IAEA Technical Meeting on Technical Aspects of Atomic and Molecular Data Processing and Exchange

23rd Meeting of the Atomic and Molecular Data Centres Network

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CURRENT ACTIVITY IN RUSSIA ON ATOMIC, MOLECULAR AND PMI DATA

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Outline

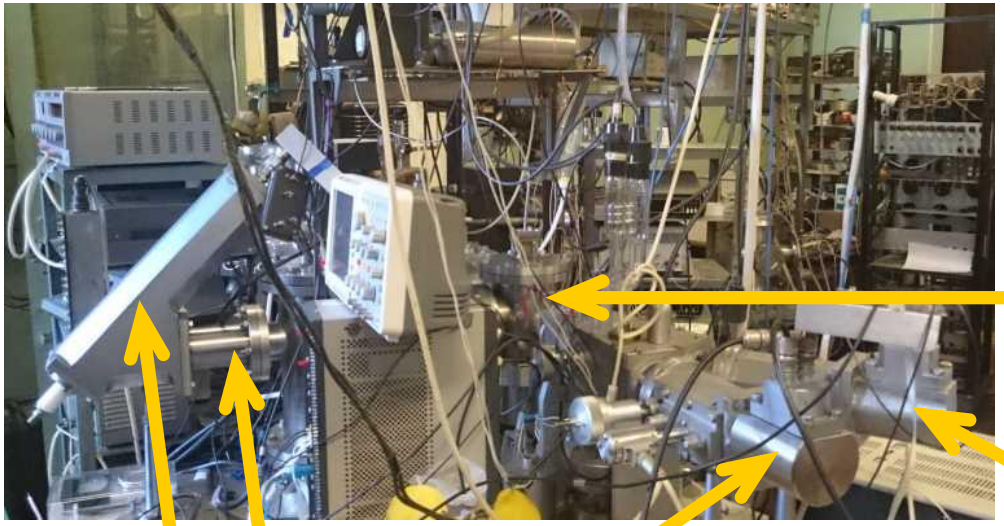
- **Generation of atomic and molecular data for nuclear fusion research needs**
- **Use of atomic and molecular data in controlled fusion research**
- **Plasma-material interaction data generation and use in magnetic confinement fusion research centres**
- **Conclusions**

1. Generation of atomic and molecular data for nuclear fusion research needs

Process	Method	Data Source / Code	Publications	Verification / Application	Problem
Charge changing collisions of H^+, D^+, He^{2+} with atoms of construction materials. SS may contain C (< 1%), Si (~0.8%), Mn (1 - 9%), Cr (~20%), Ni (< 10%), Ti (~1%), Fe (47 - 70%)	Projectile energy range E = (1 – 50)*Z keV (Z – projectile charge number). Target is prepared by thermal sputtering. Pressure 10^{-3} Torr in effusion cell for construction materials is maintained in temperature range 1146 K (Mn) - 2669 K (C).	Experimental stand described in *V.V. Afrosimov, A.A. Basalaev, M.N. Panov, O.V. Smirnov* ***Tech. Phys. Lett. 31*** *(2005) 1055-1057*	*V.V. Afrosimov, A.A. Basalaev, G.N. Ogurtsov, M.N. Panov* ***Tech. Phys. 59*** *(2014) 642-648*	Applicable in numerical modelling of physical processes in controlled fusion devices	Plasma diagnostics, plasma heating and current drive

Laboratory of Atomic Collision Physics

Ioffe Institute



Collision chamber

Magnetic analyzer of primary beam ions

Detector of fast charged particles

Primary beam collimator

Detector of fast neutral particles

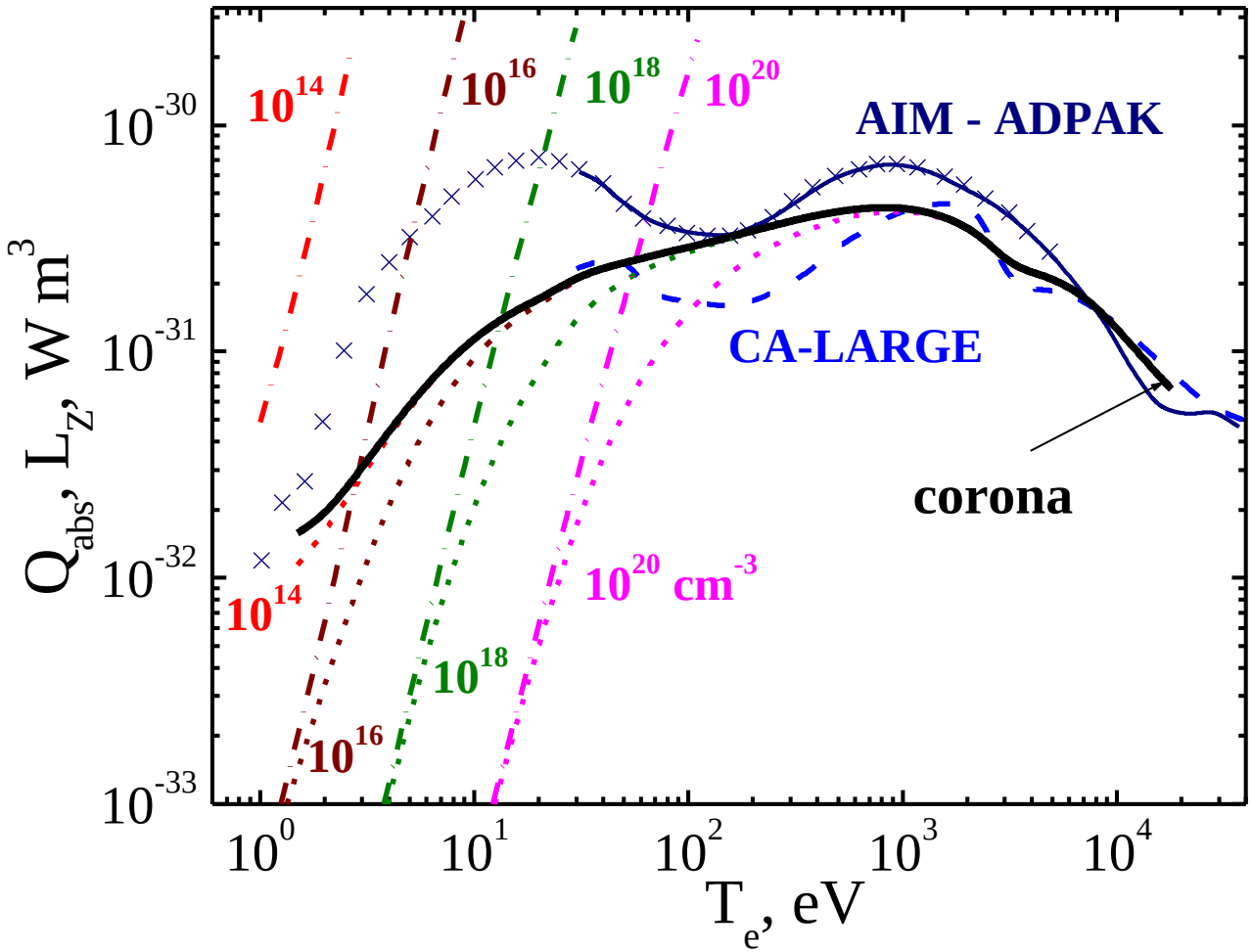
Detector of secondary particles

TOF analyzer of secondary ions

Projectile charge analyzer after interaction

Processes	Method	Data Source \ Code	Publication	Verification / Application	Problem
Multiple ionization of atoms by highly charged ions	A combination of semiclassical and quantum mechanical approaches	Codes: RICODE CAPTURE, ARSENY, DEPOSIT	*I.Yu. Tolstikhina, V.P. Shevelko* ***Phys. Scr. 90*** *(2015) 074033*	ICF driven by heavy ion beams, when a particle accelerator complex is used with equipment needed to aim and focus the beams. **F**acility for **A**ntiproton and **I**on **R**esearch (**FAIR**) in EU and **N**uclotron-based **I**on **C**ollider f**A**cility (**NICA**) in Russia	Energy losses of accelerated ions depend on their interaction cross sections with atoms and molecules of the residual gas in a wide energy range. In heavy-ion therapy, the creation of the secondary electrons due to multiple ionization may be an important effect.
Uranium ions stripping in molecular hydrogen			*V.P. Shevelko et al., submitted to* ***Nucl. Instrum. Meth. Phys. Res. Sect. B***		
Multiple Electron Losses in Uranium Ion Beams			*L. Bozyk et al., submitted to* ***Nucl. Instrum. Meth. Phys. Res. Sect. B***		

Processes	Method	Data Source \ Code	Publication	Verification / Application	Problem
Collisional-radiative processes in plasmas with multielectron ions	Thomas-Fermi and Brandt-Lundquist model of collective oscillations of atomic electron density	TFATOM	*A.V. Demura et al.* ***Atoms 3*** *(2015) 162-181* *A.V. Demura et al.* ***High Energ. Dens. Phys. 15*** *(2015) 49-58* *A.V. Demura et al.* ***J. Phys. B: At. Mol. Opt. Phys. 48*** *(2015) 055701* *A.V. Demura et al.* ***JETP Lett. 101*** *(2015) 85-88*	Comparison with (a) first-principle numerical modeling of, and (b) experimental database, on heavy impurity radiation losses	Radiation losses on W in fusion facilities (ITER et al.) Integrated modeling of fusion experiments



Radiative losses of tungsten plasmas (power per one atom/ion, per one plasma electron) versus temperature for several density values, demonstrating transition from Boltzmann equilibrium (straight dash-dotted lines) to corona limit (solid line).

Universal statistical approach (dashed lines, marked by values of electron density) vs. codes

AIM ADPAK — *D. Post et al.* ***Phys. Plasmas 2 (1995)*** *2328-2336*
K. Asmussen et al. ***Nucl. Fusion 38*** *(1998) 967-986*

ADPAK — *H.P. Summers* ***Atomic Data and Analysis Structure User Manual*** *(2007)*

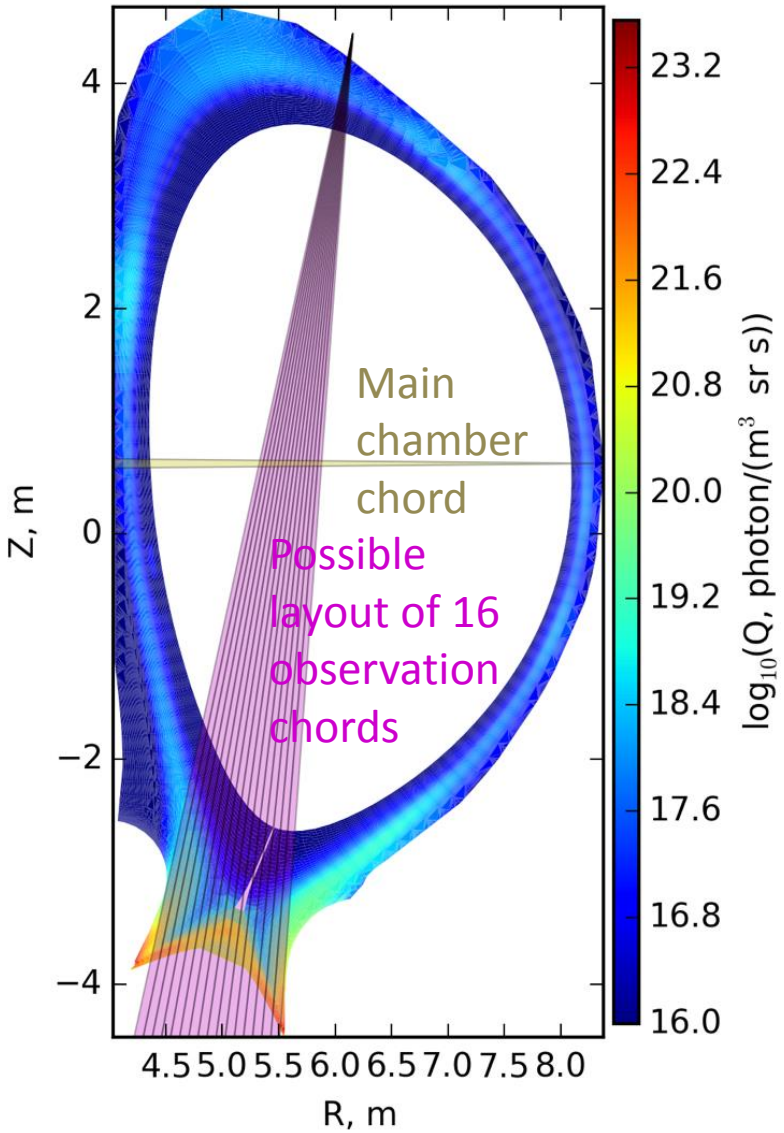
AIM - averaged ion model - *D.E. Post et al.* ***At. Data Nucl. Data Tables 20*** *(1977) 397-439*

