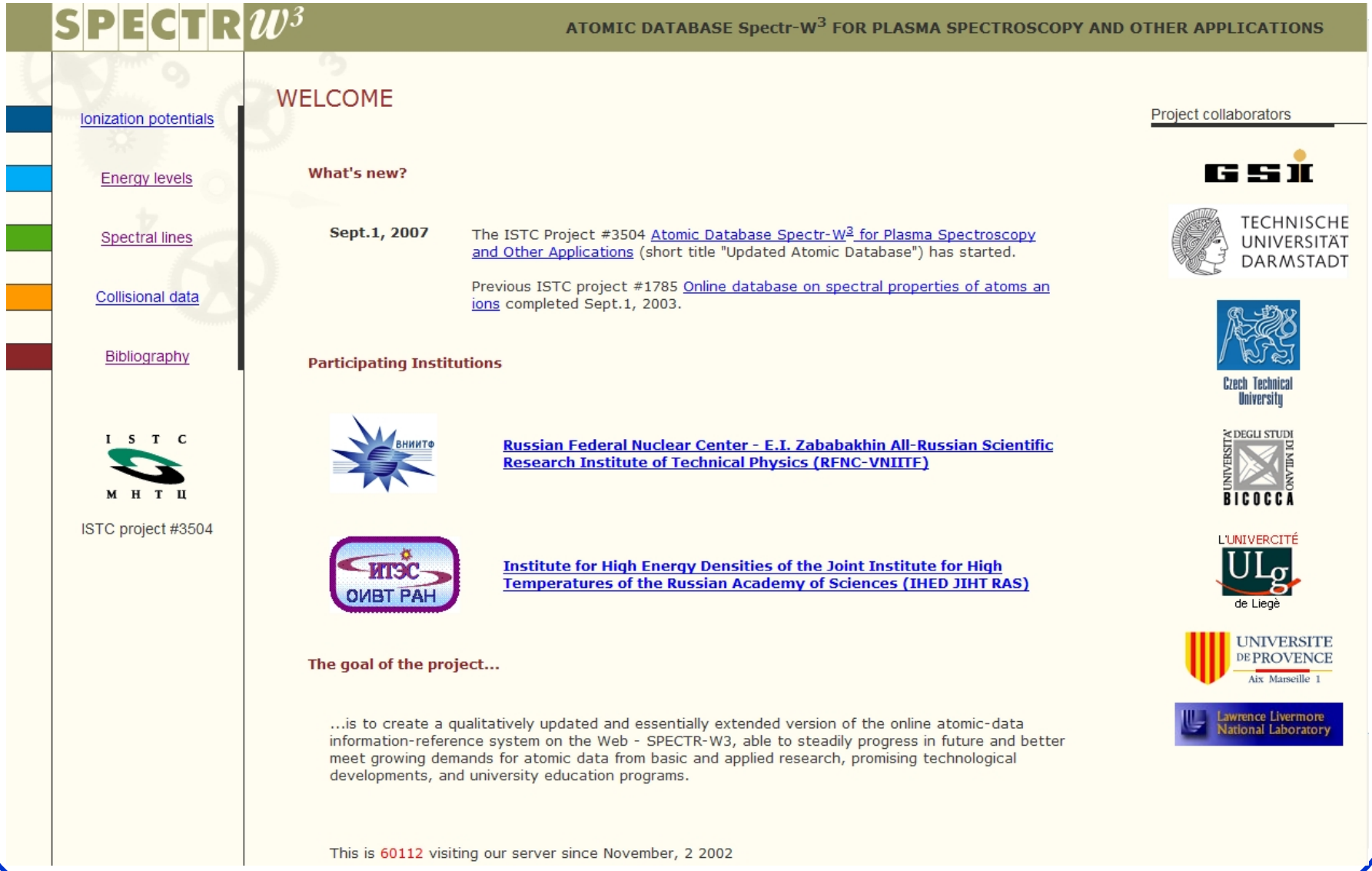
Spectroscopic-data calculations

GRASP-family MCDF packages (General Relativistic Atomic-Structure Package):

