資料9

平成19年2月21日

原子分子データ活動に関する研究会

航空会館

NIFSにおける原子分子データ活動

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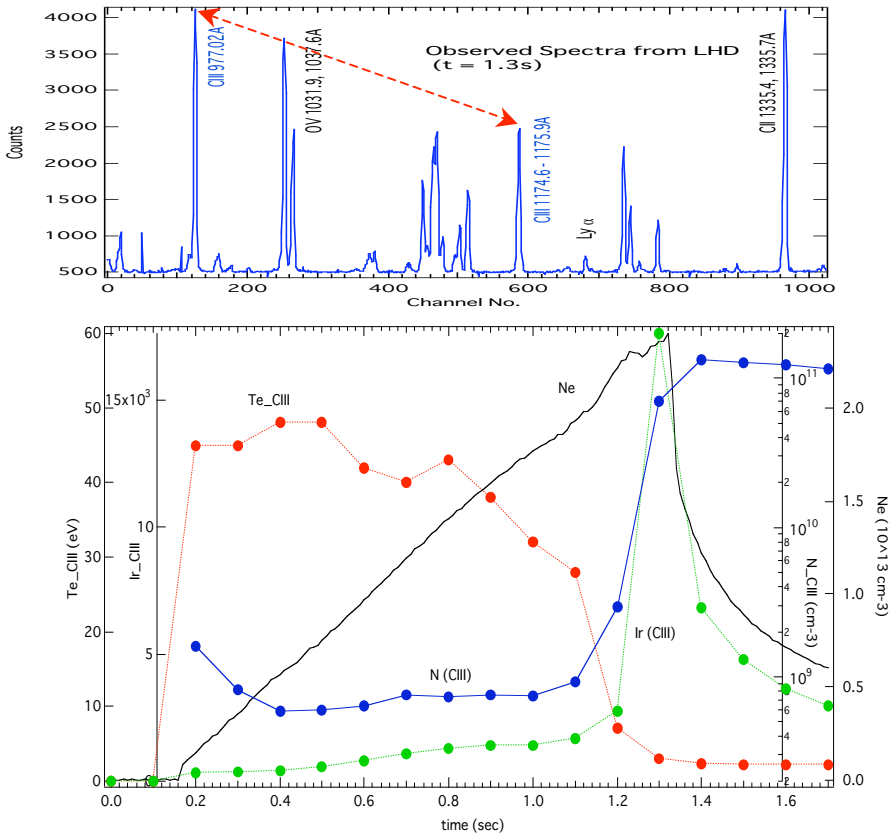
イオンのライン強度比を用いた非平衡プラズマ診断
（電子温度，電子／イオン密度など）

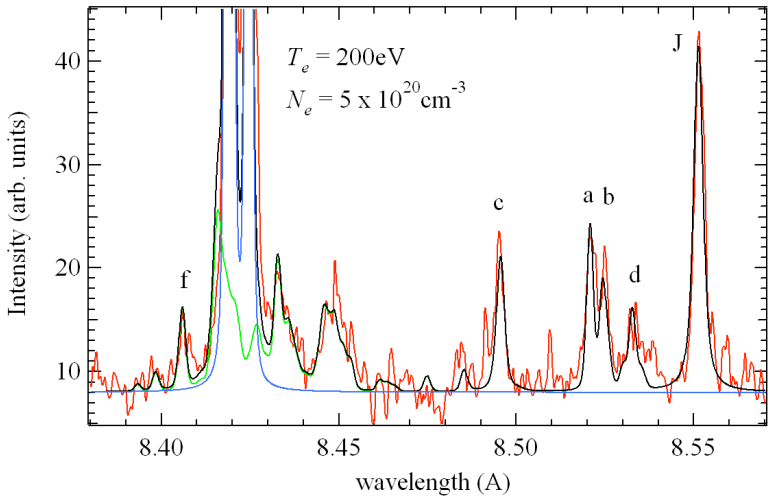
- **LHD** (Divertor plasma)



Time variation of electron temperature was derived from intensity ratios of CIII ($2s^2\ ^1S - 2s2p\ ^1P$, 977A / $2s2p\ ^3P - 2p^2\ ^3P$, 1175 A). Time variation of CIII density was obtained.

