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Survey of Atomic and Molecular Data Needs for Fusion

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Introduction

Experience with present-day fusion devices has demonstrated a critical need for numerical data information essential for the detailed understanding of the physical processes which occur in these devices. As the fusion research programs in Agency Member States progress toward design and construction of larger experimental devices, serving as prototype facilities for full-scale fusion reactors, the data requirements can only become more severe as the importance of additional physical processes is recognized and as the required level of understanding becomes more advanced.

Physicists and engineers are increasingly concerned with atomic and molecular processes which occur during particle injection, within the plasma itself and in interactions between the plasma and the interior surfaces of the confining vessel. They also continue to require nuclear data to understand nuclear processes which occur in the plasma and to evaluate the behaviour of proposed blanket and structural materials which will be required in viable energy-producing systems based on controlled fusion.

The International Fusion Research Council (IFRC) at its fifth meeting, held on 16 November 1974 in Tokyo, recognized the vital importance and need for a coordinated world-wide atomic and molecular (A+M) data service to ensure the successful development of fusion technology. On this premise, it recommended that the International Atomic Energy Agency (IAEA) perform a survey of existing atomic data banks, and consider adding atomic and molecular data for fusion to the scope of its existing nuclear data programme.

In response to the IFRC recommendation, the Nuclear Data Section (NDS) was requested to review the needs and to perform a world-wide survey of existing compilation activities concerned with atomic and molecular data for fusion. The result of this effort is the content of this report. To assist in this task, members of the International Nuclear Data Committee (INDC) and of the IFRC were invited to convey to NDS any information on existing and planned compilations, evaluations, and publications of A+M data in their own country. At the same time the IAEA convened a small consultants meeting to assess the needs and availability of A+M data for plasma research and fusion technology and to recommend the size and scope of an IAEA programme in this field.

SURVEY OF ATOMIC AND MOLECULAR DATA NEEDS FOR FUSION

by A. Lorenz, J. Phillips, J.J. Schmidt and J.R. Lemley*
International Atomic Energy Agency

This survey report on Atomic and Molecular (A+M) Data Needs for Fusion conists of two parts:

Part A: Atomic and Molecular Data Needs in Fusion Technology
Part B: Status of Atomic and Molecular Data Compilation

The review of A+M data needs (Part A) consolidates information from a number of sources, but primarily from three recent reports addressed specifically to the question of A+M data needs in fusion technology. These are:

1) draft report to the IFRC by Dr. R.S. Pease, Director of the Culham Laboratory, UK, entitled "Data on Atomic and Molecular Cross Sections for Fusion Research" dated 22 October 1974,

2) US report of the panel on atomic, molecular and nuclear physics in CTR entitled "Atomic, Molecular and Nuclear Data Needs for CTR", dated 29 March 1974, and

3) draft report by Dr. W.L. Wiese from the National Bureau of Standards, Washington, D.C., presented at the annual meeting of the American Physical Society, at Anaheim, California, on 29 January 1975, entitled "Atomic Physics Data Applicable for Toroidal Devices".

4) the final section (A5) on laser fusion compression has been contributed by staff of the Los Alamos Scientific Laboratory and the Lawrence Livermore Laboratory.

In July 1975 the IAEA convened in Vienna a consultants' meeting on A+M data for fusion. The participating consultants were:

Dr. C.F. Barnett, Holifield National Laboratory, USA;
Dr. H.W. Drawin, CEN, Fontenay aux Roses, France;
Dr. M.F.A. Harrison, Culham Laboratory, UK; and
Dr. Yu. Martynenko, Institute of Atomic Energy-Kurchatov, USSR.

The consultants made numerous contributions and suggestions which are reflected in both sections of this report. Their work is gratefully acknowledged.

A. ATOMIC AND MOLECULAR DATA NEEDS IN FUSION TECHNOLOGY

This section of the survey considers the A+M data needs in four recognized areas of plasma research and fusion technology - injection systems, interaction of plasma with surfaces, impurities and plasma cooling, and plasma diagnostics. Data requirements for laser fusion compression comprizes the fifth topic.