GRASP ⇨ GRASP^2 ⇔ GRASP92 ⇨ grasp2K

- **GRASP** (K.G. Dyall, I.P. Grant, et. al, 1989)
- **GRASP^2** (F. Parpia, I.P. Grant, C.F. Froese-Fischer, 1992)
  - ✓ errors fixed;
  - ✓ convergence of iterations to solve Dirac-Fock equations improved;
  - ✓ algorithm to calculate electron self-energy component of the QED corrections improved;
  - ✓ computation of reduced matrix elements of equivalent nonrelativistic multipole-transition operators included;
  - ✓ special-purpose program to postprocess the calculated data and generate the systematized datasets developed (to fill databases and calculate emission and absorption spectra of highly charged multielectron ions).

SPECTR-W^3: http://spectr-w3.snz.ru



Factual atomic database SPECTR-W^3

≈ 450000 records

Currently: ≈ 64000 visits to spectr-w3.snz.ru since November 2, 2002

Experimental, theoretical, and compiled values of

- **ionization potentials,**
- **energy levels,**
- **wavelengths,**
- **radiative transition probabilities and oscillator strengths,**
- **statistical weights, radiative & autoionization widths, satellite intensity factors Q_d (recently added fields),**

and also

- **fitting parameters and formulae to analytically approximate collisional cross-sections and electron transition rates in atoms and ions (*optional*)**

in free atoms & ions,

- **references to the original sources**
- **comments on the methods of the data acquisition, … etc, where necessary and available**

Data sources

- **journal papers published in the leading physical journals;**
- **datasets submitted by the authors (collaborators);**
- **high-resolution experimental and reliable theoretical data obtained by the project participants**

A technique of retrieving the atomic data from electronic and printed publications was developed on the base of the up-to-date text recognition software FineReader™.

About 200 new spectroscopic datasets were converted into HTML format & incorporated in the SPECTR-W^3 database.

Data obtained by the authors

- Satellite lines due to radiative transitions from Rydberg autoionizing states of Li-like Mg were first identified and high-resolution measurements of wavelengths performed at $\Delta\lambda/\lambda \leq 10^{-4}$ (LPP) $\Rightarrow$ new reference lines to study complex spectra of multielectron ions;
- High-resolution data on the wavelengths of Ne-like Cu & Zn in LPP $\Rightarrow$ identify 2*p*-*nd* & 2*s*-*np* Rydberg-series transitions + measure ionization potentials;
- High-resolution data on the wavelengths of N-, O-, and F-like Zn. Most of the lines were identified for the first time.
- Consistent spectroscopic datasets were generated with the GRASP[2] & FAC codes that involved the states with all possible *J* and *P* & dipole radiative transitions between them for a nr. of F-, Ne-, Na-like ions with Z~20–50 ($n \leq 4$, $n \leq 5$, $n \leq 4$, respectively), all ions of Al. The datasets are being incorporated into the **SPECTR-W[3]** database.
- Electron-collision excitation rates for some transitions in H-, He-, Li-, and N-like C, Ar, and Fe, Cu-, …Pd-like Sn were calculated using the ATOM & FAC parametric-potential codes.

Previous 2-year ISTC project # 1785 (2001–2003)

- **Fully functional CD variant of the SPECTR-W^3 atomic database — SPECTR-CD for the off-line use on PCs under Windows supplied with the automatic setup program has also been created.**
- **SPECTR-W^3 homepage was integrated into the family of special-purpose atomic databases on the Web, see http://plasma-gate.weizmann.ac.il/DBfAPP.html**

Dissemination of information & Project results evaluation

very good reaction

Objectives of the current 3-year ISTC project # 3504 (2007–2010)

In the course of work under the ISTC project # 3504

- **facilities for direct submission of new author's atomic data will be created and put into operation, a technique of supplementing SPECTR-W^3 with those data will be developed and optimized;**
- **export utilities providing the selected data output into XML (eXtensible Markup Language) and plain text format will be implemented (HTML is already available);**
- **SPECTR-W^3 and its local version SPECTR-CD will be essentially updated by:**
  - the inclusion of new experimental and theoretical information on the multicharged-ion spectra both published in literature and obtained in the participating organizations under the previous ISTC Project # 1785;
  - introduction of the new data type on the autoionization-transition rates;
  - inclusion of the results of systematic calculations and high-resolution measurements obtained by the participants as well as presented by the other authors;
  - selection and inclusion of the most important experimental and theoretical data published after 2003;
- **software and equipment of the SPECTR-W^3 website will be upgraded;**
- **functionality and informative content of the SPECTR-W^3 Web-pages will be extended;**
- **a new version of the SPECTR-CD setup package will be generated**