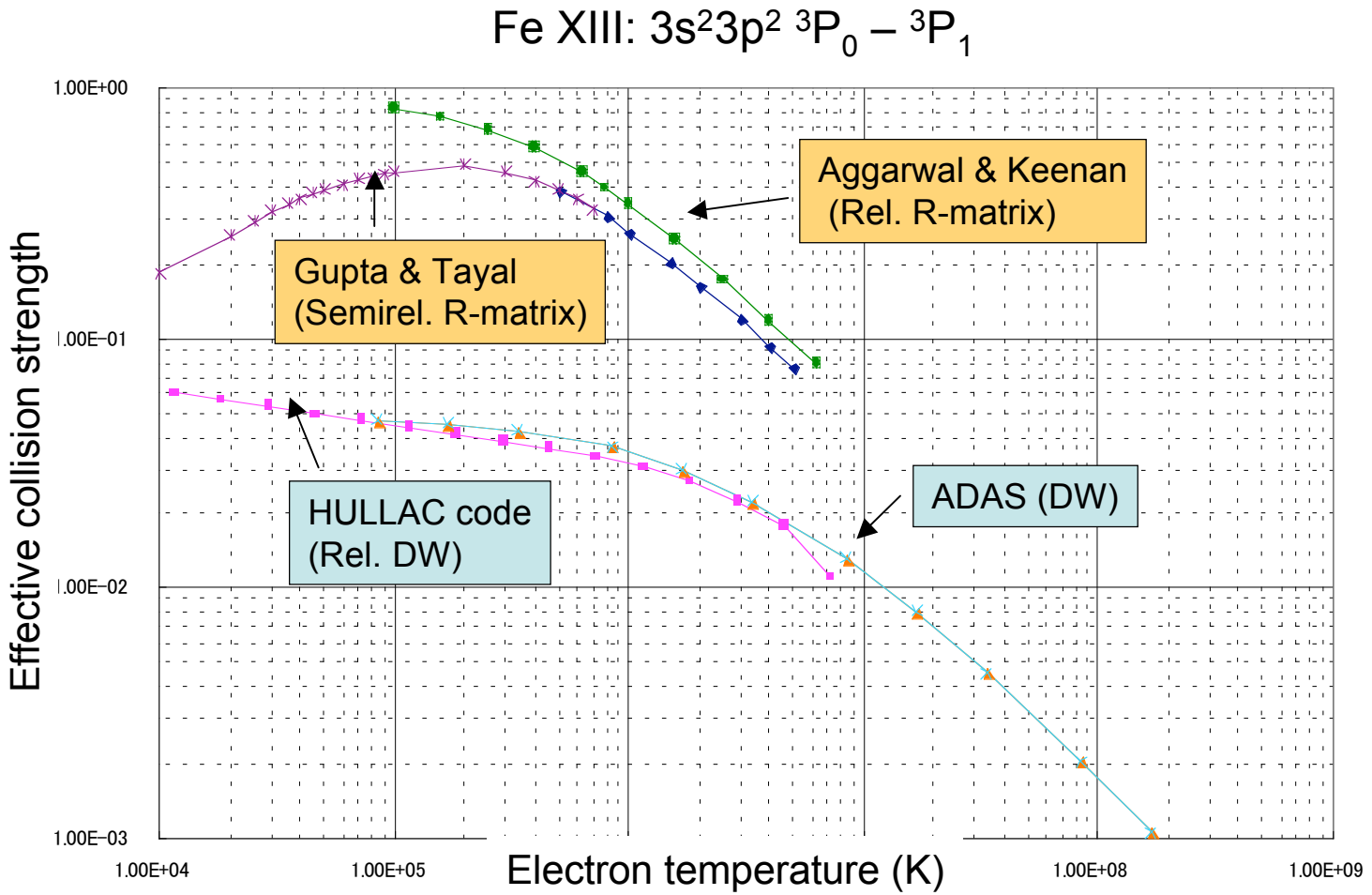
- **Laser produced plasma**

Collisional-Radiative Model (CRM) including doubly excited states



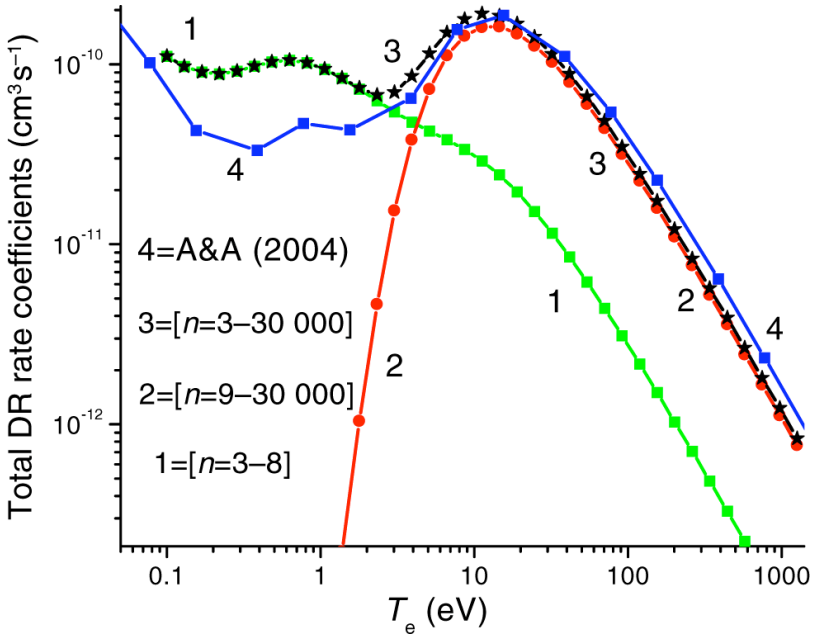
X-ray spectrum of Mg ions: Experiment (red line) and CRM. (black line:total, green line: satellite lines, blue line: Lya lines)
T_e = 200 eV and N_e = 5x10^{20}cm^{-3} were derived from spectral fit.