CA-LARGE — *T. Pütterich et al.* ***Nucl. Fusion 50*** *(2010) 025012*

➢ A.V. Demura, M.B. Kadomtsev, V.S. Lisitsa, V.A. Shurygin **High Energ. Dens. Phys. 15** (2015) 49-58

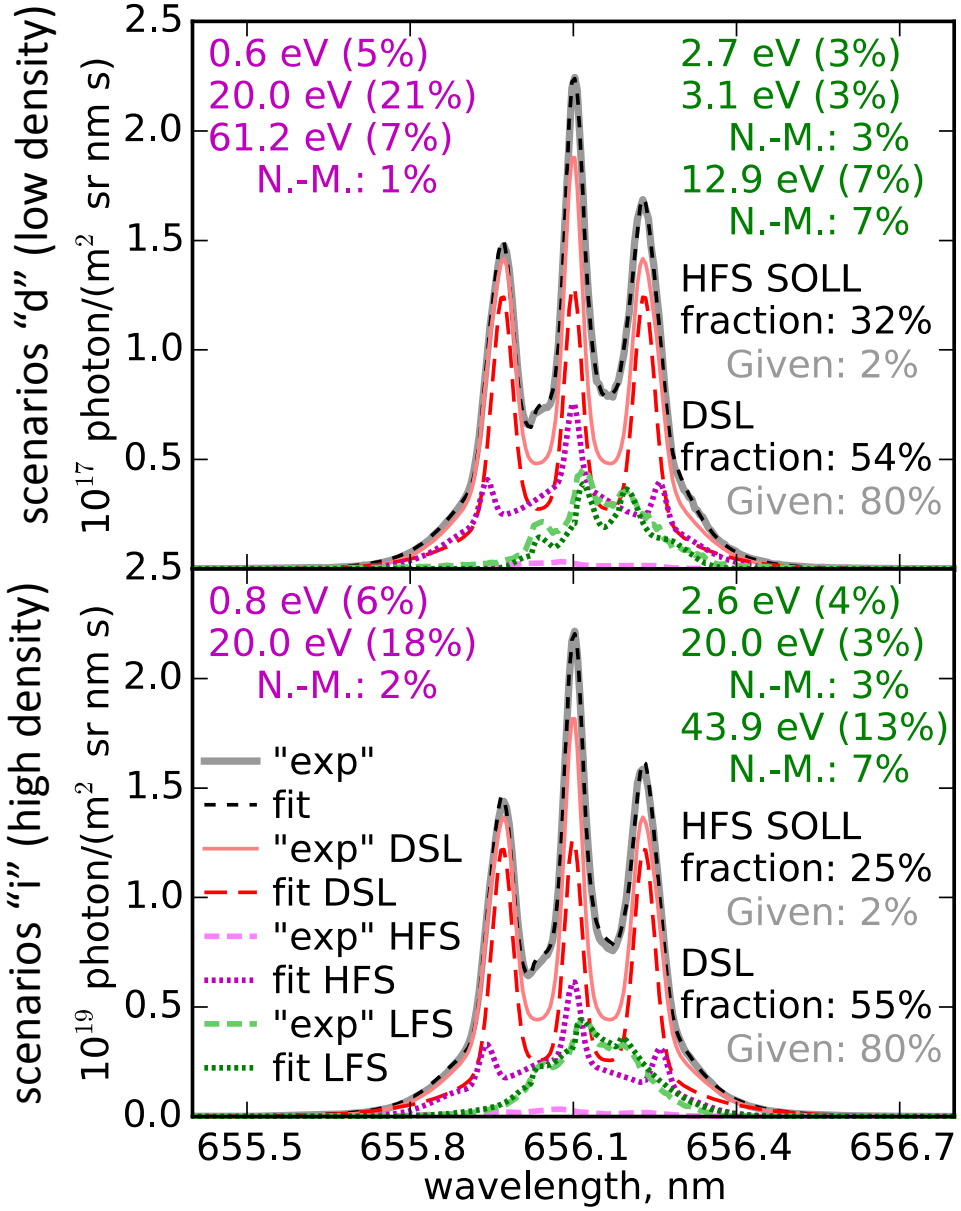
2. Use of atomic and molecular data in controlled fusion research

Problem	Task	Publication	Processes	Data Source	Data Needs
H-alpha (and Visible Light) Diagnostic in ITER: "Synthetic Diagnostics" for error assessment and hardware optimization	Divertor Stray Light problem, accuracy assessment (ITER Measurement Requirement flow down)	*V.S. Lisitsa et al.* ***Atoms 2*** *(2014) 195-206* *A.B. Kukushkin et al.* ***J. Phys.: Conf. Ser. 548*** *(2014) 012012* *V.S. Neverov et al.* ***Plasma Phys. Rep. 41*** *(2015) 103-111* *A.B. Kukushkin et al.* ***1st IAEA TM on Fusion Data Analysis*** *(2015), submitted to Fusion Sci. Technol.*	All processes with D_2 and D All processes with impurities (Be, W, etc.)	B2-EIRENE (SOLPS4.3) simulations of plasma background in divertor+SOL in ITER EIRENE simulations of neutral D velocity distribution in SOL in ITER DIVIMP simulations of impurities	Hydrogen isotope molecules dissociation with excited atoms as products Beryllium hydride molecules



2D distribution of the Balmer-alpha emissivity* in the SOL and divertor in ITER, in log-scale.

* SOLPS 4.3 (B2-EIRENE) simulation



Fitting the "phantom" experimental signal by solving an inverse problem for assumed (given) 80% fraction of DSL and 2% fraction of HFS SOL light in the total signal

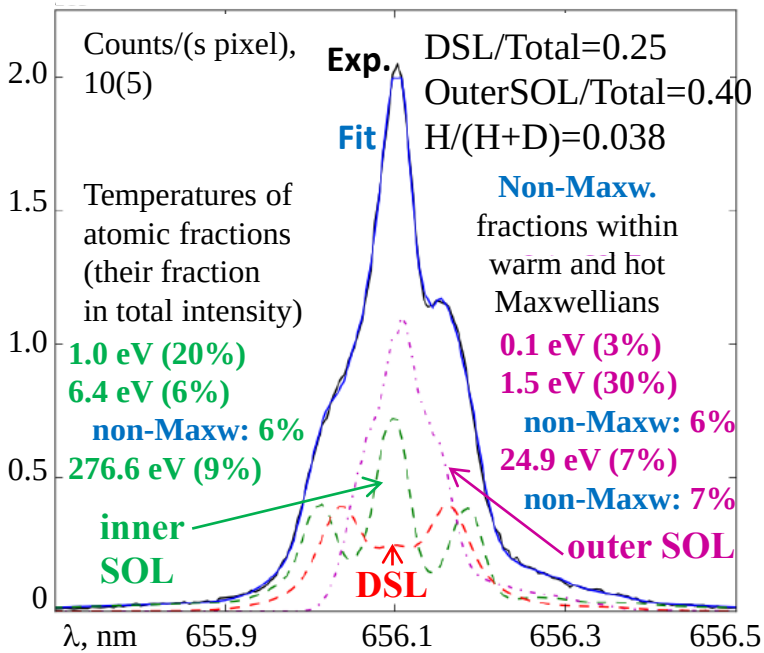
NRC Kurchatov Institute A.B. Kukushkin, V.S. Neverov, et al.
A.F. Ioffe Physico-Technical Institute E.E. Mukhin, G.S. Kurskiev et al.

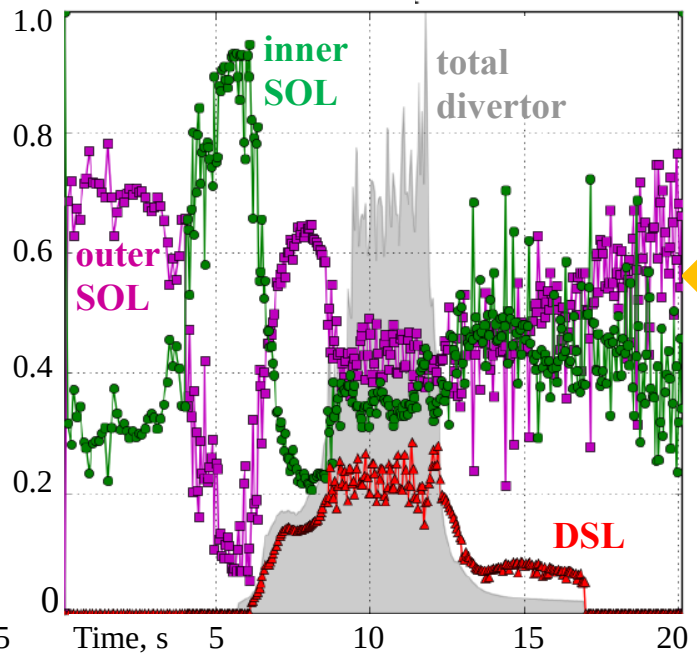
Problem	Task	Publication	Processes	Data Source	Data Needs
ITER Divertor Thomson Scattering	• Spectral Lines 900 – 1070 nm (background) • Recombination rates T_e 0.2 – 1eV (Ionization front position)	*E.E. Mukhin et al.* ***Nucl. Fusion 54*** *(2014) 043007*	All processes with D_2, DT, T_2 and D, T All processes with He and He^+ (As for example: $4HeD^+$, $3HeD^+$, He_2^+, $3He4He^+$) All processes with impurities (Be, W, etc.)	B2-EIRENE (SOLPS4.3) simulations of plasma background in divertor+SOL in ITER DIVIMP simulations of impurities	Complex impurity molecules in divertor plasmas (?)
ITER Core Thomson Scattering	Spectral Lines 400 – 1070 nm (background)	*G.S. Kurskiev et al.* ***Nucl. Fusion 55*** *(2015) 053024*			
ITER Divertor Laser-induced fluorescence (LIF)	• LIF signals (He, Be) • Spectral Lines 380 – 750 nm (background)				
D-alpha diagnostic in JET-ILW in support to ITER	Verification of H-alpha synthetic diagnostic for ITER in JET ITER-like Wall experiments	*A.B. Kukushkin et al.* ***Proc. 25th IAEA Fusion Energy Conf.*** *(2014), EX/P5-20*			

Theoretical Model of ITER High Resolution H-alpha Spectroscopy for a Strong Divertor Stray Light and Validation Against JET-ILW Experiments

A multi-parametric inverse problem with allowance for (i) a strong **divertor stray light (DSL)** on the main-chamber lines-of-sight (**LoS**), (ii) substantial deviation of neutral atom velocity distribution function from a Maxwellian in the SOL (a model for line shape asymmetry), (iii) data for direct observation of divertor.

JPN 85844: Ip=2 MA, Bt=2.8 T, Ne0=5.8 10(19) m(-3), Te0=2.6 keV, Paux(NBI)=7.5 MW, Paux(ICRH)=2 MW





- Direct observation of the divertor from top
- Observation of main-chamber inner wall along tangential and **radial LoS (KSRB Track 11)** from equatorial ports
- Analysis of HRS data on resolving the power at D+H Balmer-α spectral lines

Fitting of measured spectrum, time 10.05 s. Asymmetry of Balmer-α spectral line shapes for inner- and outer-wall SOL is due to **non-Maxwellians** (and small admixture of H).