Content

1. Injection Systems

   A. Plasma Heating by Injection of Beams of Neutral Particles
      1) Ion Source
      2) Ion Extractor and Accelerator
      3) Ion-Neutralization
      4) Trapping of neutral species in the plasma

   B. Plasma Heating by Injection of Particle Clusters

   C. Plasma Fueling
      1) Injection of neutral particles
      2) Injection of particle clusters
      3) Injection of Solid Fuel

2. Interaction of Plasma with Surfaces

   A. Sputtering

   B. Surface absorption, adsorption, reflection and evaporation

   C. Surface Emission of Electrons

   D. Interactions of atomic hydrogen isotopes

   E. Synchrotron Radiation

3. Plasma Characteristics - Impurities and Cooling

   A. Electron Impact Ionization and Excitation

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   C. Charge Exchange

   D. Reflection of (H) from wall surfaces

4. Plasma Diagnostics

   A. Atomic Structure and Transition Probabilities

   B. X-ray wavelength shift for highly ionized metals

   C. Electron Capture Collisions with H^+ and D^+

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   E. Photon Scattering

   F. Other interaction data of importance to emission spectroscopy

5. Addition problem areas related to laser-fusion compression

   A. Microexplosion Physics

   B. Diagnostics

   C. Microtarget Design

   D. Current Laser Systems Requirements

   E. Laser Development

   F. Reactor Design Needs

On each page, information about the various problem areas is presented side-by-side with the associated data needs in order to facilitate identification of the specific data requirements and at the same time to relate them to the underlying physical processes.

ATOMIC AND MOLECULAR DATA NEEDS IN FUSION TECHNOLOGY

For all indicated reactions the quantities which are of general interest are the reaction cross sections as a function of energy and the reaction rate coefficients as a function of plasma temperature. Additionally the atomic parameters for spontaneous photon emission and absorption processes are required for many of the indicated species.

Since all isotopes of hydrogen may be involved unless specifically stated, the symbol (H) is used to represent any of the isotopes H,D, or T. The symbol e is used for electrons, and the symbol X and Z may represent any other heavy particles.

PROBLEM AREAS	DATA NEEDS

1. INJECTION SYSTEMS

The designs of some fusion experiments and reactors require injection of neutral material into the plasma (core) either to raise its average temperature (plasma heating) or to supply the nuclear fuel.

Present injection techniques are restricted because little is known about the atomic and molecular collision processes which occur in the injection system. An understanding of the atomic and molecular physics of the hydrogen isotopes and of collision processes with other gases is necessary to provide data for the design of efficient sources of both positive and negative ions, for the efficient conversion of positive and negative ions to neutral atoms, and for efficient trapping of injected material in the fusion plasma.

The physical processes and data requirements which are encountered in injection systems are discussed under the following topics:

A. Plasma Heating by Injection of Beams of Neutral Particles.

   1) Ion Source

   2) Ion Extractor and Accelerator

   3) Ion Neutralization

   4) Trapping of Neutral Species in the Plasma

B. Plasma Heating by Injection of Particle Clusters.

C. Plasma Fueling

   1) Injection of Neutral Particles

   2) Injection of Particle Clusters

   3) Injection of Solid Fuel (Pellets)

At present it is not clear whether injection of neutral particles or particle clusters are likely to be useful methods for fueling a fusion reactor. Therefore the principal discussion of these topics occurs in connection with plasma heating. Both plasma heating and plasma fueling by means of neutral-particle injection involve the processes of ion-production, ion-neutralization and subsequent trapping of the neutral particles within the plasma. However the relative importance of the atomic and molecular processes which are involved might be very different depending on the energies and intensities of the beams which are required for the two purposes.

PROBLEM AREAS | DATA NEEDS

1A. Heating by Injection of Beams of Neutral Particles

1) Ion Source

The primary objective of the ion source is to produce a particular ion species by collisions of electrons with isotopes by hydrogen. These processes occur normally in competition with ion loss processes such as diffusion, ion recombination, and electron energy loss due to inelastic molecular collisions. In addition, impurities ($Z>1$) are produced as a result of the interaction of the ions and electrons with the walls and electrodes of the ion source. Together with the desired ion species these impurities may be introduced into the plasma, which they contaminate (see Impurities and Plasma Cooling below).

(i) Collisions between electrons and atomic and molecular complexes in various states of vibrational and electronic excitation

Production of positive ions - (typical processes)

$e + (H)_2 \rightarrow (H)_2^+ + e + e$

$e + (H)_2^+ \rightarrow (H)^+ + (H) + e$

$\rightarrow (H)^+ + (H)^+ + e + e$

$e + (H) \rightarrow (H)^+ + e + e$

Production of negative ions - (typical processes)

$e + e + (H) \rightarrow (H)^- + e$

$e + (H)_2 \rightarrow (H)^+ + (H)^- + e$

(ii) Some Processes affecting ion species

Ion-molecular reaction	$(H)_2^+ + (H)_2 \longrightarrow (H)_3^+ + (H)$
Association	$D + T \longrightarrow DT$
Recombination	$(H) + (H)^+ + \text{wall} \rightarrow (H)_2$

(iii) Electron energy loss processes

Atomic and molecular excitation

$e + (H) \longrightarrow (H)^* + e$

$e + (H)_2 \longrightarrow (H)_2^* + e$

$e + (H)_2 \longrightarrow (H) + (H)^* + e$

Electron-electron collisions

$e_{(fast)} + e_{(plasma)} \rightarrow (e+e)_{thermal}$

Electron recombination or detachment processes, which are the reverse reactions for production of positive or negative ions, respectively, except for the energy range involved

(iv) Interaction of ions with surfaces

- Reaction kinetics

  Some preliminary experiments show that the surfaces of the ion source walls play a dominant role in the production of $(H)^-$. A more precise knowledge of the reaction kinetics of $(H)_2^+$, $(H)^+$ and (H) particles interacting with surfaces contaminated by Cs, Mg, Na and Li in the energy range 5 - 500 eV. is required.