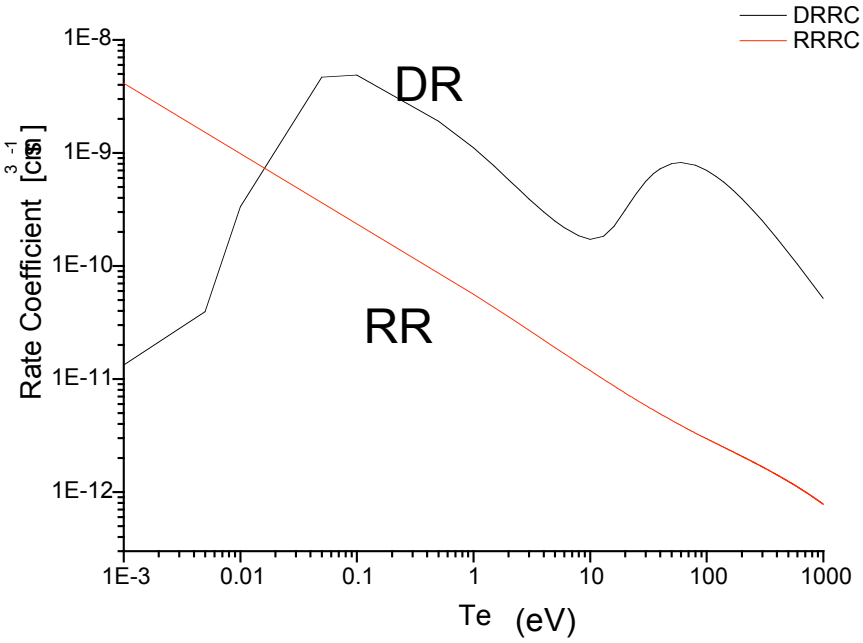
LHDにおける重元素不純物イオンの電子衝突励起速度係数の評価



LHDで計測されたEUV領域(195-210 A)の3p-3d遷移のライン強度比の解析に用いられる.

原子過程コードを用いた再結合速度係数のab initio計算
（C, O, Ne, Fe, Xe イオン）





O IVの2電子性再結合（DR）の電子温度依存性.
$O^{3+}(2s^22p) + e \rightarrow O^{2+**}(2s2p^2nl + 2p^3nl)$
$\rightarrow O^{2+*}(2s^22pnl + 2s2p^3 + 2p^4 + 2s2p^23l) + hv.$

Xe XIの2電子性再結合（DR）と放射性再結合（RR）の電子温度依存性.
$Xe^{10+}(4d^8) + e \rightarrow Xe^{9+}.$

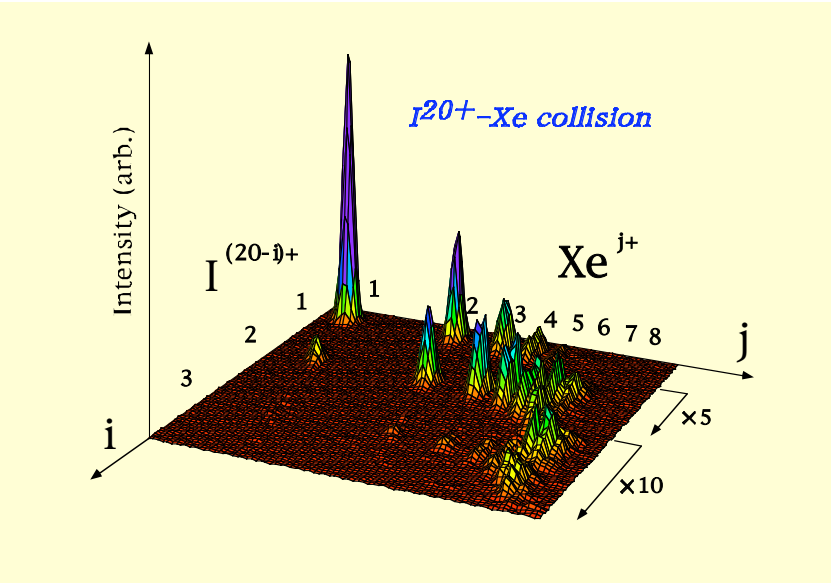
U I Safronova, Yu Ralchenko, I Murakami, T Kato and D Kato,
Phys. Scr. 73 (2006) 143.

多価イオン－原子衝突での電子捕獲断面積の系統的測定とスケーリング則の研究 （超伝導多価イオン源NICE）

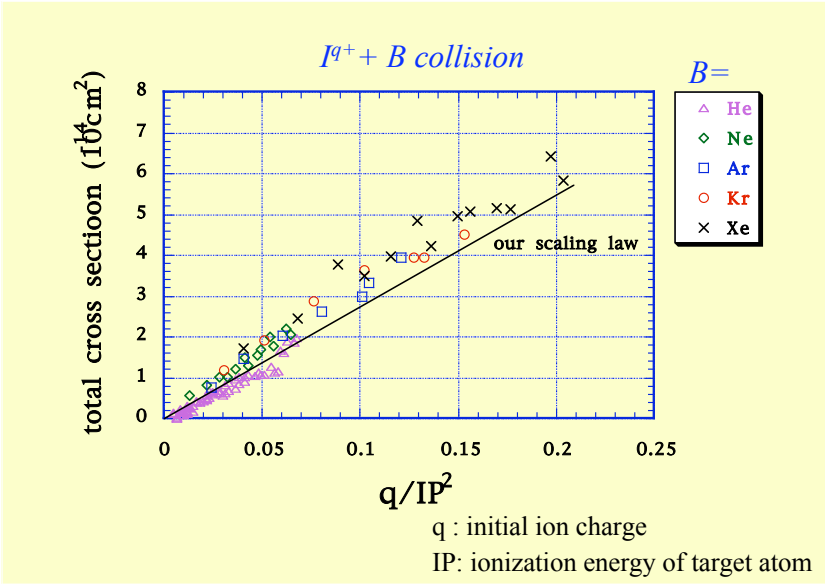
Collaborators:
N. Nakamura, S. Ohtani (UEC) etc.

$$A^{q+} + B \rightarrow A^{(q-j)+**\cdots}(n,n',\cdots) + B^{j+}$$
$$\rightarrow A^{(q-i)+} + B^{j+} + (j-i)e^- + h\nu + h\nu' + \cdots$$

5≤q≤30
A: I
B: He,Ne, Ar, Kr, Xe



Typical coincidence spectrum for the charge state distributions between the product ions and the recoil ions in I^{20+}+Xe collisions.



