RECENT WORKS ON ATOMIC AND PMI DATA FOR CONTROLLED FUSION RESEARCH IN RUSSIA

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  A.F. Ioffe Physico-Technical Institute
- A.S. Arakcheev
  G.I. Budker Institute of Nuclear Physics
• Generation of atomic data for fundamental science and controlled nuclear fusion

• Use of atomic data in controlled nuclear fusion research

• Recent works on plasma-material interaction data

• Conclusions
Generation of atomic data for fundamental science and controlled nuclear fusion

- Use of atomic data in controlled nuclear fusion research

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<tr>
<td>Overview of experimental data and theor. methods for charge-changing processes with ion beams passing through gaseous, solid and plasma targets: $e^-$ capture and $e^-$ loss processes with heavy many-electron ions, (e.g. Ar$^{a+}$, ..., U$^{q+}$) from 50 keV/u to 50 GeV/u, including multielectron processes. Stopping power is considered, and briefly isotopic effect at low energies.</td>
<td>Combined calculations using classical and quantum mechanics approaches.</td>
<td>Codes: ETACHA, GLOBAL, CHARGE, and BREIT</td>
<td>I.Yu. Tolstikhina, V.P. Shevelko <em>Influence of atomic processes on charge states and fractions of fast heavy ions passing through gaseous, solid, and plasma targets</em> Physics-Uspekhi 61 247 (2018), 33 pages</td>
<td>Cross-validation and comparisons with experimental data.</td>
<td>Detection of superheavy elements, atomic processes in stellar astrophysics, use of heavy ion beams as drivers for inertial confinement fusion.</td>
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Electron capture and electron loss processes with heavy many-electron ions; stopping power; isotopic effect at low energies (to be taken into account in modeling near-wall and divertor plasmas in facilities using hydrogen isotopes); short description of the computer programs ETACHA, GLOBAL, CHARGE and BREIT and their applications, including the use of heavy ion beams as drivers for inertial conf. fusion


Cross sections of $m$-electron ionization of Ne and Ar atoms by (a) Au$^{24+}$; (b) Bi$^{67+}$; (c) U$^{90+}$. Symbols - experiment: $m$-electron (dots) and total (circles) ionization cross sections [1, 2]. Curves - combined calculations in classical and quantum mechanical approximations [3].

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<tr>
<td>One- and two- electron capture by He$^{2+}$ ions from Ar atoms and electron capture with ionization</td>
<td>Target Ar atoms were supplied with an effusion gas jet. A collimated beam of $^3$He$^{2+}$ ions was used with energy in keV range. Calculations of cross sections using different model atomic particle interaction potentials.</td>
<td>Experimental setup described in V.V. Afrosimov, A.A. Basalaev, G.N. Ogurtsov, M.N. Panov Tech. Phys. 59 642 (2014)</td>
<td>A.A. Basalaev, G.N. Ogurtsov, M.N. Panov Tech. Phys. 63 947 (2018)</td>
<td>Verification of model interaction potentials used in the analysis of collisions of $\alpha$-particles with multielectron atoms.</td>
<td>Plasma diagnostics, numerical simulations of processes in controlled fusion devices.</td>
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<td>No.</td>
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<td>Name of the process</td>
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<tr>
<td>1</td>
<td>( \text{He}^{2+} + \text{Ar} \rightarrow \text{He}^+ + \text{Ar}^+ )</td>
<td>One-electron capture</td>
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<td>2</td>
<td>( \text{He}^{2+} + \text{Ar} \rightarrow \text{He}^+ + \text{Ar}^{2+} + e^- )</td>
<td>One-electron capture with ionization</td>
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<td>3</td>
<td>( \text{He}^{2+} + \text{Ar} \rightarrow \text{He}^0 + \text{Ar}^{2+} )</td>
<td>Two-electron capture</td>
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<td>4</td>
<td>( \text{He}^{2+} + \text{Ar} \rightarrow \text{He}^0 + \text{Ar}^{3+} + e^- )</td>
<td>Two-electron capture with ionization</td>
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<tr>
<td>5a</td>
<td>( \text{He}^{2+} + \text{Ar} \rightarrow \text{He}^+ + \text{Ar}^{n+} + (n - 1)e^- \ n \geq 3 )</td>
<td>One-electron capture with ( n )-degree ionization</td>
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<td>5b</td>
<td>( \text{He}^{2+} + \text{Ar} \rightarrow \text{He}^0 + \text{Ar}^{n+} + (n - 2)e^- \ n \geq 4 )</td>
<td>Two-electron capture with ( n )-degree ionization</td>
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<tr>
<td>5c</td>
<td>( \text{He}^{2+} + \text{Ar} \rightarrow \text{He}^{2+} + \text{Ar}^{n+} + ne^- \ n \geq 1 )</td>
<td>( n )-Degree ionization</td>
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</table>