Current SPECTR-W^3 project-related collaborations

XSAMS

XML Schema for Atoms, Molecules, and Solids

a new versatile standard for atomic, molecular and particle surface interaction data exchange (AM/PSI) based on XML is being developed under the IAEA support

www-amdis.iaea.org/xsams/documents

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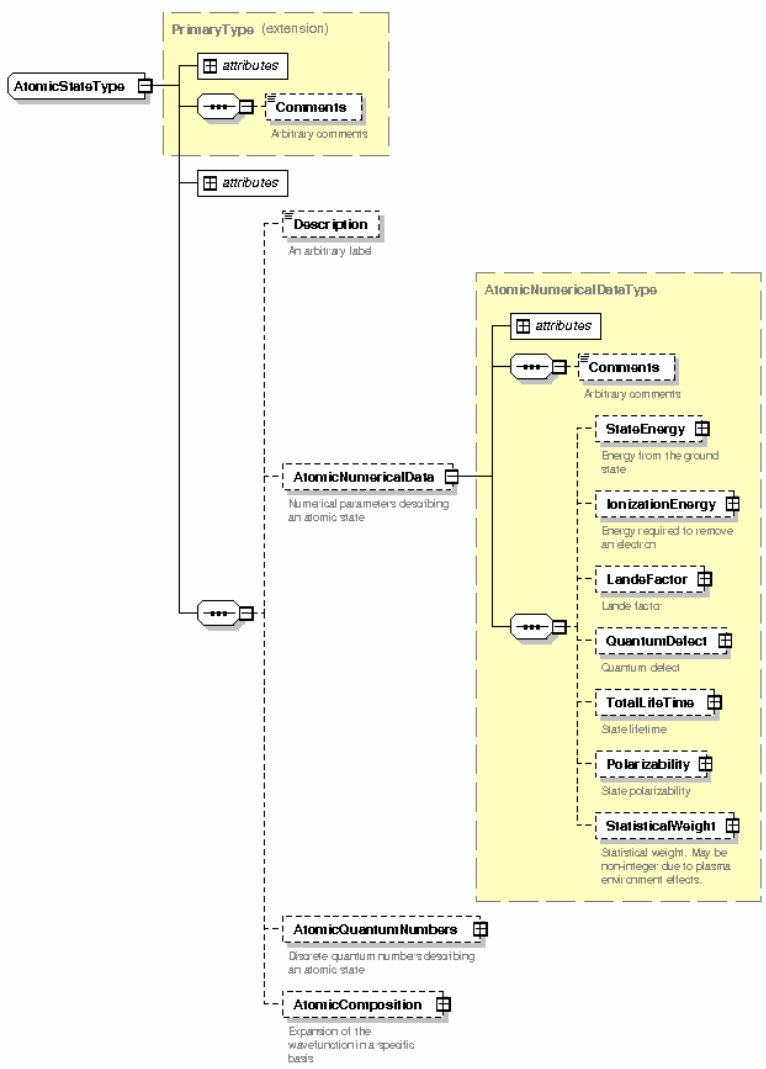
- N. Moreau (Observatoire Paris-Meudon, France)

Presented @ ICAMDATA-2008

Yu. Ralchenko et al. AIP Conf. Proc. 1125, 207–216 (2009).