q : initial ion charge
IP: ionization energy of target atom

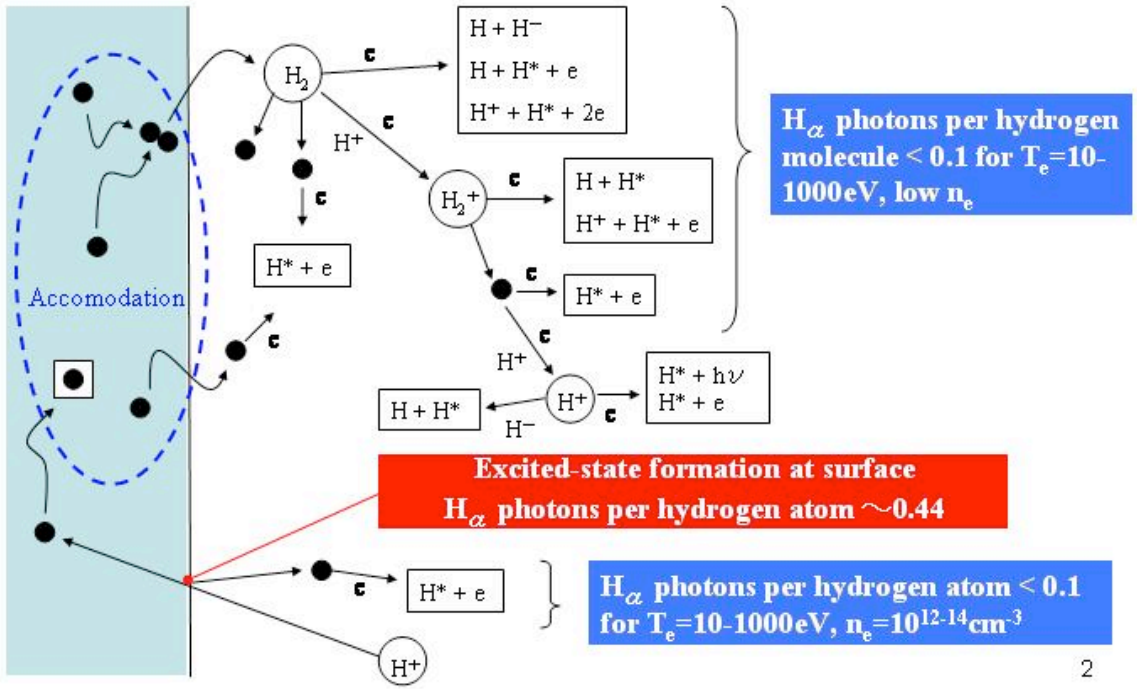
Total electron transfer cross sections scaled by q/IP^2.The solid line represents the our scaling law.

- **The electron transfer processes of up to eight electrons (j=8) were clearly observed.**
- **The absolute total electron transfer cross section σ_q , partial cross section σ_q^j and $\sigma_{q,q-i}^j$, and the branching ratios of decay processes were experimentally determined.**
- **We proposed a simple scaling law for the electron transfer cross sections systematically.**

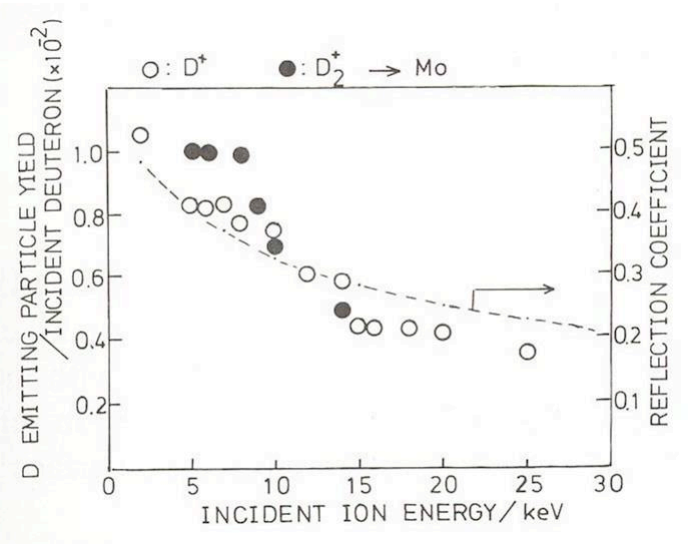
$$\sigma_q = 2.6 \times 10^{-13} \cdot q/IP^2 (cm^2)$$

q : initial ion charge
IP: ionization energy of target atom

Excited state formation and H_α emission above refractory metal surface



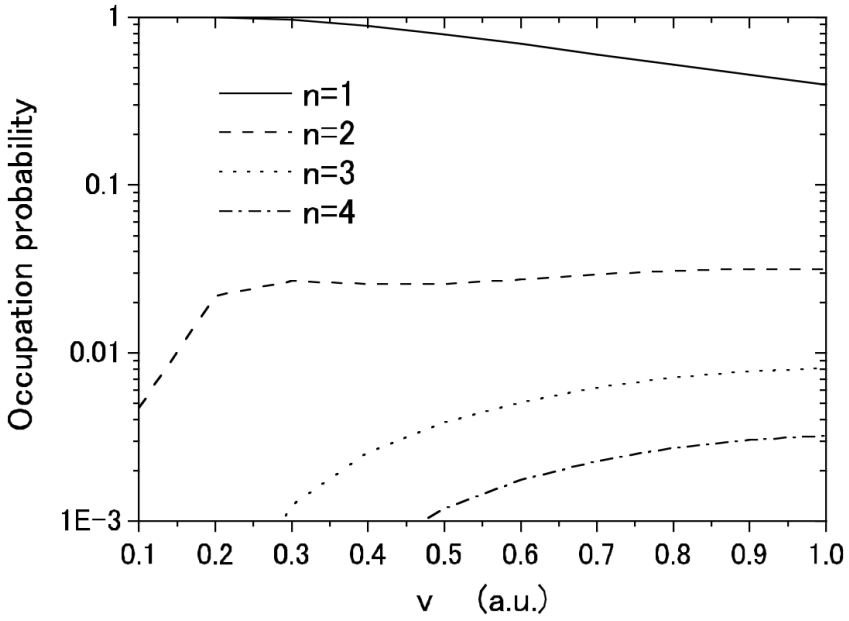
D_α (656.1 nm) emission from high energy neutrals of a deuteron beam reflected at Mo surfaces