Total cross sections of capture of one or two electrons in collisions of \( \text{He}^{2+} \) ions with \( \text{Ar} \) atoms

Sum of cross sections of processes 1+2: dots – [*], triangles – [1], circles – [2].
Sum of cross sections of processes 3+4: solid squares – [*], open squares – [3].


The contribution of process 5 to the total cross section can be disregarded.
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Reflection coefficients for D atoms scattered from amorphous W. Dots – experiment [1]


Reflection coefficients for D atoms scattered from amorphous C. Experimental data are from [2].


Additional bibliography:


The interatomic potential determines the nuclear stopping power in materials. A review of the most recent papers concerning the study of interatomic potentials is given.
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<tr>
<td>Statistical modeling of heavy ions quasicontinuum in thermonuclear plasmas</td>
<td>Slater approximation for electron subshells</td>
<td>The statistical model of quasicontinuum of heavy ions</td>
<td>A.V. Demura, D.S. Leontyev, V.S. Lisitsa, V.A. Shurygin ECA 2019 V. 43C P1.1066</td>
<td>Comparison with experim. data and data from level-by-level computations</td>
<td>Integrated modeling of fusion experiments</td>
</tr>
<tr>
<td>Radiative losses of alpha particles on tungsten impurities in thermonuclear plasmas</td>
<td>Local plasma frequency model of collective oscillations of atomic electron density</td>
<td>The statistical model of the radiation losses of electrons and alpha particles</td>
<td>A.V. Demura, D.S. Leontyev, V.S. Lisitsa, V.A. Shurygin JETP Letters 106 429 (2017)</td>
<td>Refinement of the critical concentration of heavy-ion impurities in fusion plasma</td>
<td>Diagnostics of thermonuclear plasma</td>
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</table>
Quasicontinuum from tungsten ions at T=1.5 keV

Statistical model predicts a sharp cut of quasicontinuum at short wavelengths, that satisfactorily coincides with experimentally observed spectra

1 - statistical model [1] with $<Z_i>=23$ calculated by the statistical approach in coronal equilibrium;
3 – experimental data from LHD [3]


Courtesy D.S. Leontyev
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V.A. Astapenko, A. Calisti, V.S. Lisitsa High Energy Density Physics 31 59 (2019)  
F.B. Rosmej, V.A. Astapenko, V.S. Lisitsa, X. Li, E.S. Khramov Contributions to Plasma Physics 59 189 (2019) | Atomic spectra for different broadening mechanisms, with optical depth effects.  
Diagnostics of matter, including the inertially confined fusion plasmas, using free-electron lasers. |
Outline

- Generation of atomic data for fundamental science and controlled nuclear fusion

- Use of atomic data in controlled nuclear fusion research

- Recent works on plasma-material interaction data

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Electron Capture and Loss Processes in Hydrocarbon and Li Pellet Clouds