- Sputtering (see 2A and 2B)
- Charge exchange
- Charge exchange processes of hydrogen with impurities (e.g. Fe, Ni, Cr, Cu, C, W and Mo), which may enter the ionizing discharge due to sputtering from the walls and other surfaces.

PROBLEM AREAS | DATA NEEDS

2) Ion Extractor and Accelerator

Positive and negative ions extracted from the ion source are accelerated to energies ranging from ~10 keV to ~1 MeV. The ion beam is accelerated in a low density gas diffusing out of the ion source. In addition to the interaction of the accelerated ions with the gas, in which charge exchange, charge stripping, detachment and dissociation can occur, part of the beam interacts with metallic surfaces creating the attendant surface effects, such as sputtering and outgassing, thereby introducing additional impurities.

Secondary electrons, produced in the extractor and accelerator by particle impact and X-rays, can be accelerated back towards the ion source so that additional ion production takes place but at much higher electron energies; the production of X-rays by these electrons may introduce a significant hazzard to health. The presence of arcs in the extractor system introduces collisions with impurity atoms.

(i) Particle interaction in the beam. X is the neutralizer species.

Charge exchange $(H)^+ + X \longrightarrow (H) + (X)^+$

Ionization $(H) + X \longrightarrow (H)^+ + X + e$

Detachment $(H)^- + X \longrightarrow (H) + e + X$

Dissociation $(H)_2^+ + X \longrightarrow (H)^+ + (H) + Y$

(ii) Surface effects

$(H)^+$ + surface $\longrightarrow$ radiation emission

$(H)^+$ + surface $\longrightarrow$ electron emission

$(H)^+$ + surface $\longrightarrow$ X-ray production

$(H)^+$ + surface $\longrightarrow$ outgassing

$(H)^+$ + surface $\longrightarrow$ sputtering

3) Ion Neutralization

a) Energetic neutral particles in the range 5 to 100 keV, which present injection concepts envisage, are most efficiently obtained by neutralization of accelerated positive ions in a gas cell.

(i) Production of neutrals from positive ions - typical processes:

Collisions with heavy species:

$$(H)^+ + X \longrightarrow (H) + X^+$$

$$(H)_2^+ + X \longrightarrow (H) + (H)^+ + X$$

Collisions with electrons:

$$(H)_2^+ + (X^+ + e) \longrightarrow (H) + (H)^+ + e + X^+$$

(ii) Some re-ionization processes:

$$(H) + X \longrightarrow (H)^+ + e + X$$

$$(H) + e \longrightarrow (H)^+ + e + e$$

b) In about five to ten years, however, larger experimental devices and prototype fusion reactors may require injected-particle energies ranging between 100 keV and 1 MeV. Several methods have been proposed to obtain intense atomic (H) beams in this energy range for heating and, possibly, fueling such devices. At these energies it will be more desirable to neutralize a beam of negative ions since the neutralizer efficiency is almost independent of ion energy and can be as high as 10 - 20 % in the case of a cesium-vapor-cell neutralizer. The following two methods have been proposed to obtain negative ions:

- use of a conventional positive ion source to produce a low-energy (1.5 keV) beam which is passed through an alkali vapor cell to form the required negative ions,
- development of a suitable negative ion source to produce the negative ions directly.

The negative ions are then accelerated to the desired energy and neutralized by stripping the excess electrons in a suitable target.

(iii) Formation of $(H)^-$ from positive ions and stripping of $(H)^-$ to form neutrals in gas or vapor cells.

- Interaction of $(H)_2^+$, $(H)^+$ ions with Cs, Na and Li in the energy region 0.5 - 5 keV. Little information is available for collisions of $(H)_2^+$ and $(H)_3^+$ ions in these vapors. Needed are the total cross sections, equilibrium fractions, and differential interaction cross sections to form $(H)^-$.
- No information is available concerning the cross section for the formation of D from D^+, D_2^+, and D_3^+ in target plasmas of either deuterium or Li. This may be a mechanism to produce 0.1 to 1 MeV D without resorting to the D^- cycle.
- Cross sections for the formation of (H) from $(H)^-$ collisions in gaseous targets of H_2, He, N_2, O_2, Ne, Ar and H_2O, in energy region between 50 and 300 keV.
- Peak fraction of (H) formed from $(H)^-$ in energy range 0.1 to 1 MeV.
- Formation of (H) from passage of $(H)^-$ through target plasma of deuterium or lithium in energy range 0.1 to 1 MeV.
- Stripping of $(H)^-$ in electromagnetic fields.