Fractions of **inner-wall SOL**, **outer-wall SOL**, and **DSL**, in total signal vs. time. **Normalized total power of H+D Balmer-α emission in divertor**.

The results support the expectation of a strong impact of the DSL upon H-alpha (and Visible Light) Spectroscopy Diagnostic in ITER.

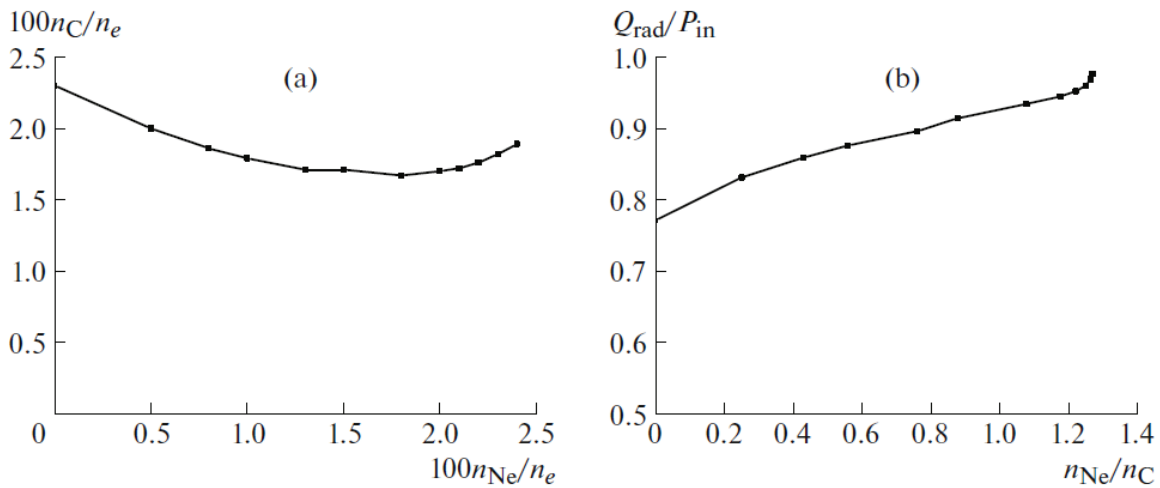
A.B.Kukushkin, V.S.Neverov, M.F.Stamp, A.G.Alekseev, S.Brezinsek, A.V.Gorshkov, M.vonHellermann, M.B.Kadomtsev, V.Kotov, A.S.Kukushkin, M.G.Levashova, S.W.Lisgo, V.S.Lisitsa, V.A.Shurygin, E.Veshchev, D.K.Vukolov, K.Yu.Vukolov, and JET Contributors

ITER RF DA S.N. Tugarinov et al. (TRINITI + NRC Kurchatov Institute)

Problem	Task	Publication	Processes	Data Source	Data Needs
CXRS-edge diagnostic in ITER **Test of design at T-10 tokamak**	W lines' influence on the CXRS spectral profiles	*L. Klyuchnikov et al.* ***Proc. 25th IAEA Fusion Energy Conf.*** *(2014), EX/P1-44*	All processes with W	ADAS simulations of plasma radiation in divertor+SOL in ITER; *S. Menmuir et al.* ***Rev. Sci. Instrum. 85*** *(2014) 11E412*	W lines intensity for all kinds of ionization stage in CXRS ranges: 468±8 nm 529±8 nm 656±10 nm

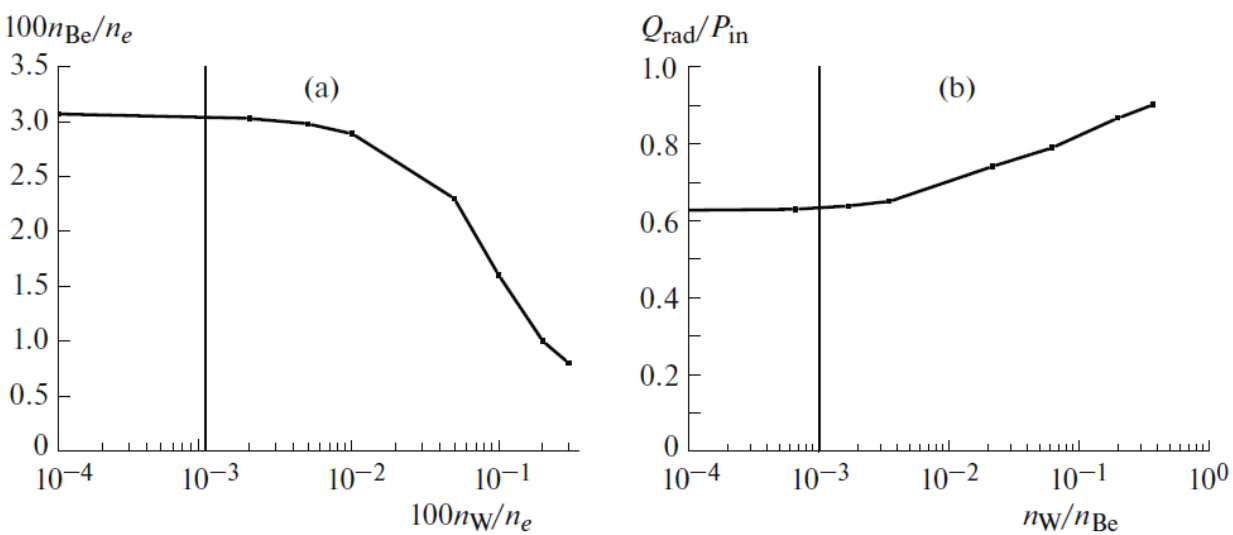
NRC Kurchatov Institute D.Kh. Morozov et al.

Problem	Task	Publication	Processes	Data Source	Data Needs
Radiation-condensation instability in tokamak edge plasmas	Light impurity radiation losses for m=n=0 mode Li radiation losses for edge turbulence	*D.Kh. Morozov et al.* ***Contrib. Plasma Phys. 54*** *(2014) 570-574* *R.V. Shurygin et al.* ***Plasma Phys. Rep. 40*** *(2014) 919-931*	Elementary processes with low-Z impurities	*D.A. Verner et al.* ***At. Data Nucl. Data Tables 64*** *(1996) 1-180*	
	MARFE development for ITER-like impurity mixture	*D. Kh. Morozov et al.* ***Plasma Phys. Rep. 41*** *(2015) 599-606*	Elementary processes in a mixture of low-Z and high-Z impurities	ZIMPUR code simulations	Elementary processes with high-Z impurities (W)



(a) Critical carbon impurity concentration corresponding to the Radiation-Condensation Instability marginal stability as a function of the neon concentration near the wall and

(b) radiated fraction of the power incoming into the layer from the core plasma as a function of the neon-to-carbon density ratio.

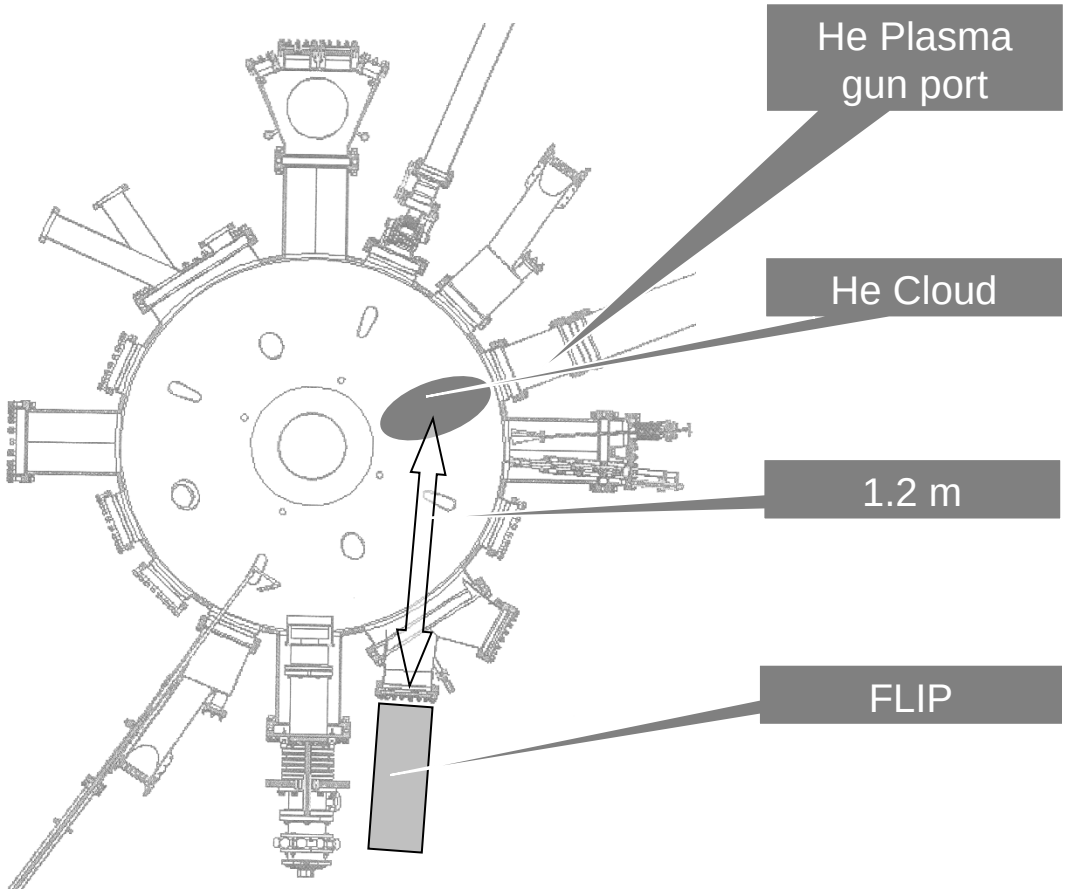


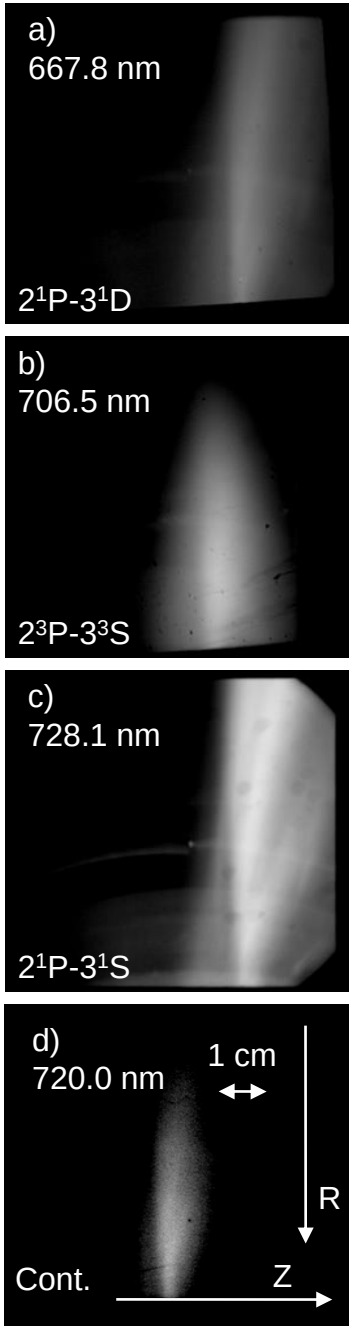
The same as above, but for a beryllium–tungsten mixture.