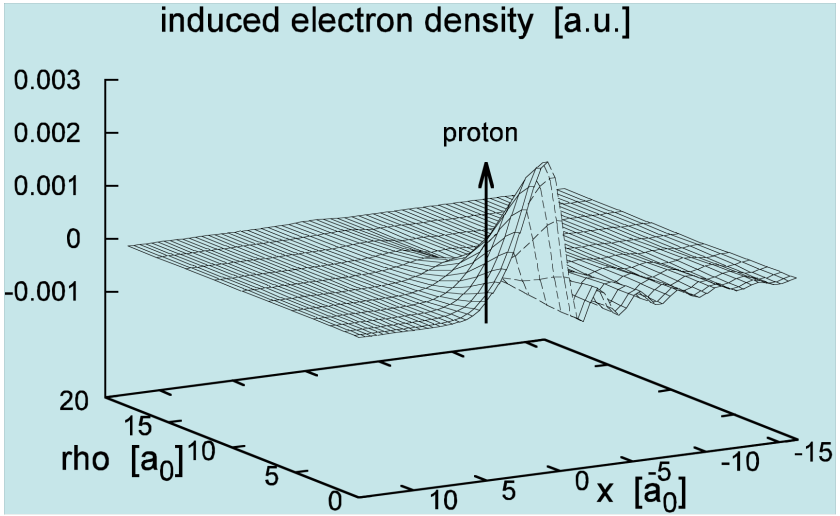
T. Tanabe et al.; J. Nucl. Mater. 220-222 (1995) 841.

- **One excited H atom would emit more photons than one H atom at the ground state in boundary plasmas.**
- **Excited states would be ionized before reaching a core plasma boundary; Less charge-exchange neutral particle loss.**
- **Excited states in sputtered particles (*e.g.* Be), H^- formation in NBI source, ionization/excitation of He ash at PFM surfaces are also to be studied.**

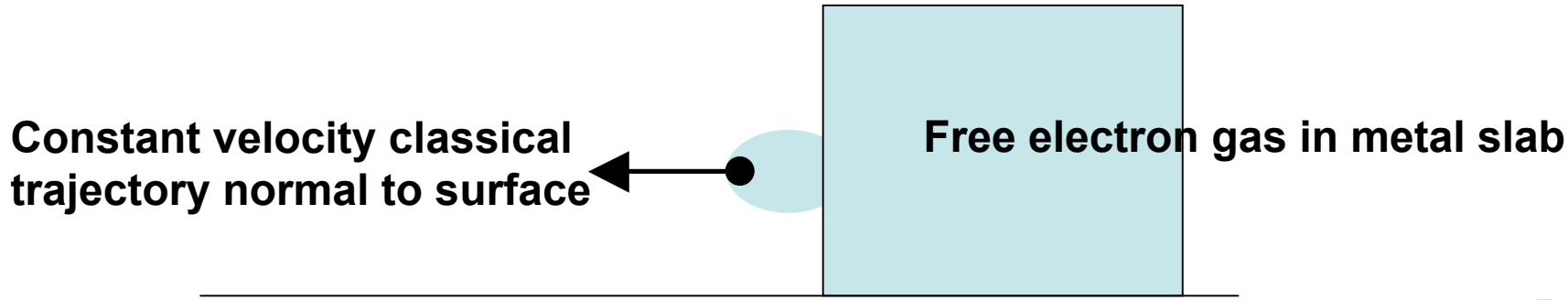
Semi-classical and quantum statistical calculations of electron transfer to excited atomic levels at metal surface



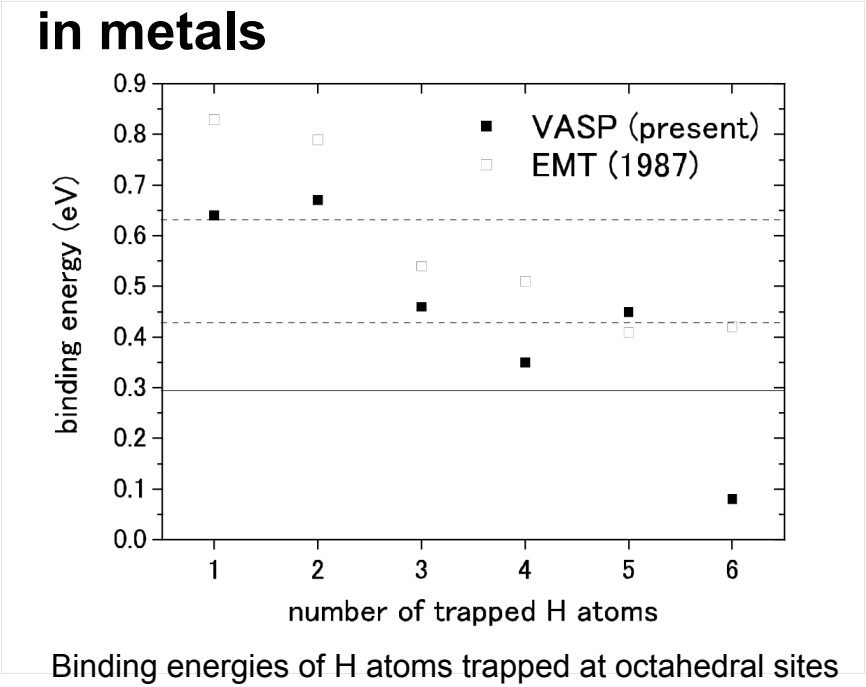
Level occupation of atomic hydrogen emitted from tungsten surface. 1D model calculation.