Current SPECTR-W^3 project-related collaborations

XSAMS = XML Schema for Atoms, Molecules & Solids



Energy levels

N	Atom	Ion	Znuc	Zspec	Level name	Configuration	Energy cm^{-1}	Γ_{rad} s^{-1}	Method	Reference	Comment
1	La	Ga	57	27	$(4s^24p)\,^2P_{3/2}$	4s(2)4p	1.90054e5	6.2137e4	Thr	R530	All-order single-double method
2	Gd	Ga	64	34	$(4s^24p)\,^2P_{3/2}$	4s(2)4p	3.61913e5	4.3147e5	Thr	R530	All-order single-double method
3	Sn	Ga	50	20	$(4s^24p)\,^2P_{3/2}$	4s(2)4p	8.8357e4	6.2137e3	Thr	R530	All-order single-double method
4	Sb	Ga	51	21	$(4s^24p)\,^2P_{3/2}$	4s(2)4p	9.9545e4	8.9332e3	Thr	R530	All-order single-double method
5	Te	Ga	52	22	$(4s^24p)\,^2P_{3/2}$	4s(2)4p	1.11738e5	1.2579e4	Thr	R530	All-order single-double method
6	I	Ga	53	23	$(4s^24p)\,^2P_{3/2}$	4s(2)4p	1.24999e5	1.7623e4	Thr	R530	All-order single-double method
7	Xe	Ga	54	24	$(4s^24p)\,^2P_{3/2}$	4s(2)4p	1.39392e5	2.446e4	Thr	R530	All-order single-double method
8	Cd	Ga	48	18	$(4s^24p)\,^2P_{3/2}$	4s(2)4p	6.8763e4	2.917e3	Thr	R530	All-order single-double method
9	Ba	Ga	56	26	$(4s^24p)\,^2P_{3/2}$	4s(2)4p	1.71848e5	4.5881e4	Thr	R530	All-order single-double method
10	Ag	Ga	47	17	$(4s^24p)\,^2P_{3/2}$	4s(2)4p	6.0245e4	1.975e3	Thr	R530	All-order single-double method

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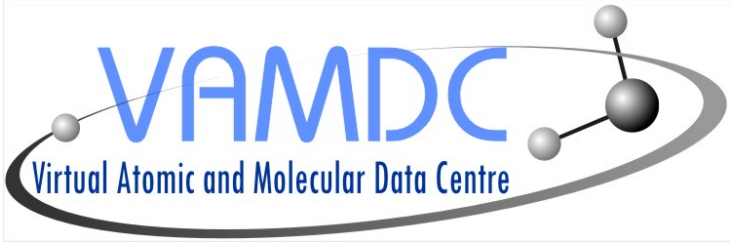
Current SPECTR-W^3 project-related collaborations



www.vamdc.eu

Collaborative 3.5-year EC project Virtual Atomic & Molecular Data Centre (VAMDC) has started

Project Coordinator: Marie Lise Dubernet, UPMC/CNRS, France

VAMDC aims to build a secure, documented, flexible and interoperable e-science environment based interface to the existing A&M data.
The **VAMDC** will be built upon the expertise of existing A&M databases, data producers, and service providers with the specific aim of creating an infrastructure that is easily tuned to the requirements of a wide variety of users in academic, governmental, industrial or public communities both within and outside the European Research Area (ERA).

The project will cover the building of the core consortium, the development and deployment of the infrastructure and the development of interfaces to the existing A&M databases as well as providing a forum for training potential users and dissemination of expertise across the ERA.

Current SPECTR-W^3 project-related collaborations

VAMDC participants

1. Centre National de la Recherche Scientifique (CNRS), France: coordinator
2. Cambridge University (UCAM), UK
3. University College London (UCL), UK
4. Open University (OU), UK
5. Universität Wien (UW-A), Austria
6. Uppsala Universitet (Uppsala), Sweden
7. Universität zu Köln (Koln), Germany
8. Istituto Nazionale di Astrofisica (INAF-OAC), Italy
9. The Queen's University of Belfast (QUB), UK
10. Astronomical Observatory of Belgrade (AOB), Serbia
11. Institute of Astronomy of RAS (INASAN), Russia
12. Russian Federal Nuclear Centre All-Russian Institute of Technical Physics (RFNC-VNIITF), Russia
13. Institute of Atmospheric Optics, SB of RAS (IAO), Russia
14. Venezuelan Institute for Scientific Research (IVIC), Venezuela
15. Institute for Spectroscopy of RAS (ISAN), Russia