PROBLEM AREAS	DATA NEEDS
c) Intense beams of ions cause the neutralizer target gas to become partially ionized so that charge-exchange (etc.) takes place in a plasma. Since "thick target" conditions may prevail in the neutralizer, cascading collisions are important. The balance between charge exchange and ion production are further complicated by the presence of excited atoms and molecules.	(iv) Charge exchange rates for (H), $(H)_2$ and $(H)_3$ in partially ionized neutralizer target gases are required. (v) It is important to know the rate at which impurity atoms from the ion source enter the plasma confinement region. Required are cross sections for charge-exchange processes of C, N, O, Fe, Ta and Pt atoms with neutralizer gases over the energy range 5 to 100 keV and the rates for these processes in the environment of the neutralizing gas cell.
d) Trapping in the plasma core. After passing through the confining magnetic field, the injected (neutral) particles must be ionized before significant heating can occur. The importance of various ionization processes depends upon beam energy and plasma temperature.	(vi) Typical trapping processes: For beams < 50 keV: $(\underline{H})_{(beam)} + (H)^+_{(plasma)} \longrightarrow (H)^+_{(trapped)} + (H)$. At higher beam energies: $(\underline{H})_{(beam)} + (H)^+_{(plasma)} \longrightarrow (H)^+_{(trapped)} + e + (H)^+$. (The underscores indicate energetic particles.) (vii) Processes which result in trapping of heavy-ion impurities from the ion source within the plasma.

1B. Plasma Heating by Injection of Particle Clusters

Clusters of $(H)_2$ molecules can be produced by expanding cold $(H)_2$ gas into a vacuum. The clusters have a crystalline structure and may contain up to 10^5 atoms although the mass distribution depends upon the conditions of the expansion.

The clusters are ionized (positive charge) by means of electron collisions. In this process they dissociate into clusters of smaller size, many of which still contain $10^2 - 10^3$ atoms. On the average each cluster is singly charged. The clusters are accelerated to energies of several keV per atom in an electrostatic accelerator. (The energy per atom depends on the accelerating potential and the number of atoms in the cluster.)

After acceleration the energetic clusters are allowed to penetrate into the plasma. Very little is known about the distribution of charge and energy within the cluster or about the mechanisms of evaporation or dissociation of the clusters in the plasma.

Both the penetration distance in the plasma and the trapping efficiency depend strongly on the cluster dissociation history and on the nature of interactions between the accelerated clusters, neutral particles and plasma components.

In interactions between clusters and primary plasma components - electrons and ions such as $(H)^+$, $(H)_2^+$ and $(H)_3^+$ - the following processes occur:

(i) Excitation of the electronic, vibrational and rotational levels of the clusters molecules;

(ii) Dissociation of cluster molecules;

(iii) Ionization of cluster molecules;

(iv) Elastic momentum transfer to cluster molecules.

The secondary particles which are produced may induce the same reactions and escape from the cluster if they reach the surface with sufficient energy. Processes of recombination, ionization and charge exchange also occur. Processes which cause internal excitation are energy - loss mechanisms unless the excitation energy is subsequently converted to translational energy within the plasma.

In order to calculate plasma heating resulting from injection of clusters, it is necessary to calculate the rate of evaporation or break up of the clusters and the distributions of charge and energy of particles resulting from interactions of the cluster particles with each other and with the plasma components. The models for cluster evaporation and break up require cross-section and reaction-rate data for the processes which have been described.

PROBLEM AREAS | DATA NEEDS

1C. Plasma Fueling

1) Plasma fueling by injection of neutral particles.

For fusion reactors based on certain confinement systems it has been proposed to supply the nuclear fuel to the plasma by injecting neutral particles although it is not yet clear whether this method of fueling will be feasible. Many of the processes involved in plasma heating by neutral injection are also involved in fueling; however the relative importance of the various atomic and molecular processes may be different because of differing beam energies and intensities.

In addition to injection of isotopes of hydrogen, another possibility for fueling a fusion reactor may be injection of ^{3}He particles.

(i) As discussed in connection with plasma heating data related to the processes of ion-production, ion-neutralization and charge exchange with plasma constituents and impurities are required for atomic and molecular species composed of the isotopes of hydrogen.