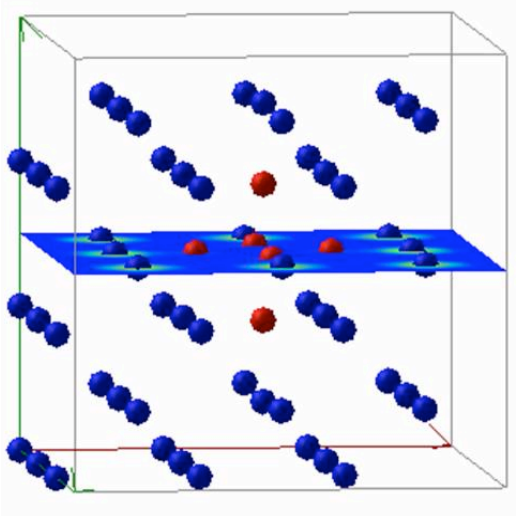
Dielectric response of the electron gas for tungsten. Random phase approximation of linear density response theory. Proton is placed at 5 a.u. above the tungsten surface.



Ab initio study on atomic structures of vacancy-hydrogen clusters in metals



Binding energies of H atoms trapped at octahedral sites around a mono-vacancy in ferritic iron (bcc). Dotted lines are deduced from experimentally observed hydrogen retention. Solid line stands for solution energy of interstitial H atom (tetrahedral-site). □: effective medium theory (EMT).



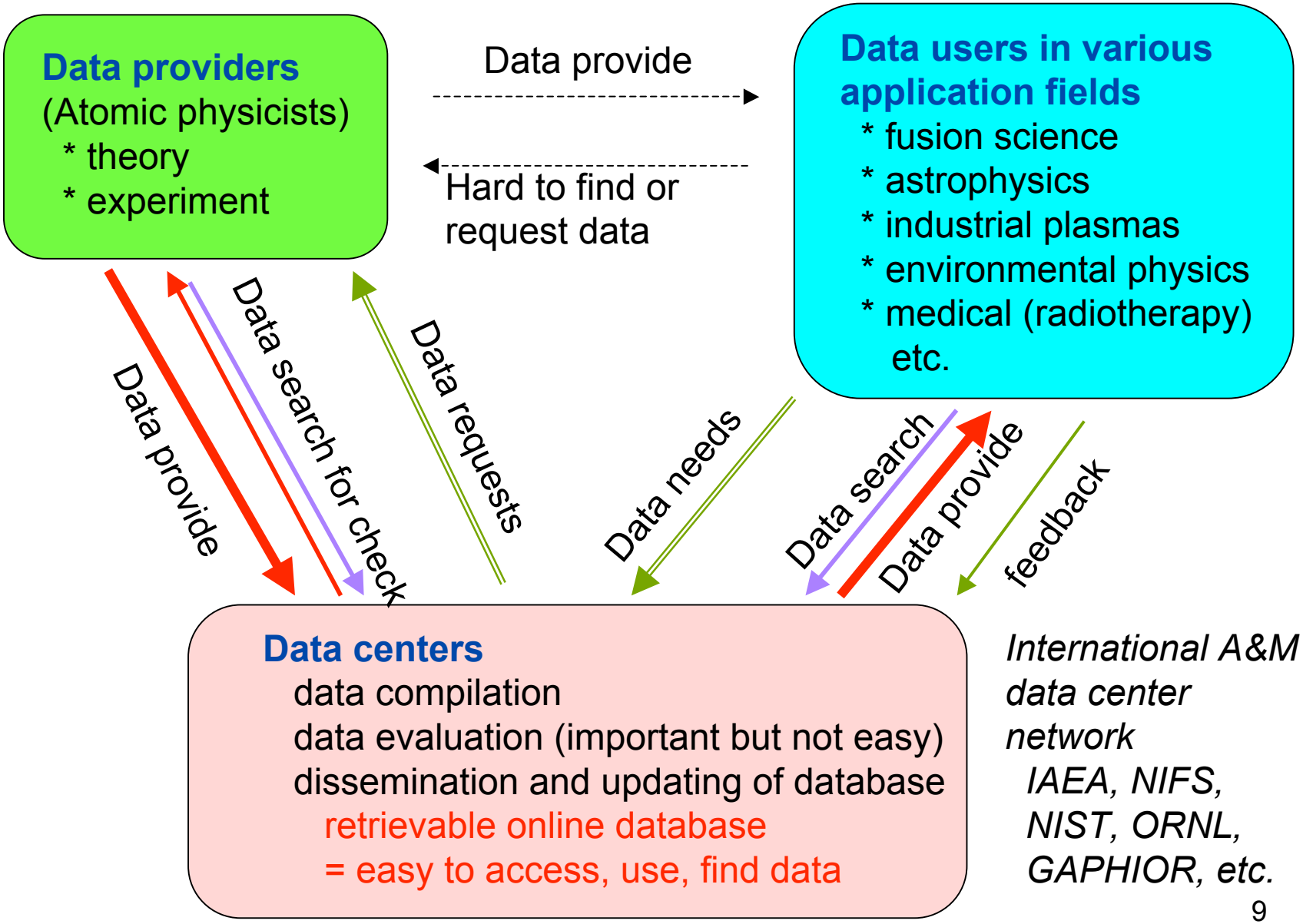
Atomic structure of mono vacancy-hydrogen cluster in ferritic iron. Blue: Fe atoms, Red: H atoms.