D. Kh. Morozov et al. ***Plasma Phys. Rep. 41*** *(2015) 599-606*

Problem	Task	Publication	Processes	Data Source	Data Needs
Diagnostics of edge plasma parameters on Globus-M/M2 spherical tokamak	Measurements of peripheral plasma parameters using ratios of line intensities of neutral Helium	*V.M. Timokhin et al.* ***Tech. Phys. Lett. 42*** *(2016), in press*	$He^* \rightarrow He^{*\prime} + \hbar\omega$ $\lambda_{3^1d\rightarrow 2^1p}$= 667.8 nm $\lambda_{3^1s\rightarrow 2^1p}$= 728.1 nm $\lambda_{3^3s\rightarrow 2^3p}$= 706.6 nm Rn_e = 667.8/728.1 RT_e = 728.1/706.5	ALADDIN	Improved data are needed for transition rates in the range of $2.0\times10^{18}\ \mathrm{m}^{-3} < n_e < 2.0\times10^{19}\ \mathrm{m}^{-3}$ and $10\ \mathrm{eV} < T_e < 250\ \mathrm{eV}$

Test experiments on Globus-M spherical tokamak





References

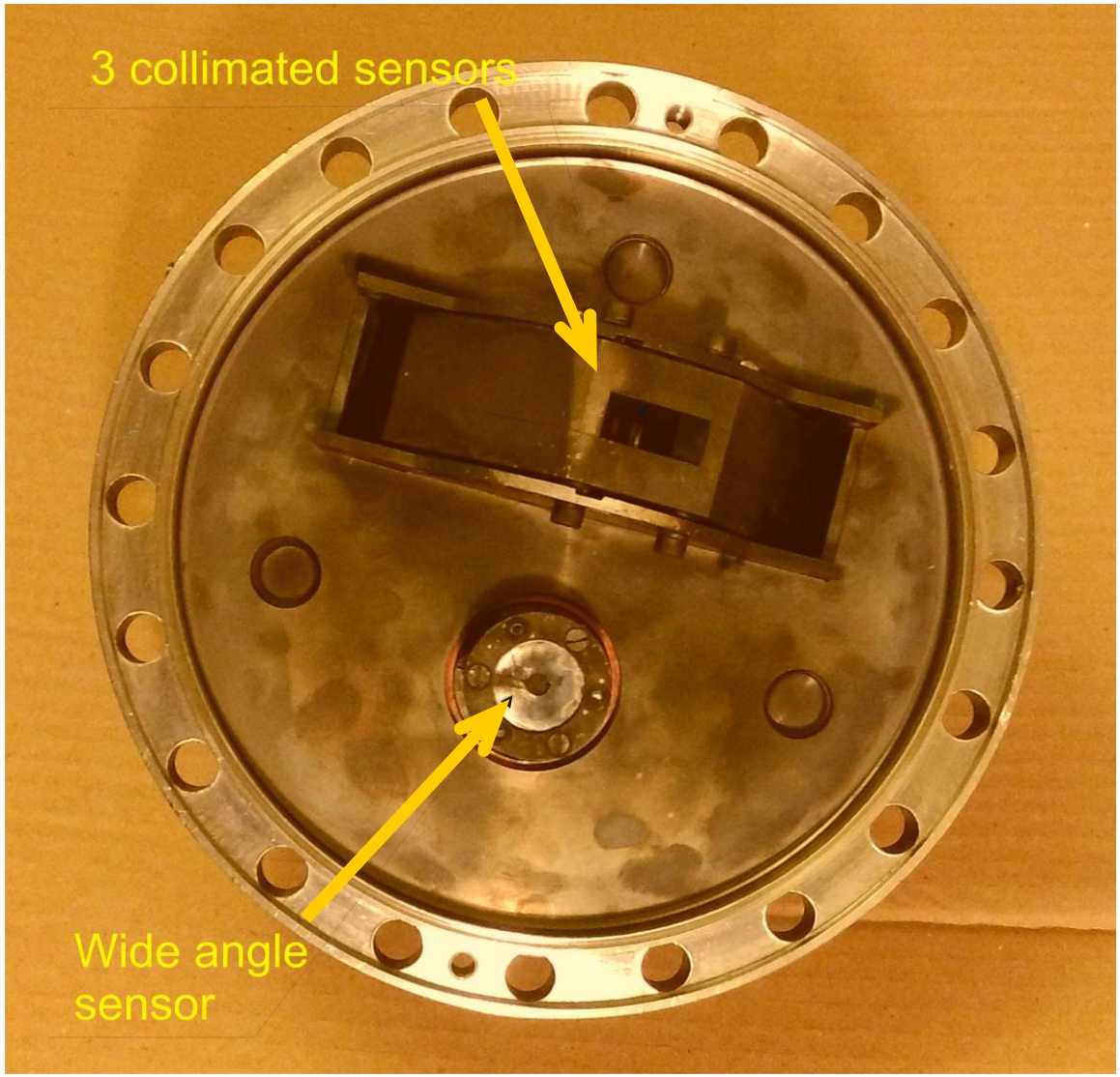
J.-W. Ahn et al. ***Phys. Plasmas 14*** *(2007) 083301*

B. Schweer ***Fusion Sci. Technol. 45*** *(2004), Number 2T, 434-441*

M. Brix ***Berichte des Forschungszentrums Jülich 3638*** *(1998)*

Problem	Task	Publication	Processes	Data Source	Data Needs
Modelling of radiative losses from divertor region with tungsten tiles for various discharge termination scenarios	Selection of processes predominantly contributing to radiative losses in the viewing regions of collimated channels of the bolometric diagnostic	*V.G. Kapralov et al.* ***43rd Zvenigorod Conf. on Plasma Phys. Control. Fusion*** *(2016)*	Ionization and recombination in collisions involving W, H, D	NIST ASD	

Flange of the bolometric diagnostic on Globus-M spherical tokamak



Problem	Task	Publication	Processes	Data Source	Data Needs
Development of gas discharge methods for cleaning of diagnostic mirrors in ITER. **Development of gas discharge methods to study tritium retention in ITER.** **Optimization of plasma technologies for microelectronics.**	Modelling of gas discharge plasma	*A.G. Razdobarin et al.* ***Nucl. Fusion 55*** *(2015) 093022* (RF discharge for in situ mirror surface recovery) *E.E. Mukhin et al.* ***Nucl. Fusion 52*** *(2012) 013017* (deposition prevention and cleaning techniques)	Elastic and nonelastic collisions of neutral and charged particles in a gas discharge plasma and with solid surfaces	NIST ASD	

Peter the Great Polytechnic University (in collaboration with NIFS, Japan)

Problem	Task	Publication	Processes	Data Source	Data Needs
Measurements of the ion distribution function with an active PCX diagnostic	Measuring of the spatial distributions of T_e, n_e, ionization states abundances of H and C in the cloud of cold secondary plasma around a solid polystyrene pellet ablating in high temperature plasma in a magnetic confinement device.	*I.A. Sharov et al.* ***Tech. Phys. Lett. 40*** *(2014) 361–363* *I.A. Sharov et al.* ***Rev. Sci. Instrum. 86*** *(2015) 043505* *S. Sudo et al.* ***Plasma and Fusion Research 9*** *(2014), 1402039*	**1)** Radiative recombination of H^+, C^+, C^{2+}, C^{3+}, C^{4+} **2)** Radiative attachment to H^0 and C^0 **3)** $H^0 + e \rightarrow H^+ + e + e$ $C^{k+} + e \rightarrow C^{(k+1)} + e + e$ **4)** Collisional and radiative processes involved in excitation and deexcitation of the singly ionized carbon. Necessary for experimental study of the **C II 723** nm line radiation from pellet cloud. **5)** Data on the Stark-broadened hydrogen Balmer beta line	NIST ASD K.L.Bell et al. J.Phys. Chem. Ref. Data 12 (1983) 891-916 C. Stehl'e and R. Hutcheon, Astron. Astrophys., Suppl. Ser. 140, 93 (1999) and earlier published sources	Hydrogen Balmer-beta line shapes (in the vicinity of the line center 486.12 ±5 nm) in the multicomponent plasma can improve results. Required temperature range 0.5 – 15 eV Required electron density range 10^{16} - 10^{18} cm^{-3}

Principle of PCX Measurements with a Compact NPA

local flux of ions with energy E, [cm^{-2}s^{-1}]

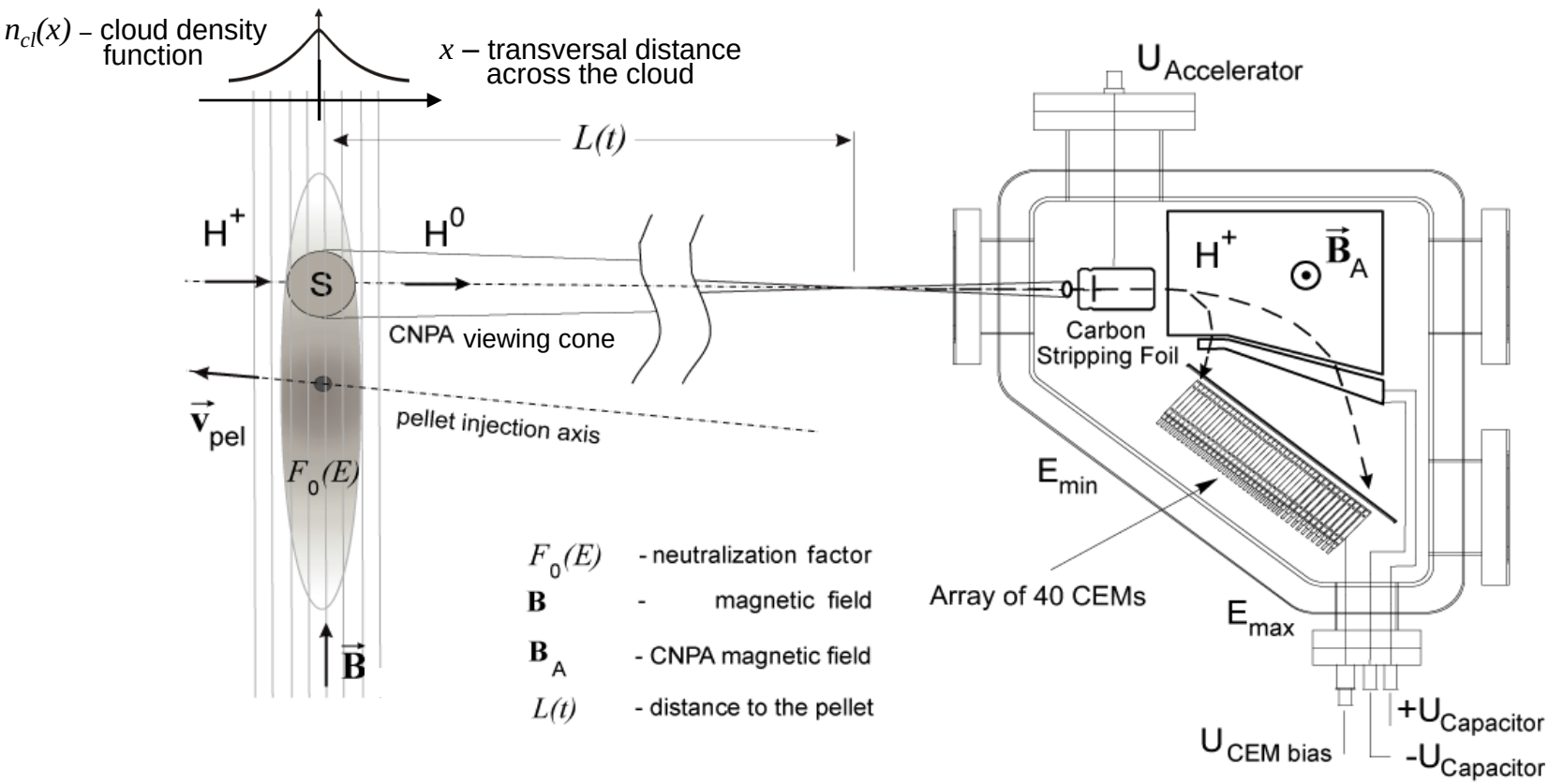
$$\Gamma_{H^+}(E) = n_i \mathrm{v}_i f_i(E,\mathbf{r})\, dE$$

local emission of atoms, [erg^{-1}cm^{-2}s^{-1}] from the unit area of the cloud

$$\gamma(E,\mathbf{r}) = F_0(E)\, n_i(\mathbf{r})\, \mathrm{v}_i f_i(E,\mathbf{r})$$

$$\Gamma_{H^0}^{(PCX)}(E,\mathbf{r}(t)) = \frac{S_a S}{4\pi L^2}\gamma(E,\mathbf{r})\, e^{-\tau(E,L)}$$

Measured H^0 Flux, [erg^{-1}s^{-1}]