I. Electron capture by H$^+$ ions

$$H^+ + C^q \to H^0 + C^{(q+1)+}, \quad q = 0, \ldots, 5$$

$$H^+ + H^0 \to H^0 + H^+$$

$$H^+ + Li^q \to H^0 + Li^{(q+1)+}, \quad q = 0, 1, 2$$

II. Electron loss by H$^0$ atoms

$$H^0 + C^q \to H^+ + C^{(q-1)+}, \quad q = 1, \ldots, 6$$

$$H^0 + C^q \to H^+ + C^q + e^-, \quad q = 0, \ldots, 6$$

$$H^0 + H^+ \to H^+ + H^0$$

$$H^0 + H^+ \to H^+ + H^+ + e^-$$

$$H^0 + H^0 \to H^+ + H^0 + e^-$$

$$H^0 + e^- \to H^+ + e^- + e^-$$

$$H^0 + Li^q \to H^+ + Li^{(q-1)+}, \quad q = 1, 2, 3$$

$$H^0 + Li^q \to H^+ + Li^q + e^-, \quad q = 0, 1, 2, 3$$

$$H^0 + e^- \to H^+ + e^- + e^-$$


NIFS-DATA-102 Research Report, ISSN 0915-6364
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| Verification of experimental data interpretation methods proposed for ITER Main Chamber H-alpha and Visible Spectroscopy on the data from JET | Interpretation of high-resolution spectra of hydrogen isotopes (Balmer-alpha) and beryllium in JET-ILW (passive spectroscopy) | *The results for beryllium are not published yet.*  
Balmer-alpha data: V.S. Neverov, A.B. Kukushkin, U. Kruezi, M.F. Stamp, H. Weisen and JET Contributors,  
Be II 527 nm spectral line: signal decomposition

The program fits the signal on the line of sight (LoS) in the main chamber and separates the contributions from high field side and low field side scrape-off layer (SOL).

ADAS603 code is used to simulate the line shape under combined action of Zeeman splitting and fine structure.

B - magnetic field, $\alpha$ - angle between the directions of magnetic field and the line of sight (LoS),

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<td>ADAS database <a href="https://open.adas.ac.uk/">https://open.adas.ac.uk/</a></td>
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ITER charge-exchange recombination spectroscopy (CXRS) diagnostics of the core and edge plasmas (NRC «Kurchatov Institute», TRINITI, Troitsk, Moscow Region, in cooperation with ITER Organization, France)

The problem of passive signal simulation

\[ \text{Be}^{4+} + \text{H}(1s) \rightarrow \text{Be}^{3+} + \text{H}^+ \]

5. ADAS database, https://open.adas.ac.uk/
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<td>Massive gas injection for discharge quenching in fusion facilities, including ITER</td>
<td>The problem of using the data for fine structure of atomic level in radiative-collisional kinetics and radiation losses simulation for edge plasmas in fusion facilities, including the radiation losses during massive gas injection for discharge quenching in ITER</td>
<td>P.A. Sdvizhenskii, A.B. Kukushkin, et al. Proc. 45th EPS Conference on Plasma Physics, 2-6 July 2018, Prague, Czech Republic, ECA, Vol. 42A, P4.1083</td>
<td>The transitions, corresponding to high intensity spectral lines of ions of gases used in massive gas injection disruption mitigation</td>
<td>ADAS database <a href="https://open.adas.ac.uk/">https://open.adas.ac.uk/</a></td>
<td>Radiated Power Data PLT - Line Emission from excitation under ADF11 derived data class (updated 2019 data for Argon plt42_ar.dat) was used. Updated data for Neon would be beneficial.</td>
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The problem of using the data for fine structure of atomic level in radiative-collisional kinetics and radiation losses simulation for edge plasmas in fusion facilities, including the radiation losses during massive gas injection for discharge quenching in ITER (NRC «Kurchatov Institute»)


Figure. Spatial profiles of plasma parameters at time $t = 12.31$ ms from the MGI start for ion $\text{Ar}^{+3}$. Lines:

1. $(3p \rightarrow 3s), \lambda = 702.867 \text{ Å}$
2. $(3d \rightarrow 3p), \lambda = 532.718 \text{ Å}$

The optical thickness $\Theta$ over the path along major radius for lines (*) and (***) is: $\Theta_{532} \approx 16.30, \Theta_{702} \approx 6.88$.

Curve 1 – local emissivity in the lines (*) and (**), calculated with account of the exact structure of atomic energy levels and the respective coronal limit of radiative-collisional model without opacity effect;

Curve 2 – the same but for the simplified radiative collisional model with the opacity effect;

Curve 3 – total emissivity of $\text{Ar}^{+3}$ ion in the coronal limit for the approximate structure of atomic energy levels, used in the ZIMPUR code.