•Modeling hydrogen cluster, bubble and hydride formation is important concerning hydrogen retention and embrittlement of metals.

•First principle molecular dynamics was used to study atomic structures of mono vacancy-hydrogen clusters in ferritic iron and tungsten.

•Present *ab initio* calculation favors a conjecture that hydrogen trapping observed at ion-beam experiments is due to mono vacancy-hydrogen cluster formation for irons.

Views from Database *assessed data on AM collision cross sections*



International A&M data center network
IAEA, NIFS, NIST, ORNL, GAPHIOR, etc.

Data compilation

We compile atomic and molecular data with help of working groups of atomic physicists from Japanese universities. Some of compiled data were published as NIFS-DATA series.

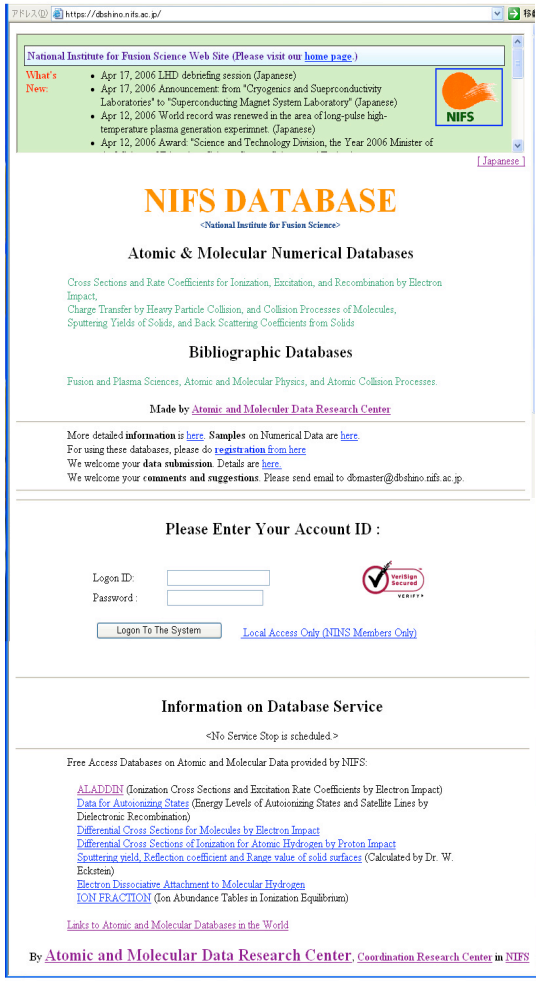
Recent works:
(1) Cross sections for electron and ion collisions with molecules of hydrogen, hydrogen isotopes, nitrogen, oxygen, hydrocarbons, water and carbon oxides (M. Kimura et al., NIFS-DATA-98 (2006))
(2) Cross section data for low energy ion-molecule reactions in hydrogen systems and for charge transfer of multiply charged ions with atoms and molecules (K. Okuno, NIFS-DATA submitted)
(3) Fe ions data (excitation, recombination) are being compiled in 2005-2006.

Data evaluation

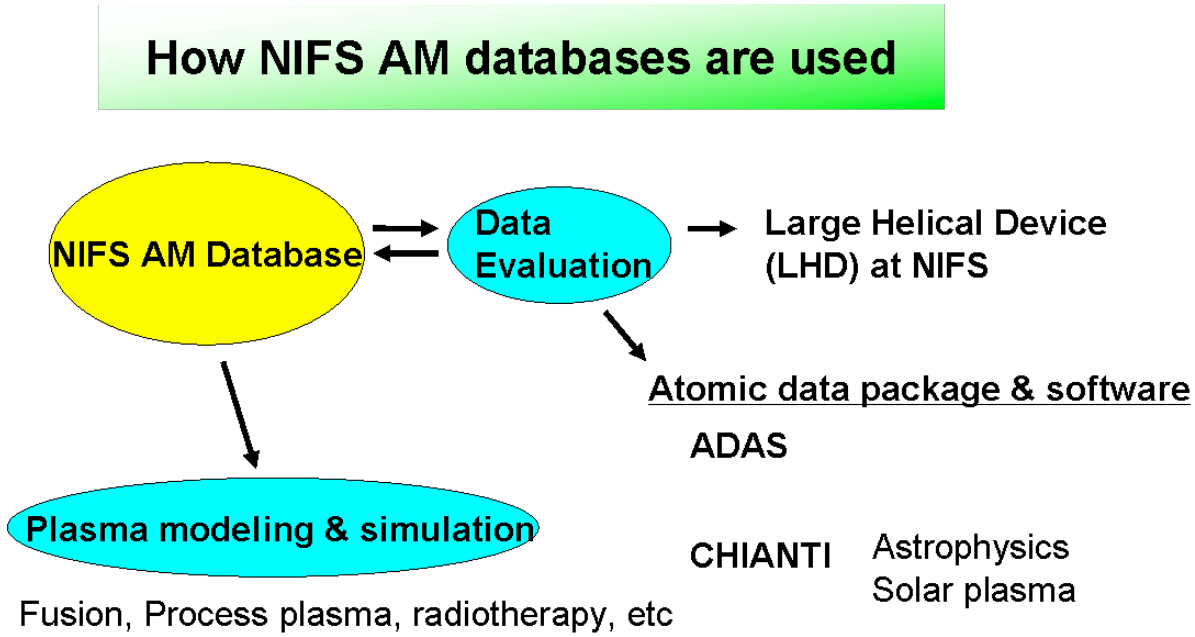
For data evaluation, we search data, compile data, examine data, select or estimate recommended data, and fit to an analytic formula.