Electron Capture and Loss Processes in Hydrocarbon and Li Pellet Clouds

I. Electron capture by H^+ ions

$H^+ + C^{q+} \rightarrow H^0 + C^{(q+1)+}$, q = 0, …, 5

$H^+ + H^0 \rightarrow H^0 + H^+$

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

II. Electron loss by H^0 atoms

$H^0 + C^{q+} \rightarrow H^+ + C^{(q-1)+}$, q = 1, …, 6

$H^0 + C^{q+} \rightarrow H^+ + C^{q+} + e^-$, q = 0, …, 6

$H^0 + H^+ \rightarrow H^+ + H^0$

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

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

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

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

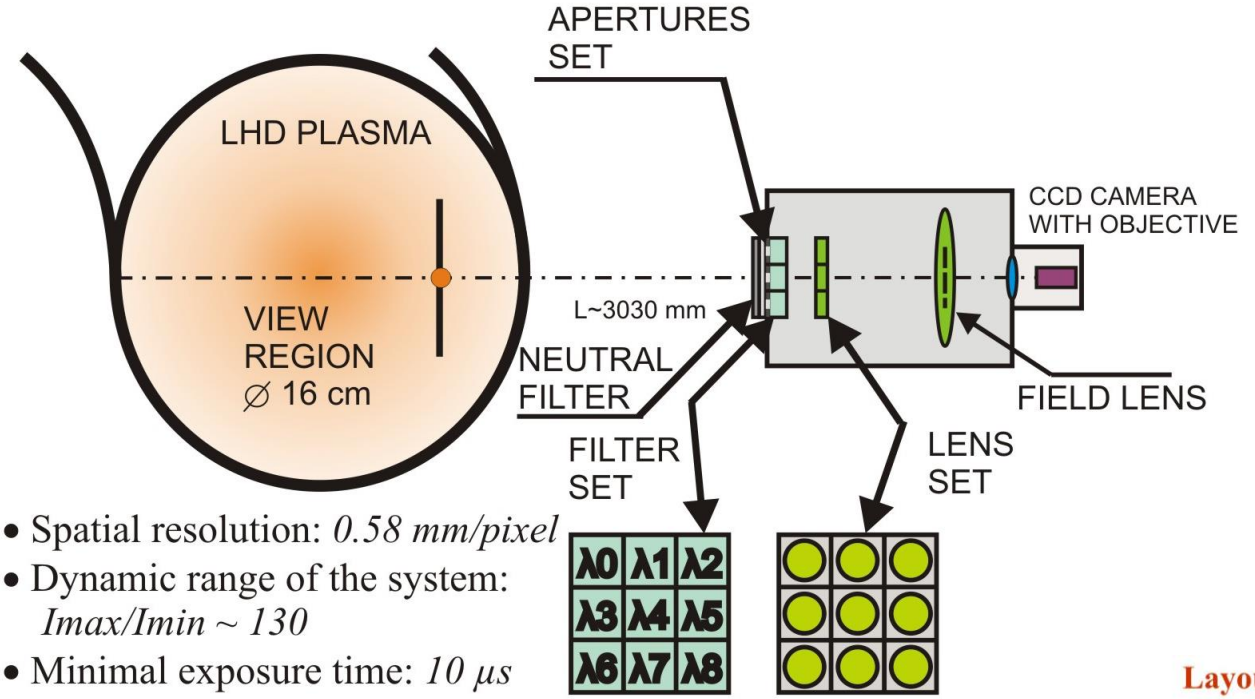
$H^0 + Li^{q+} \rightarrow H^+ + Li^{q+} + e^-$, q = 0, 1, 2, 3

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

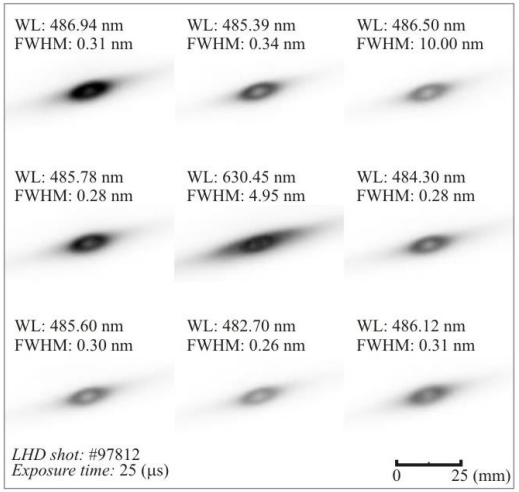
I.Yu. Tolstikhina, P.R. Goncharov, T. Ozaki ,S. Sudo, N. Tamura, V.Yu. Sergeev
***NIFS-DATA-102 Research Report**, ISSN 0915-6364*

NIOS 9-channel filter-lens imaging polychromator

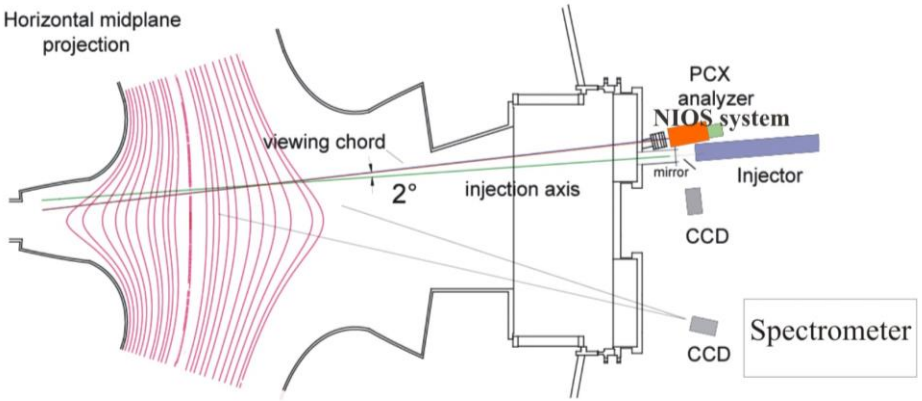
I.A. Sharov et al. Imaging Spectroscopy of Pellet Clouds in a Helical Plasma ***IEEE Trans. Plasma Sci. 39*** *(2011) 2476-2477*



- Spatial resolution: *0.58 mm/pixel*
- Dynamic range of the system: *Imax/Imin ~ 130*
- Minimal exposure time: *10 μs*
- *1 frame* per injection



Layout of pellet ablation diagnostics



- Pellet type: *polystyrene* (C_8H_8)
- Vp = 400 - 500 m/s
- Dp= 900 microns,

I.A. Sharov et al. Imaging polychromator for density measurements of polystyrene pellet cloud on the Large Helical Device ***Rev. Sci. Instrum. 86*** *(2015) 043505*

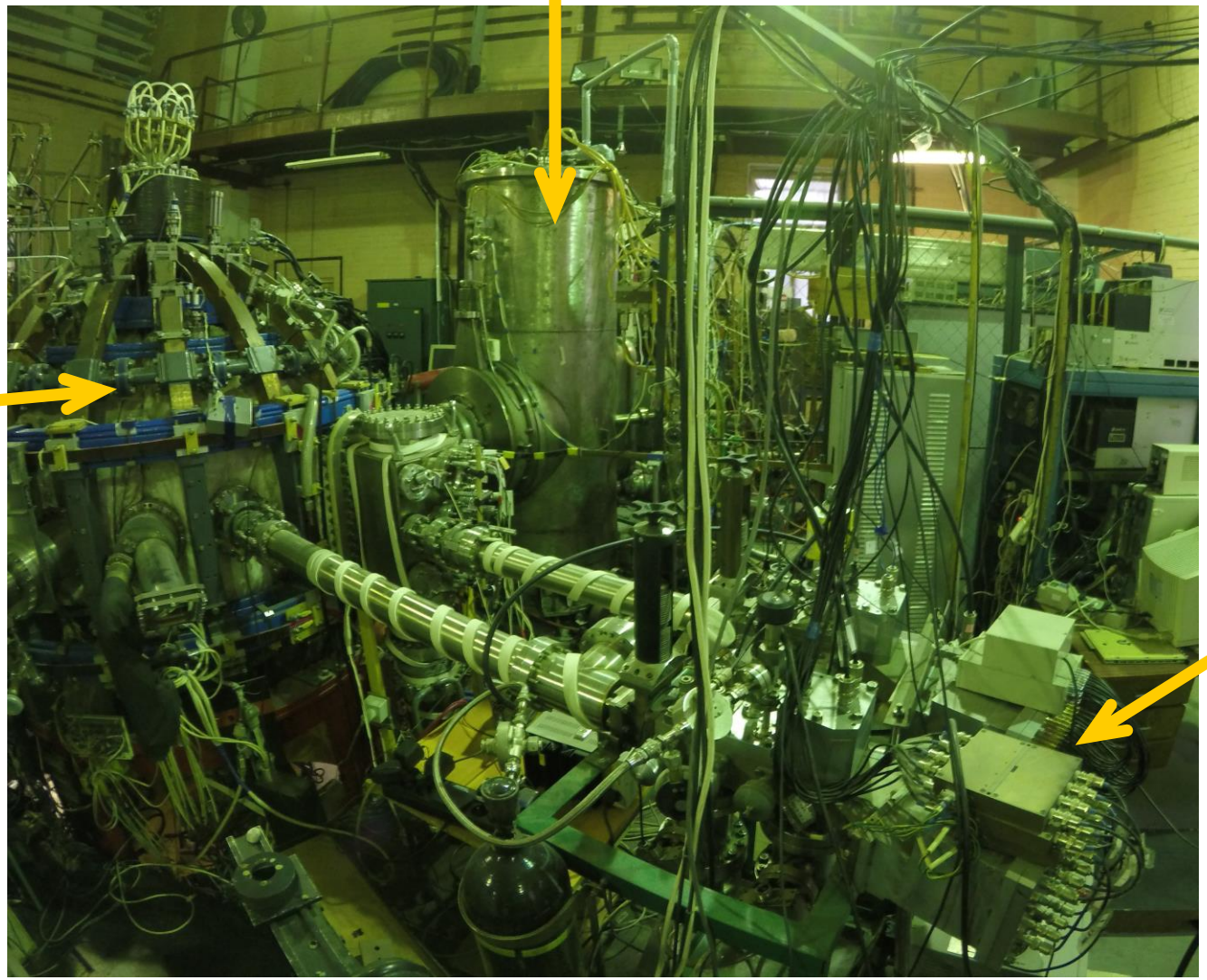
Problem	Task	Publication	Processes	Data Source	Data Needs
Numerical modelling and measurements of the ion distribution function on Globus-M and ITER	Calculations of penetration of heating and diagnostic neutral beams into plasma. Formation of the flux of escaping fast neutral atoms.	*N.N. Bakharev et al.* ***Nucl. Fusion 55*** *(2015) 043023* *V.G. Nesenevich et al.* ***Plasma Phys. Control. Fusion 56*** *(2014) 125002*	Charge changing reactions involving **H, D, T**	*R.K. Janev et al.* ***Nucl. Fusion 29*** *(1989) 2125-2140* *S. Suzuki et al.* ***Plasma Phys. Control. Fusion 40*** *(1998) 2097–2111* *R.K. Janev et al., Eds.* ***ATOMIC AND PMI DATA FOR FUSION****, Suppl. to Nucl. Fusion (IAEA 'green books')* *and other published data*	