(ii)

- Measurements have been made on the formation of He and H atoms through the dissociative collisions of H_2^+, H_3^+ and HeH^+ in H_2, He, N_2, O_2, Ne, Ar and H_2O targets in the energy range greater than 500 keV. These measurements should be extended to include the energy range 50 - 500 keV.
- Data for ionization processes leading to trapping of ^{3}He in the plasma core are also required.

2) Injection of clusters of hydrogen isotopes.

At present it is not clear whether injection of clusters ($< 10^5$ atoms) of hydrogen isotopes, as discussed in connection with plasma heating, might also be used to fuel a fusion reactor.

(iii) See discussion in Section 1B. Plasma Heating by Injection of Particle Clusters.

3) Injection of solid hydrogen isotopes.

Another proposal for fueling is the injection of solid hydrogen isotopes in the form of pellets into the plasma. A "pellet" may be rather arbitrarily defined as an aggregate of $(H)_2$ molecules consisting of more than about 10^9 atoms for which a fluid-like model of evaporation would be valid.

(iv) Effects of electrons and $(H)^+$ on solid $(H)_2$.

In addition to ionization, charge exchange and stripping processes ablation is of major importance.

Ablation: $e + (H)_2\,(solid) \longrightarrow e + (H)_2\,(gas)$
$\longrightarrow e + (H) + (H)$

$(H)^+ + (H)_2\,(solid) \longrightarrow (H)^+ + (H)_2\,(gas)$
$\longrightarrow (H)^+ + (H) + (H)$

The range of the ablation atmosphere is important. It is essential to consider all the energy loss processes for e and $(H)^+$ (at $\sim$ 10 keV) through an atmosphere consisting essentially of (H) and $(H)_2$ together with their ionization products.

PROBLEM AREAS | DATA NEEDS

2. INTERACTION OF PLASMA WITH SURFACES

In a fusion reactor charged and neutral particles (ions, electrons, neutrons, protons...) of energies ranging from a few eV to tens of MeV, and radiation escape from the plasma and impinge onto the surfaces of the vacuum wall surrounding the plasma. The surface processes of most concern include sputtering, desorption, adsorption, absorption, secondary emission and the interaction of atomic hydrogen isotopes with oxide layers or insulators.

2A. Sputtering

Sputtering is a mechanism whereby wall material under the bombardment of energetic particles or radiation is released into the plasma. Sputtering is important since the presence of high Z material causes plasma cooling by emission of radiation from spontaneous bound-bound transitions, dielectronic recombination and bremsstrahlung processes. Severe sputtering also may necessitate the replacement of the vacuum wall at frequent intervals. Although current conceptual designs of vacuum walls are envisaged to be made of refractory metals such as Nb or V, the first operating reactors will most probably have vacuum walls made of either Ni- or Fe-based alloys and other materials.

One of the most important wall reactions in toroidal plasma devices is the sputtering by hydrogen, deuterium and impurities on plasma limiters*, which are usually fabricated of Mo or W. Another approach, proposed to reduce impurities in the plasma, is the use of magnetic divertors**. In both cases, the designs of these limiters and divertors will require optimization in selection of materials and treatment of their surfaces to minimize sputtering.

It is clear that the atomic data required are for those materials used in the first wall or in limiters and divertors, i.e. for all surfaces which may come in contact with plasma.

In addition to sputtering caused by heavy and light ion impact, a number of other processes have been identified:

- In chemical sputtering, hydrides, formed when hydrogen isotopes react with wall materials, are easily sputtered off by energetic particle impact;
- Electron sputtering, caused by the interaction of 0.01 - 5 MeV electrons with the wall material;
- Sputtering by high energy neutrons, a process not yet completely understood;
- α-particle bombardement leading to blister formation.

A large quantity of sputtering data has been generated in the past 30 to 40 years, with most of the data taken for heavy ion impact on common metallic surfaces. Emphasis on heavy ion impact rather than on hydrogen impact results from the fact that the sputtering yield for light projectiles is relatively small compared to heavy projectiles. The low yield has been difficult to determine quantitatively. However, in the past three years, ion backscattering techniques have been developed that greatly increase the ease and accuracy in the determination of sputtering yields.

Present operating plasmas are usually surrounded by stainless steel walls. Sputtering yields for hydrogen on gold are very well known for energies in excess of 0.5 keV. Data for Ni or Fe based alloys and other materials need to be extended over the energy range of interest.

The following additional data are of importance to the reactor designer:

- sputtering of elements and alloys at energies below 2 keV.
- Blistering of wall surfaces, including heating and evaporation of blister covers by radiation and bombardment by particles.
- Trapping, re-emission and backscattering of plasma particles from solid surfaces.

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* Limiters confine the plasma discharge to the central part of the discharge tube.