Recent work:
(1) Collision processes of Li^{3+} with atomic hydrogen: cross section database (Murakami et al., NIFS-DATA-86 (2004))
(2) Cross section data for C atom and ions: electron-impact ionization, excitation, and charge exchange in collision with hydrogen atoms (Suno & Kato, ADNDT, 92, 407 (2006))
(3) Recommended data on proton-ion collision rate coefficients for Fe X-Fe XV ions and FeXVII-FeXXIII ions (Skobelev, Murakami, Kato, NIFS-DATA-95 (2006) and one in preparation)
(4) Evaluation of electron-impact excitation rates of Fe M-shell ions (Murakami, Skobelev, Itikawa, Kato, in preparation)

Promote interdisciplinary research between atomic physics and plasma physics



NIFS DB homepage (https://dbshino.nifs.ac.jp)

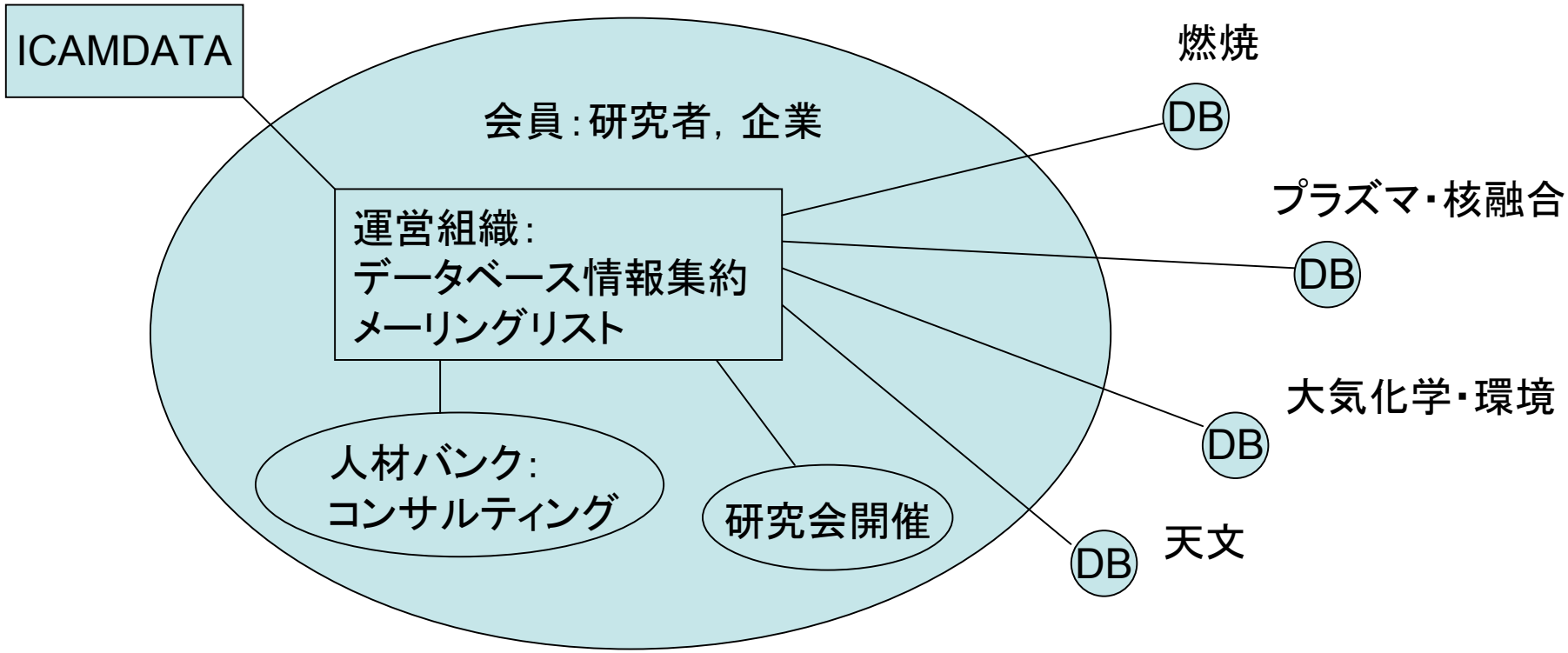


Other data activities

- We correspond to **data requests** or **inquiries** on atomic and molecular data. We use Human network in the World to answer.
- We are providing other databases made by domestic and international collaboration programs.
- New study for making software which automatically searches atomic data from internet resource are studied as a collaboration with computer scientists (A. Sasaki, JAEA).

原子分子データベース協会（仮称）

- 原子分子データベース活動の情報の集約（ウェブサイト）
- 情報交換のための人材バンク（コンサルティング），メーリングリスト作成
- 研究会等の開催
- 国内外連携のための窓口



NIFS一般共同研究で準備会を立ち上げ有識者（大学，研究所，企業）と意見交換を進めている．