Ioffe Institute

POLYTECH
Peter the Great St.Petersburg Polytechnic University

Neutral Beam Injector

Globus-M Spherical Tokamak

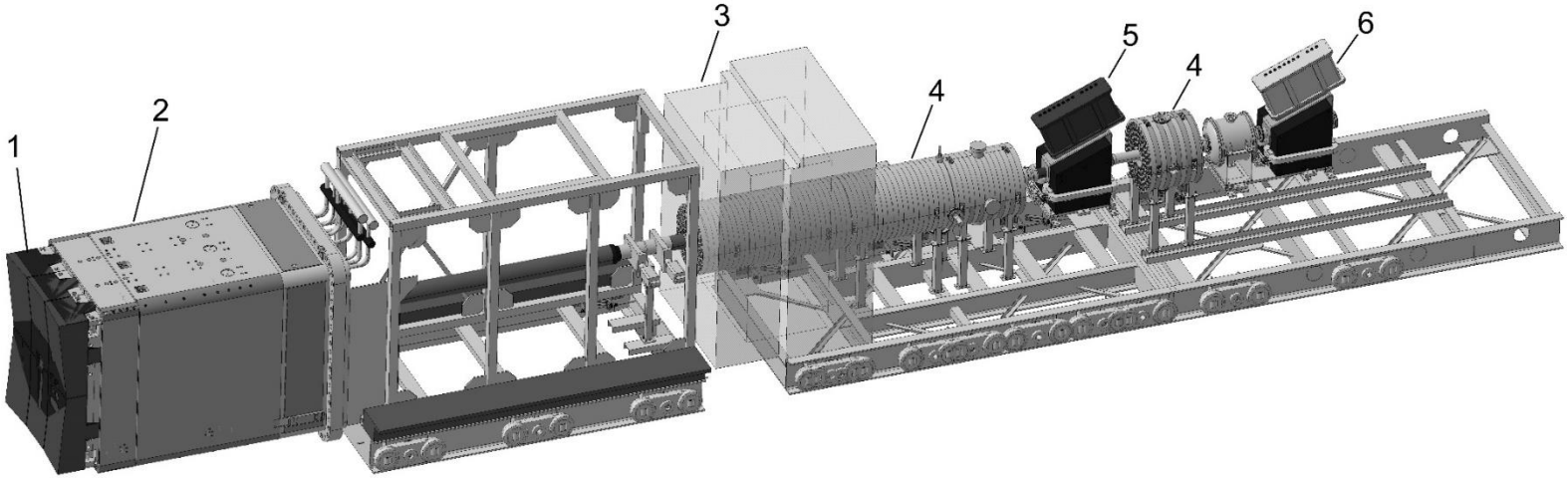


Neutral Particle Analyzers

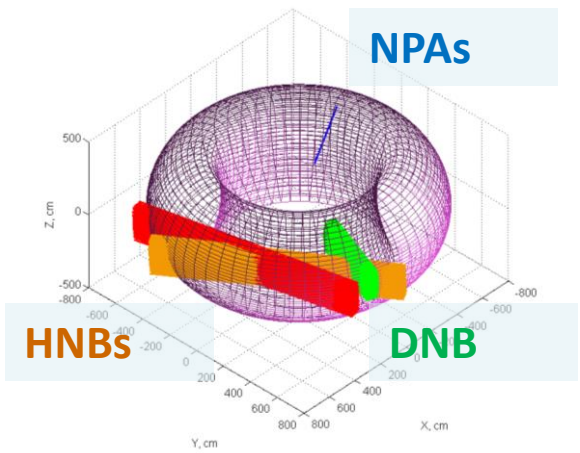
V.K. Gusev et al. ***Nucl. Fusion 55*** *(2015) 104016*

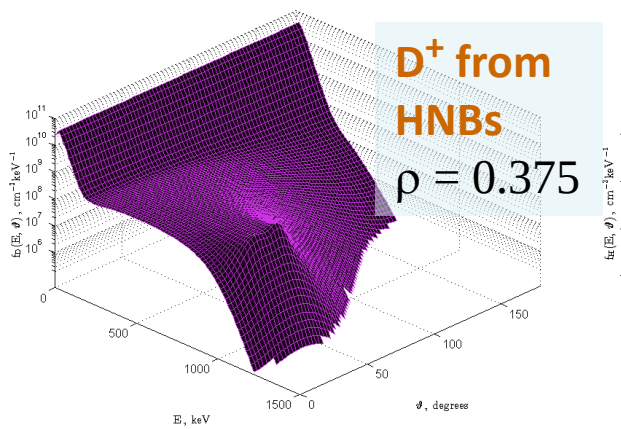
LENPA and HENPA on ITER

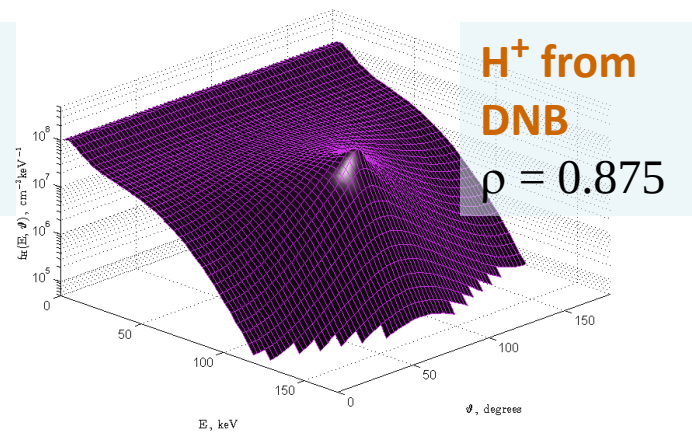
- Design and manufacturing by A.F. Ioffe Institute, numerical modelling by Peter the Great Polytechnic University



1 – equatorial port 11; ***2*** – blanket; ***3*** – bioshield; ***4*** – neutron shield; ***5*** – HENPA; ***6*** – LENPA







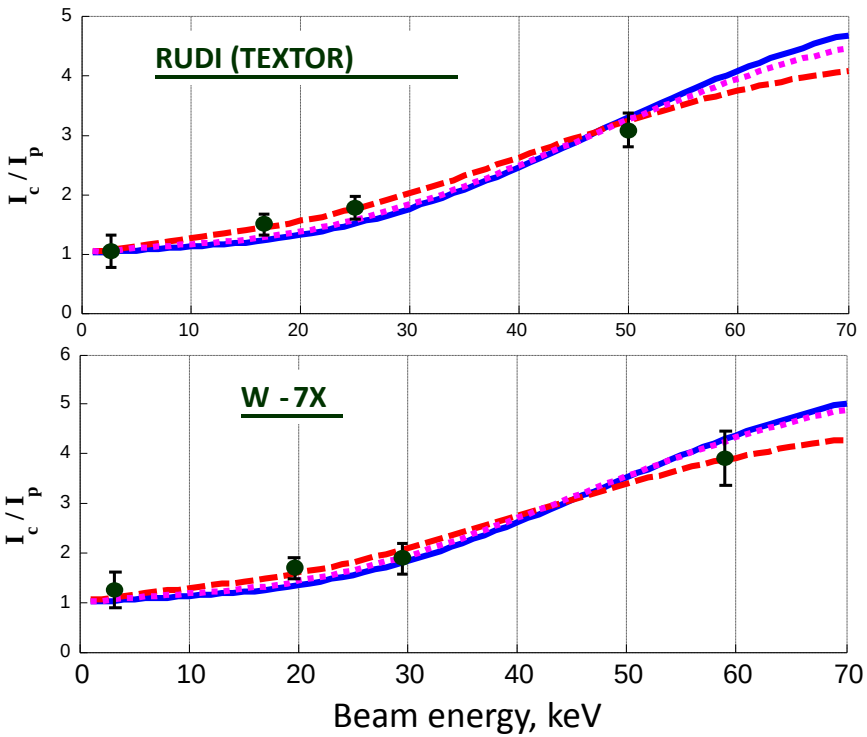
V.G. Nesenevich et al. ***Plasma Phys. Rep. 41*** *(2015) 1062-1068, in press*

Problem	Task	Publication	Processes	Data Source	Data Needs
Doppler-shift measurements of NB species content	Study of influence of l-mixing of hydrogen n=3 level population to interpretation of DSS measurements	S.V. Polosatkin **J. Instrum. 8** (2013) P05007 S.V. Polosatkin et al. **Rev. Sci. Instrum. 85** (2014) 02A707	$H+H_2 \rightarrow H^*+H_2$ $H+H_2 \rightarrow H^*+H^+_2$	ALADDIN ORNL-6086	Sublevel-resolved cross-sections of hydrogen excitation in collisions with H_2

e-mail:s.v.polosatkin@inp.nsk.su

L-Mixing Effects in Hydrogen Neutral Beams Emission

- **Doppler-shift spectroscopy (DSS) is a routine tool for measuring species content in the hydrogen neutral beams for fusion**
- **Interpretation of DSS measurements depends on excitation cross-sections and de-excitation branching ratios**
- **Several weak effects can cause L-mixing of n=3 sublevels that result in changes of DSS correction factors**
- **Model of sublevel population was studied by the measuring of a ratio of H_α intensities w/ and w/o separating magnet in the NB injectors of TEXTOR and W-7X**



Models:

solid – no L-mixing

dashed – moderate L-mixing *(3s-3p transition)*

doted – strong L-mixing *(thermal equilibrium between 3s, 3p, and 3d)*

Points – experimental measurements

Comparison of experimental data with model calculation points out that traditional coronal model of sublevel population must be rejected on the significance level 10%

3. Plasma-material interaction data generation and use in magnetic confinement fusion research centres

- A comprehensive review of PMI activity in RF was done by V. Kurnaev at the 18th Russian Conference on Plasma-Surface Interaction in Moscow.
- This review and a number of other results presented at this conference have been published in **Physics Procedia,** vol. **71** (2015).

Modelling and Calculations

Processes	Method	Data Source \ Code	Publication	Verification / Application	Problem
Vapor Shielding of Solid Targets Exposed to High Heat Flux	Analytical models	Experimental results on QSPA device	*A.A. Pshenov et al.* ***Physics Procedia 71*** *(2015) 14–19*	Experiments at QSPA	Erosion of materials under high heat loads
The Role of the Adatom Diffusion in the Tungsten Fuzz Growth	Analytical models, MD calculations	Baldwin et al. Nucl. Fusion 48 (2008) 035001/ LAMMPS	*D. Trufanov et al.* ***Physics Procedia 71*** *(2015) 20–24*	Experiments at PISCES-B	Mechanism of fuzz growth on tungsten surface under He irradiation
Modelling of Charged Particle Dynamics in the Sheath and Plasma-facing Surface Sputtering	Analytical model, computer simulation	PIC code SPICE2	*I.E. Borodkina et al.* ***Physics Procedia 71*** *(2015) 25–29*		Influence of oblique magnetic field on sheath structure and the first wall irradiation
Ab-initio Simulation of Hydrogen Atom Interaction with Tungsten	DFT modelling		*N. Degtyarenko et al.* ***Physics Procedia 71*** *(2015) 30–34*		Definition of parameters characterizing hydrogen isotope retention and transport in materials

Experiments

Processes	Method	Data Source \ Code	Publication	Verification / Application	Problem
Radiation damage of tungsten and new generation of low-activated steels and their influence on the deuterium retention	Experiment, analytical model and numerical code		*O.V. Ogorodnikova et al.* ***Physics Procedia 71*** *(2015) 41-46* *O.V. Ogorodnikova et al.* ***J. Nucl. Mater. 460*** *(2015) 60-71* *Yu.M. Gasparyan et al.* ***J. Nucl. Mater. 463*** *(2015) 1013-1016* *O.V. Ogorodnikova* ***J. Appl. Phys. 118*** *(2015) 074902* *Y. Hatano et al.* ***Fusion Sci. Technol. 67*** *(2015) 361-364* *O.V. Ogorodnikova et al.* ***J. Nucl. Mater. 442*** *(2013) 518-527* *O.V. Ogorodnikova et al.* ***J. Nucl. Mater. 415*** *(2011) S661-S666*	Experiment and model of D retention dependence on the ion energy, and ion flux. Validation of DFT predictions of multiple occupation of traps.	Deuterium retention in a presence of high density of defects in W and ODS steels under plasma exposure, predictions of the fuel retention in ITER and DEMO.
Interaction of Li-D Films with Water Vapor	Experiment (TDS)		*A.S. Popkov et al.* ***Physics Procedia 71*** *(2015)* 88-92 *S.A. Krat et al.* ***Vacuum 105*** *(2014) 111-114*	Low temperature removal of D from Li films in the presence of water.	Hydrogen isotopes removal from lithium.