** In divertors, energetic impurities and plasma ions near the wall are led out by the magnetic field into side cavities where they are allowed to bombard surfaces remote from the reacting plasma volume.

PROBLEM AREAS | DATA NEEDS

2B. Surface absorption, adsorption, reflection and evaporation

The wall surfaces absorb, adsorb and reflect energetic plasma particles and suffer themselves evaporation of material under the influence of the impinging plasma particles. Hydrogen isotopes and impurity particles (especially alpha particles and oxygen) trapped on and below the wall surface are released by photon and particle bombardment and diffuse back into the plasma, which is thus continuously contaminated and cooled. It is important to have direct control over these effects.

Adsorption, absorption, reflection and evaporation are also of great importance for understanding operation of the divertors.

(i) Absorption, adsorption, desorption and solubility measurements should be directed to the study of photon, hydrogen-isotope, impurity-particle and electron impact on currently used wall materials in the energy range 0.1 to several hundred keV as a function of the surface temperature.

(ii) Quantitative data as a function of surface temperature are urgently needed for the fraction of hydrogen isotopes, helium and other impurity atoms absorbed or adsorbed on, or dissolved in, surfaces of Li, Na or K, and also Nb, V or Ti.

(iii) The reflection coefficients and the charge state of the reflected particles are also needed as a function of their initial and final energies.

2C. Surface Emission of Electrons

Electrons are released by secondary emission which occurs when an energetic particle strikes a solid surface. One impinging particle can liberate one or more low energy electrons. Surface emission of electrons can also occur due to strong local heating of the confining walls and limiter surfaces (thermal emission).

(i) A data base of secondary emission coefficients in the presence of a plasma needs to be established for impingement of electrons, hydrogen isotopes and other particles found in a plasma on materials such as Fe, Cr, Ta, Mo, W, etc., and currently used alloys. The energy range of interest is 100 eV to several hundred keV and will extend eventually to several MeV.

(ii) Since the presence of a plasma may modify the usual thermal emission of surfaces in vacuum, data for thermal emission in the presence of a plasma are also needed.

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3. PLASMA CHARACTERISTICS IMPURITIES AND PLASMA COOLING

Ideally, plasma in a fusion reactor would be composed uniquely of hydrogen isotopes; in reality, however, typical plasmas observed today in toroidal confinement contain 5 percent (but as high as 16 %) [1] oxygen and approximately 0.2 percent metal impurities[2]. It has been shown [3] that a 0.2 percent heavy metal plasma impurity component radiates about 40 percent of the total radiation mainly in the form of line radiation for the various stages of ionization. If one assumes that the total power input during the steady phase of the discharge is 200 kW, (the other losses originating mainly from charge exchange processes and charged-particle losses) the total power loss due to heavy ion impurities is about 10 percent [1].

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1 W.L. Wiese, Atomic Physics Data Applicable for Toroidal Devices. Presentation to the Annual APS Meeting in Anaheim, California, 29 January 75.

2 E. Hinnov, Princeton Plasma Physics Laboratory Report MATT-1022 (k974).

3 D.L. Meade, Nucl. Fusion 14, 289 (1974).

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Heavy metal impurities also have a significant effect on plasma resistivity. Multiplied by the effective ionic charge (which under the given circumstances could be 7 for oxygen and 20 for metals), the small number densities of these impurities contribute significantly to an increase in electrical resistivity of the plasma. It has been estimated that an impurity concentration of only 0.1 percent, if allowed to accumulate gradually, is sufficient to cause a 30 percent increase in resistivity. [2]

Another detrimental effect of heavy ion impurities in plasma arises from ionization which introduces cold electrons which have an adverse effect on the density and temperature distribution of the plasma. Although quantitative estimates about the importance of this additional ionization are difficult to make, an estimate by Hinnov [2] indicates that concentrations of less than 0.1 percent are sufficient to make this effect significant.

Under fusion reactor conditions, the plasma temperature and the rate of the processes described above will be proportionately higher; heavy-element impurities may not only be more abundant but may be ionized up to seventy times instead of the 20-times ionization encountered in the contemporary Tokamak experiments. In the presence of large fractions of heavy metal impurities such as tungsten, the power loss by radiation may be so large that the temperature necessary to meet the fusion criterion may never be reached. [3]

Bremsstrahlung radiation, in the form of electromagnetic radiation, is given off when electrons are accelerated as they pass close to a nucleus. Bremsstrahlung losses in a hot ionized plasma constitute an important cooling mechanism which may limit the attainable temperature in operating thermonuclear plasmas, after plasma instabilities are brought under control. Bremsstrahlung losses due to highly charged heavy-ion impurities are particularly damaging. Furthermore, bremsstrahlung losses, even in a relatively clean plasma, will be significant if the plasma is heated by techniques which principally heat the electrons.