Opacity effect gives $\sim 25\text{-}30\%$ corrections

Courtesy P.A. Sdvizhenskii
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<tr>
<td>Laser-Induced Quenching diagnostics of H (D,T) atoms</td>
<td>Collision-radiative model of HI</td>
<td>E.E. Mukhin, G.S. Kurskiev, A.V. Gorbunov et al., Nuclear Fusion, 2019, 59(8), 086052</td>
<td>All processes for H/D atoms</td>
<td>ADAS: EIE, EII NIST: radiative transitions R.K. Janev et al., Collision Processes in Low-Temperature Hydrogen Plasmas: other processes</td>
<td>EIE, EII rates for fine structure transitions ($nl$-splitting)</td>
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EII - Electron Impact Ionisation, EIE - Electron Impact Excitation
LIQ diagnostics of HeII for ITER*

HeII LIQ spectroscopic scheme

Laser pumping:
\[ n = 4 \rightarrow 5 \]
\[ \lambda_l = 1012.3 \text{ nm} \]

Quenching obs.:
\[ n = 4 \rightarrow 3 \]
\[ \lambda_l = 468.6 \text{ nm} \]

Expected LIQ and background signals
(HelI CRM calculations for ITER)

LIQ diagnostic test at Globus-M tokamak**

HI LIQ

H\(\alpha\) LIQ signals detected at Globus-M tokamak

H\(\alpha\) quenching

OPO laser: (gray area)
\[ \lambda = 1005 \text{ nm}, \]
\[ n = 3 \rightarrow 7 \]
\[ \Delta \lambda = 2000 \text{ pm} \]
\[ \tau = 10 \text{ ns} \]
\[ E = 2.2 \text{ mJ} \]

*Courtesy A.V. Gorbunov

**E.E. Mukhin, G.S. Kurskiev, A.V. Gorbunov et al., Nuclear Fusion, 2019, 59(8), 086052

Outline

• Generation of atomic data for fundamental science and controlled nuclear fusion

• Use of atomic data in controlled nuclear fusion research

➢ Recent works on plasma-material interaction data

• Conclusions
Russia Conferences on Plasma Surface Interaction are mostly attended by domestic participants reporting on activities in Russia


(Annual conference organized by Moscow Eng. Physics Institute)
Newest PMI activities in Russia and in the world were reported at the 24th International Conference on Ion-Surface Interactions


A biennial conference organized and sponsored by
- Russian Academy of Sciences
- Ministry of Education and Science
- Moscow Eng. Physics Institute
- Moscow State University
- St. Petersburg Polytechnic University
and other institutions

Book of Abstracts is currently available on demand
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<td>Helium retention in W irradiated with He+ ions at elevated temperatures (300-1200 K)</td>
<td>Ion beam implantation and thermal desorption spectroscopy (up to 2500 K). Secondary electron microscopy</td>
<td>Medion facility (MEPhI)</td>
<td>S. Ryabtsev et al. <em>Nuclear Instruments and Methods in Physics Research, Section B: Beam Interactions with Materials and Atoms</em>, <a href="https://doi.org/10.1016/j.nimb.2019.01.051">https://doi.org/10.1016/j.nimb.2019.01.051</a></td>
<td>Low fluence experiments in well controlled conditions can used as a reference for modeling</td>
<td>Influence of He plasma irradiation of PFM on H isotope retention and surface morphology</td>
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Add-on: 
Database Activities in Snezhinsk and Novosibirsk
SPECTR-W3 database on spectroscopic properties of atoms and ions (http://spectr-w3.snz.ru/index.phtml) developed at E.I. Zababakhin All-Russian Scientific Research Institute of Technical Physics in Snezhinsk was earlier reported in the context of VAMDC activity.

The virtual atomic and molecular data centre (VAMDC) consortium*

Current status was reported at I.Yu. Skobelev, P.A. Loboda

Database SPECTR-W3 on spectroscopic properties of atoms and ions
17th International Workshop “Complex Systems of Charged Particles and their Interactions with Electromagnetic Radiation 2019”
Moscow, Russia, 25-27 March 2019
https://cscpier.org/
G.I. Budker Institute of Nuclear Physics

Russian atomic spectroscopy, information system electronic structure of atoms (IS ESA) (http://grotrian.nsu.ru) was described in
V.V. Kazakov et al. Phys. Scr. 92 105002 (2017)
An update was published in
V.V. Kazakov et al. AIP Conference Proceedings 2052, 020010 (2018)
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➢ Conclusions
Conclusions

- Works on atomic data in the past two years were motivated by both fundamental science and controlled nuclear fusion research.
- Further development of ITER diagnostics in Russia reveals new data needs.
- Priorities of Russian research programme on controlled fusion determine the activity on PMI data.
- Activities on SPECTR-W3 and IS ESA databases are continuing.