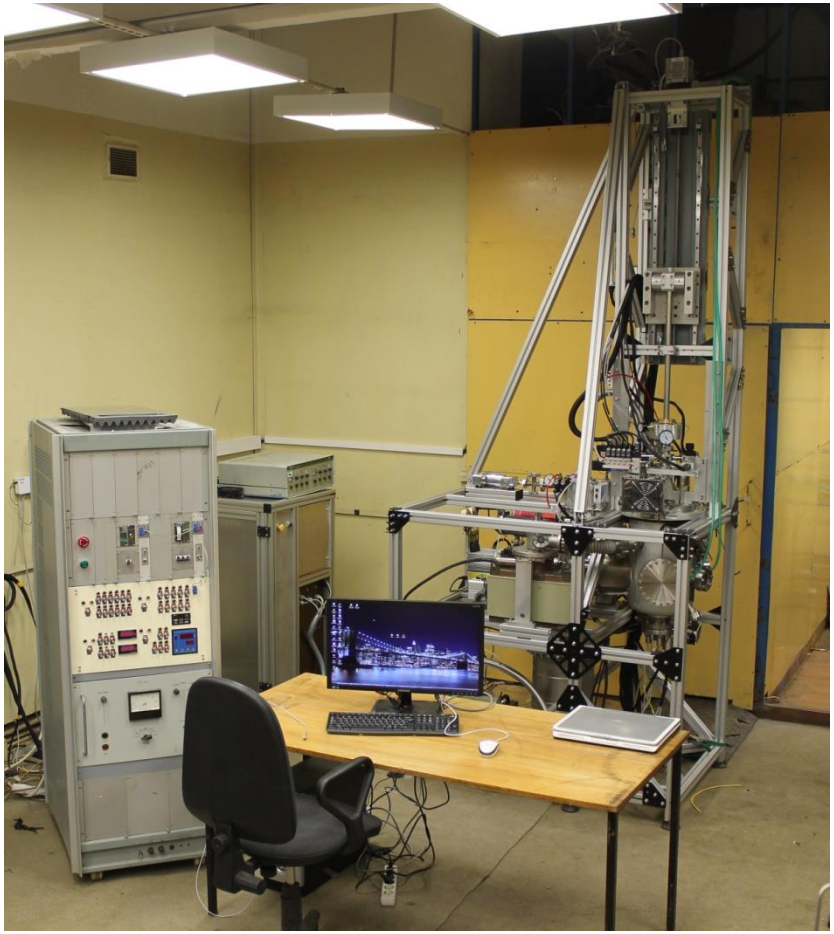
Experiments (continued)

Processes	Method	Data Source \ Code	Publication	Verification / Application	Problem
Surface Processes and Hydrogen Transport through the Stainless Steel Surface Under Atom and Ion Irradiation	Experiment: irradiation of vacuum chamber wall surface with D, O atoms and/or ions		*O. Dvoichenkova et al.* ***Physics Procedia 71*** *(2015) 93–98* *L. B. Begrambekov et al.* ***J. Surf. Inv. X-ray, Sync. Neut. Tech. 9*** *(2015) 190–195*	Laboratory plasma devices, fusion research	Outgassing of metal surface under low temperatures
Plasma Influence on Tungsten Powder	Experiment	*J. Ma et al.* ***J. Nucl. Mater. 438*** *(2013) 199–203*	*A. Zakharov et al.* ***Physics Procedia 71*** *(2015) 99–104* *L. Begrambekov et al.* ***Nucl. Instrum. Meth. Phys. Res. Sect. B 354*** *(2015) 282-286*	Investigations of dust production and its behavior in fusion devices	Dust production and its influence on the plasma. Dust related hydrogen isotopes retention
Film Deposition and their Removal in Gaps and Regions Shaded from the Plasma in the Presence of RF Fields	Experiment at PR-2 facility with plasma-beam discharge		*K. Gutorov et al.* ***Physics Procedia 71*** *(2015) 68–72*	Removal of CH-films	Hydrogen retention in redeposited films

Processes	Method	Publication	Verification / Application	Problem
Acceleration of vacuum vessel wall outgassing due to simultaneous irradiation with flux of hydrogen and oxygen atoms or ions	Experiment: irradiation of vacuum chamber wall surface with deuterium and oxygen atoms and/or ions	*L. B. Begrambekov et al.* ***J. Surf. Inv. X-ray, Sync. Neut. Tech. 9*** *(2015) 190–195*	Laboratory plasma devices, fusion research	Outgassing of metal surface under low temperatures

Oxygen concentration in D_2+ x % O_2 gas, %	Amount of H released from vacuum vessel walls in 40 min, 10^{21} at/m^2	Amount of D trapped in vacuum vessel walls in 40 min, 10^{21} at/m^2	Ratio $H_{release.}/D_{trapp.}$
0,5	0,6	0,3	2,0
2	1,0	0,5	2,0
10	1,7	0,9	1,9
20	2,0	1,1	1,8
30	2,9	1,5	1,9

The Stand for film deposition and material irradiation



L.B. Begrambekov, E.A. Azizov, O.I. Buzhinsky et al. ***Proc. 25th IAEA Fusion Energy Conf.*** *(2014), MPT/P4-17*

The goals of the Stand construction

- Investigation of conditions of boron carbide (**B_4C**) coating deposition on tungsten;
- Testing of materials and thing films under thermal cycles and high power density ion and electron beam irradiation.

The method of B_4C coating deposition

- The B_4C coating is formed on tungsten substrate through deposition of boron and carbon atoms sputtered by plasma ions from boron and carbon targets

The conditions of B_4C deposition

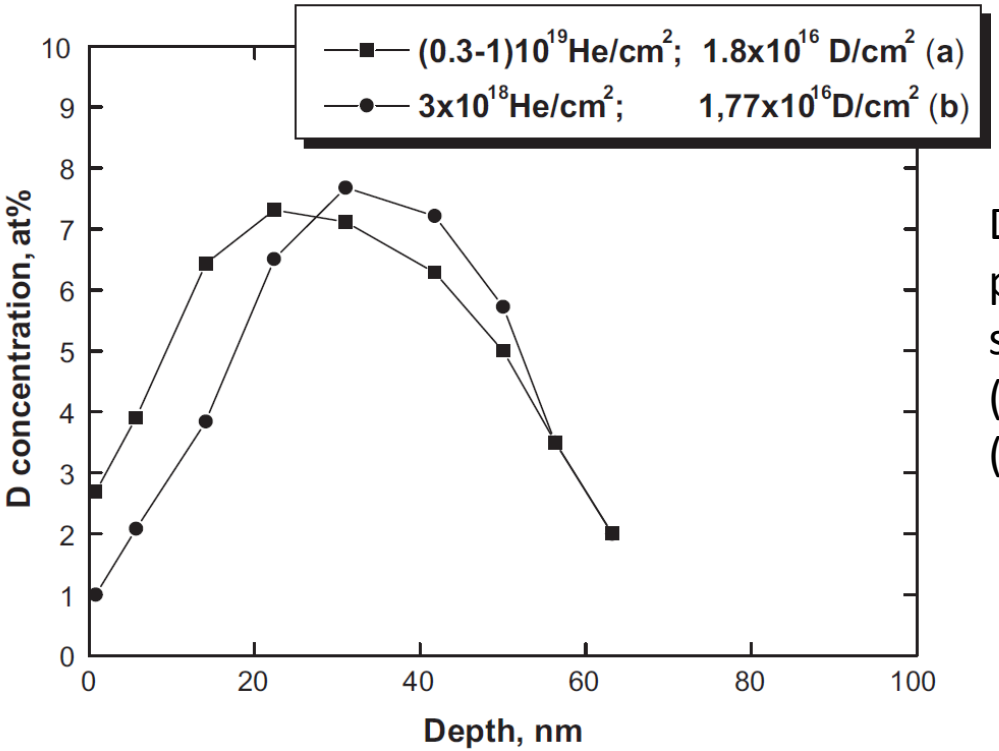
Residual vacuum	$\leq 2\times10^{-8}$ Pa
Energy of sputtering ions	$\leq$ 20 KeV
Current of sputtering ions	$\leq$ 200 mA
Temperature	500 - 900°C

The conditions of high heat load test

Quasy-stationary ion/electron beam with power density	$\leq$ 40 MW/m^2
Testing cycle frequency	$\geq$ 1msec
Temperature of testing material	$\leq$ 2200°C

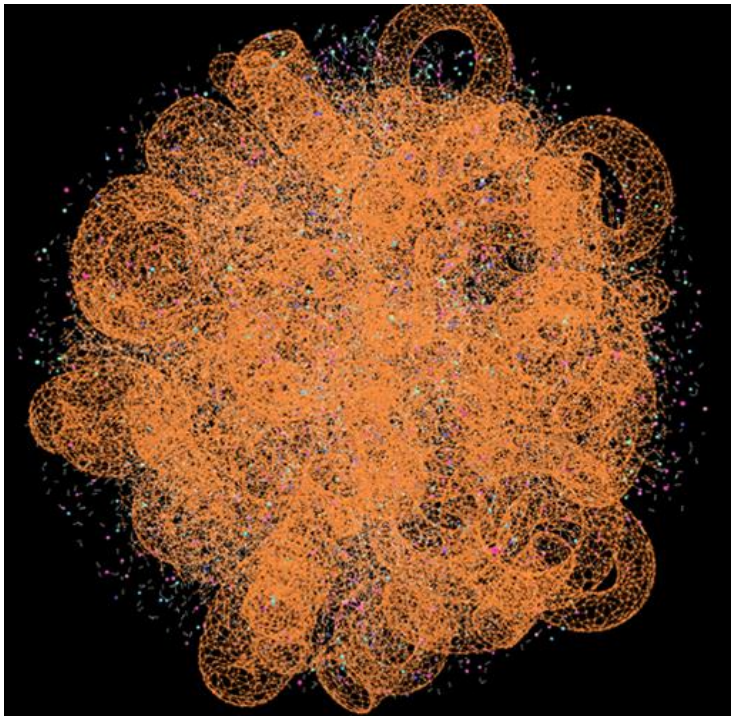
Processes	Method	Data Source \ Code	Publication	Verification / Application	Problem
Sputtering of metals at simultaneous ion and electron irradiation	Experiment and analytical model		*Yu.V. Martynenko et al.* ***JETP Lett. 98*** *(2014) 853-857*		Decrease of sublimation energy and an increase of sputtering due to excitation of surface atoms
Recrystallization and cracking under remelting and heating	Experiment on QSPA and analytical model		*V.P. Budaev et al.* ***J. Nucl. Mater. 463*** *(2015) 237-240*		Tungsten recrystallization and cracking under ITER-relevant heat loads
Motion of molten metal layer and droplet erosion under the influence of plasma flow parallel to metal surface	Analytical model		*Yu. V. Martynenko* ***Problems of Atomic Science and Technology, Thermonucl. Fusion Series, 37*** *(2014), issue 2, pp. 53-59*	Experiments on QSPA in TRINITI	Impact of a plasma flow on metal surfaces under conditions typical for transient regimes in ITER

Processes	Method	Data Source\ Code	Publi-cation	Verification / Application	Problem
Production of damage in plasma facing materials, erosion of damaged materials and hydrogen isotope retention	Experiment and analytical models		*B. Khripunov et al.* ***J. Nucl. Mater. 463*** *(2015) 258-262*	Experiments on Kurchatov Inst. facilities: cyclotron, LENTA linear divertor simulator	Erosion and deuterium retention in ion-irradiated tungsten under plasma exposure



Deuterium concentration in He-irradiated plasma exposed tungsten (RT): 2 dpa at the surface.
(a) Plasma 2.9 10^{21} D+/cm^2 (1.2 μm eroded);
(b) plasma 1.0 10^{21} D+/cm^2 (0.7 μm eroded).