In summary, it can be concluded that very small concentrations of heavy ion impurities may have extremely serious effects on the success of fusion plasma experiments, particularly in toroidal (tokamak-type) confinement. It is therefore of utmost importance to understand the role of heavy ion impurities, and to find ways to control them.

PROBLEM AREAS | DATA NEEDS

3A. Electron-Impact Ionization and Excitation

The important transitions between atomic energy levels in CTR plasmas consist of excitation or ionization by electron collisions and de-excitation by radiative transitions. The excitation cross sections are proportional to the radiative transition probabilities and at high electron energies (much larger that the excitation potential) are adequately calculable from the Born approximation. However, in the range up to several times the threshold, where the cross section is largest and of most interest, the Born approximation is not adequate, and more sophisticated calculations and experimental checks are necessary. At present, available information is adequate only in a few special cases.

There is a growing need for information on the behaviour of medium and heavy element ions in plasmas with the characteristics of the present most advanced experiments and of reactors. Initially such ions will always be multiply-ionized, and there is virtually no direct experimental data for key processes involving such ions.

Much of the presently available data relies on calculations. It is difficult to assess the accuracy of these calculations; they can probably be relied on to an order of magnitude, and in some cases they may be more accurate than a factor of two. However, more accurate data will definitely be needed, both for interpretation of experiments and estimates of reactor performance.

Of special interst are transitions between low-lying terms of multiply-ionized C, N, O, Ne, Ar, Kr and Xe, the latter four being important because they are readily added in known quantities to CTR plasmas. Of equal importance are transitions between bound states of all types of impurity ions originating from surface desorption, wall evaporation and sputtering (Fe, W, Ti, Ta ...). Knowledge of the excitation (and ionization) cross sections of multiply charged particles is vital for spectroscopic plasma diagnostics, for plasma modeling and for insight into loss of plasma energy via line radiation.

Theoretical and experimental investigations should be made along isoelectronic sequences with special emphases on:

- The resonance lines of the copper and zinc isoelectronic sequences all the way to the upper end of the periodic table, but with immediate attention to W and Au as most likely heavy impurity components of Tokamak plasmas. With somewhat less urgency, the programme should be extended to the Mg, Na, Be and Li sequences and other sequences that are expected to provide strong resonance lines (with large transition probabilities or $f \gtrsim 0.1$).
- The systematic investigation of the atomic structure for the first forty states of ionization of W (and Au) for the existence of simple electron configurations (e.g. 5 S + closed shells) that will lead to strong resonance lines.

Both of these tasks are partly theoretical and partly experimental. The experimental work should extend presently available isoelectronic sequences to as high Z-values as possible (using vacuum sparks and tandem accelerators) with the objective to identify theoretically predicted lines. Due to the high particle energies, simultaneous excitation of several bound electrons can lead to enhanced radiative losses. Practically nothing is known about such processes (see also dielectric recombination).

These investigations should be combined with detailed crossed-beam measurements of cross-section versus energy for multiply charged ions and with rate-coefficient measurements for specified energy distributions in plasmas with higher states of ionization.

3B. Recombination Processes

1) Radiative Recombination

Radiative recombination is a common type of electron-ion recombination in which an electron coming within a close distance of an ion drops into a low-lying electronic orbit and radiates its excess energy. Because of its strong Z dependence, radiative recombination is a significant energy loss process.

The appropriate Gaunt factors are important at least for a few representative cases (e.g. Nb or W) for all the states of ionization in plasmas up to electron temperatures of about 50 keV to 100 keV.

PROBLEM AREAS | DATA NEEDS

2) Dielectronic Recombination

An electron colliding with an ion with at least one bound electron may be captured into an autoionizing doubly-excited state which may subsequently decay into a bound state by emission of two or more photons:

$$e + X^{n+} \longrightarrow [X^{(n-1)+}]^{**} \longrightarrow [X^{(n-1)+}]^{*} + h\nu_1$$

$$[X^{(n-1)+}]^{*} \longrightarrow X^{(n-1)+} + h\nu_2$$

Under high-temperature conditions this process can be much faster than the purely radiative recombination. For example, in the solar corona where the electron temperature is high, the dielectronic recombination of He^+ is reputed to be over 10^2 times faster than radiative recombination. It is possible that similar factors apply to heavy elements in reactor type plasmas, thereby reducing the equilibrium charge-state and significantly increasing the power loss caused by these elements. In other words, this may be the most important power loss mechanism in a fusion reactor, and may necessitate still further reduction of the maximum allowable concentrations of the heavy elements beyond the present estimates based on radiation recombination.

Dielectric recombination rates on partially stripped heavy atoms are required. Due to the importance of this effect it is urgent to have numerical data, which are necessary both for spectroscopic diagnostics and for plasma modelling.