Processes	Method	Data Source \ Code	Publication	Verification / Application	Problem
Clusterization of hydrocarbon and sp^2 carbon molecules	Rigid Body Molecular Dynamics of various molecules, including flat and curved sp^2 carbon molecules	*L.A. Chernozatonskii, **Phys. Lett. A 170** (1992) 37-40* *J.D. Gale et al. **Mol. Simul. 29** (2003) 291-341*	*V.S. Neverov et al. **Phys. At. Nuclei 78** (2015) 38-45, in press*	Characterization of big carbon molecules and their agglomerates in the hydrocarbon film deposits in tokamak T-10	Diagnostics of deposits (particles and films) in fusion facilities

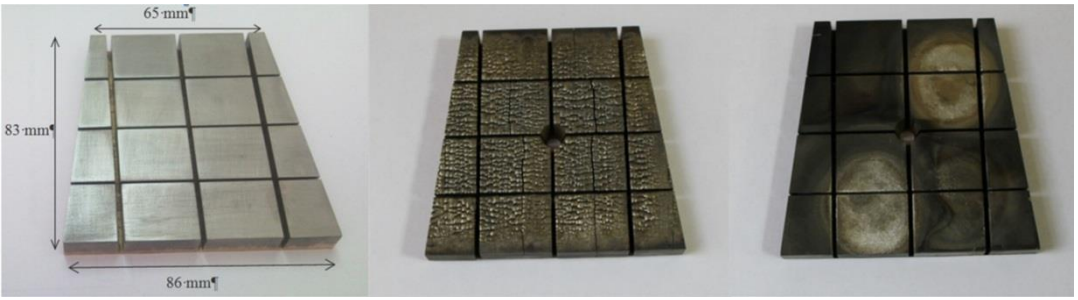


Model sample of 84 500 atoms after the MD simulation for variable packing of molecules in the film deposit in tokamak T-10. The average mass density of 1.1 g/cm^3 (the density in the central part is higher).
Hydrocarbon component: $C(D, H)_4$ (60%), $C_2(D, H)_4$ (30%), $C_6(D, H)_6$ (10%).
The carbon molecules content is taken from [Chem. Phys. Lett., 506, 265 (2011)] (inverse-problem-based recovery from high-resolution X-Ray Diffraction data): fullerenes, nanotubes, toroidal nanotubes.
Carbon (orange), hydrogen (grey), heavy impurities (other colours)

Process	Method	Data Source / Code	Publications	Verification / Application	Problem
Interaction of Hydrogen, Deuterium and Helium plasma with Tungsten	Scanning Electron Microscopy (SEM), Secondary Ion Mass Spectrometry (SIMS), Roentgen structural analysis (RSA), spectral analysis	Globus-M spherical tokamak, coaxial plasma gun	*A.V. Voronin et al.* ***Tech. Phys. Lett. 40*** *(2014) 1146-1149* *A.V. Voronin et al.* ***Tech. Phys. 59*** *(2014) 981-988* *A.V. Ankudinov et al.* ***Tech. Phys. 59*** *(2014) pp. 346-352* *V.K. Gusev et al.* ***Nucl. Fusion 55*** *(2015) 104016* *A.V. Voronin et al.* ***Tech. Phys. 61*** *(2016), in press*	Aimed at collecting a database on the behavior of tungsten exposed to hot plasma	Divertor and first wall of magnetic confinement fusion devices

Materials

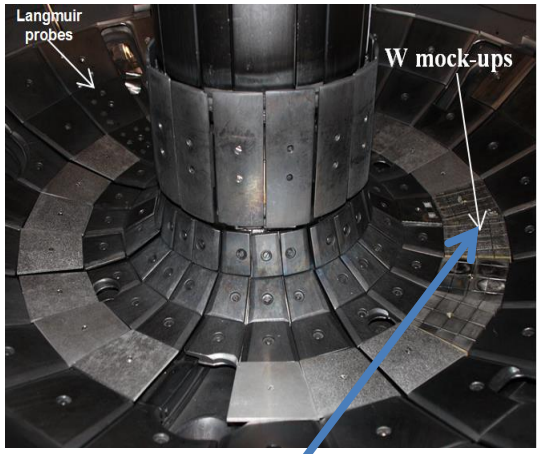
ITER-like tungsten tiles were installed in the divertor region



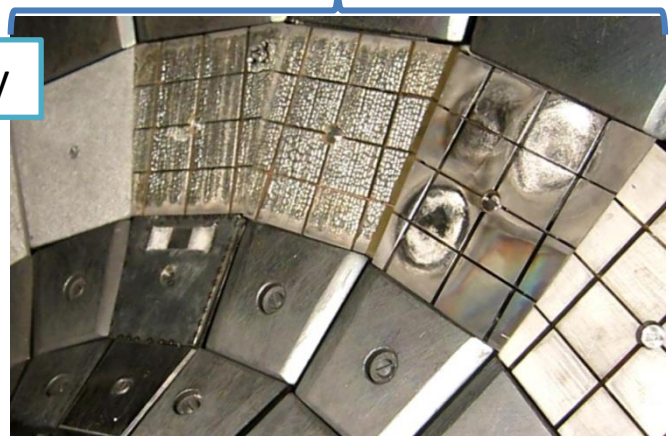
undamaged

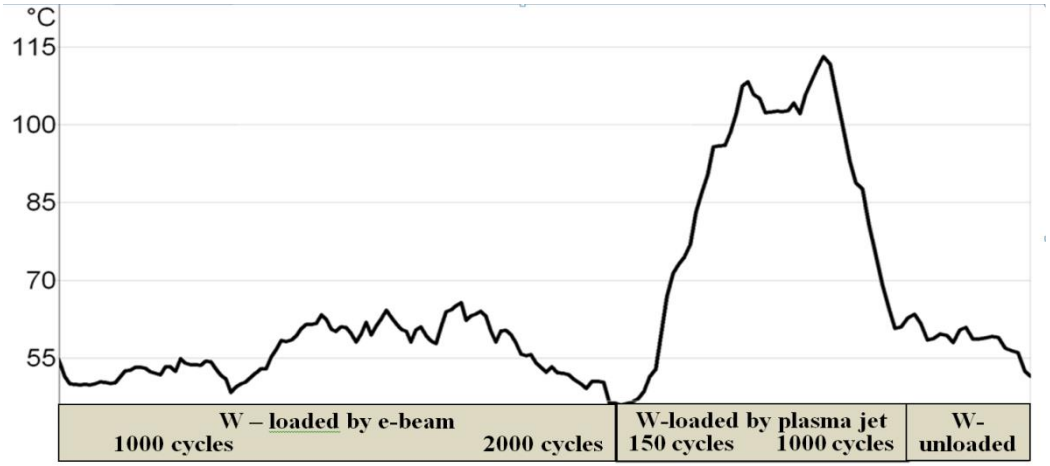
electron beam
1000/2000 pulses

plasma gun
150/1000 pulses



tiles damaged by the plasma gun were heated significantly





[Voronin A.V. et al. *TPL* 40 (2014) No 24]

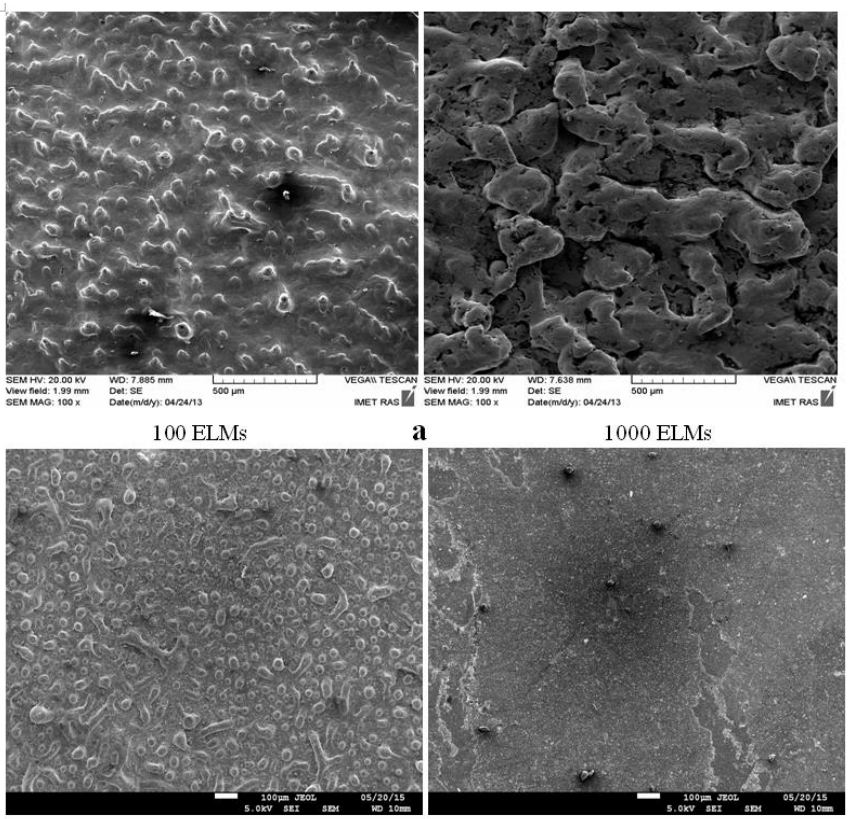
Materials

After 2370 pulses of Globus-M (total duration ~ 200 s) samples were taken out for analysis.

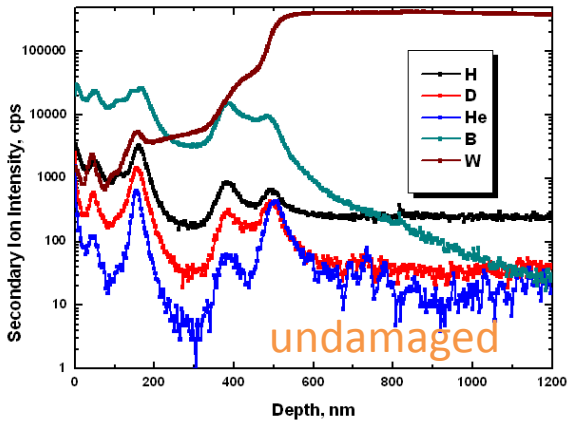
SEM images of the surface

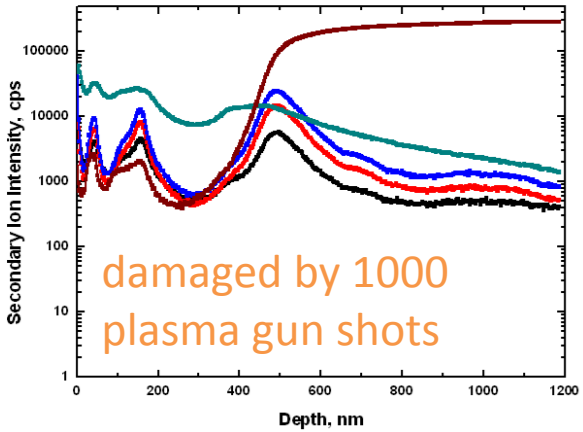
before

after



SIMS in-depth profiles of the elements





W did not change plasma performance in Globus-M

P5-175 A.V. Voronin et al. Experimental studies of cyclical plasma effects on tungsten

Chemical element accumulation is greater in the damaged sample

G.I. Budker Institute of Nuclear Physics, Novosobirsk A.S. Arakcheev et al.

Processes	Method	Data Source \ Code	Publication	Verification / Application	Problem
Crack formation on tungsten after pulsed heat load	Analytic model, experimental verification		A.S. Arakcheev et al. **J. Nucl. Mater. 463** (2015) 246-249 A.S. Arakcheev et al. **J. Nucl. Mater. 467** (2015) 165-171	Compared with laser and e-beam-based divertor ELM simulaton experiment	

Conclusions on A+M Data

- **The use of A-M data covers both the recognized databases (IAEA AMDU Databases, NIST, ADAS) and newly generated data.**

- **The results of simulations by the suites of codes, like B2-EIRENE (SOLPS-ITER), for reference scenarios of ITER operation have become a database widely used by ITER component designers.**

- **New A+M data may come from semi-analytic models for arising complicated problems (e.g. elementary process rates for many-electron, heavy-impurity atom and ions like, e.g., W in ITER) where the direct numerical modeling is either too cumbersome for providing the extensive databases or not very reliable for partially simplified simulation.**

Conclusions on PMI Data

- **The use of available PMI data, as a rule, assumes interpolation and/or extrapolation because of much less universality compared to A+M data.**

- **Generation of PMI data is rapidly growing along many lines. The benchmarking is more complicated compared to that for A+M data, however, is feasible for critical problems, e.g. melting of tungsten tiles.**

- **Experiments emulating ITER conditions (heat load, sputtering, etc.) seem to be the major line.**