3C. Charge Exchange

(i) One possible source of plasma cooling occurs through the following charge exchange reaction and its reverse:

$$(H)^+ + X^{n+} \rightleftharpoons (H) + X^{(n+1)+}$$

where X can be C, O, N, Fe, Nb, W or Mo.

The assessment of the rate of plasma cooling by this process is impossible since not even fragmentary data are available. These cross sections have been difficult to measure because it is only recently that adequate sources of X^{n+} ions have been developed.

(ii) As an alpha-particle slows down in a plasma, charge exchange reactions of the following type are of importance to particle and energy loss from the plasma:

$$He^{++} + (H) \rightleftharpoons He^+ + (H)^+$$

Although some data exist at energies greater than 10 keV, definitive experiments are needed to cover the region between 0.1 keV to several MeV.

3D. Reflection of (H) from wall surfaces

When energetic (H) atoms escape the plasma, they impinge on the vacuum wall. Past measurements have indicated an ion reflection coefficient (ions out to ions in) of 5 to 10 percent in the energy range of a few keV. Also, reflected ions are known to have an energy distribution ranging from incident energy down to thermal. If one assumes that a charge equilibrium exists in the reflected beam then the reflection coefficient of neutral (H) atoms at low energies may be as high as 0.5 to 0.6. These energetic particles will penetrate the plasma, and form an energy transport mechanism for energy loss to the vacuum wall.

Measurements of reflection coefficients, energy and charge distribution, and ratios of $(H)/(H)_2$ coming off surfaces of stainless steel, Nb, Au and W will permit a better understanding of particle and energy loss from plasmas. The excited-state population of (H) reflected from surfaces, and surface conditions that influence the excited population, should also be determined.

PROBLEM AREAS | DATA NEEDS

4. PLASMA DIAGNOSTICS

In contrast to the preceeding three problem areas which were directed towards the understanding of the effect of individual physical processes and overall plasma behaviour, plasma diagnostics aim at the quantitative determination of the plasma parameters (i.e. spatial distribution of temperature, particle density and magnetic/electric fields). Also of importance is the identification of the various plasma components and impurities, the measurement of their characteristics, (such as temperature, density, degree of ionization), and their effect on the overall energy balance. This latter problem calls for the development of diagnostic techniques to study plasma-wall interactions.

Present diagnostic techniques make use of injected beams of atoms and very fast ions, photon scattering and spectroscopic observation of emitted radiation. Consequently many processes described in sections 1 - 3 are of direct relevance to diagnostics. The following are a limited selection of some current requirements.

Of particular interest is the measurement of highly ionized heavy ion impurity concentrations, their degree of ionization, their spatial plasma potential and relative particle densities.

4A. Atomic Structure and Transition Probabilities

Of primary importance to plasma diagnostics by emission spectroscopy are the atomic structure and transition probabilities of all plasma components.

- High Z impurities

For quantiative measurements of impurity concentrations and for the predicition of radiation intensities and power losses, it is necessary to know the transition probabilities of the resonance lines of the various states of ionization of heavy elements. Special emphasis should be on isoelectronic sequences of simple configurations which are particularly important for diagnostic purposes. There remains some work to be done on atomic structure of likely impurities such as the molybdenum ions stages Mo XX to Mo XL, which could be calculated by Hartree-Fock-Slater techniques. Other ions of importance are Fe XVII to Fe XXIV, Ni XIX to Ni XXVI, etc.

- Low Z Impurities

Although they are not necessarily detrimental to the plasma properties in the same ways which heavier elements are, oxygen, carbon and perhaps nitrogen are numerically the most abundant impurities and exert a considerable influence on plasma behaviour. Further accurate theoretical calculations and studies of systematic trends along isoelectronic sequences are needed to provide a more accurate transition probability data base.

PROBLEM AREAS | DATA NEEDS

4B. X-ray wavelength shift for highly ionized metals

When an atom (Fe or Nb) is stripped of its outer electrons, the X-ray wavelengths of its K-lines of L-lines shift. A measurement of the wavelength as a function of radius (in a toroidal discharge for example) could provide information on the cross-field transport rates and ionization/recombination relationships in the plasma.

Expected x-ray wavelength shifts should be determined for elements likely to be present in Tokamak discharges, e.g. Fe. Mo, Nb, Au and W. Extrapolation to neighbouring elements, e.g. Fe to Cr and Ni, or Mo to Nb, should be a relatively simple matter.

4C. Electron capture collisions with H^+ and D^+

Spatial ion temperature distribution may be obtained by projecting an energetic beam of hydrogen or deuterium atoms across a plasma region. Electron capture collisions with H^+ or D^+ in the plasma result in the formation of H atoms in various electronic excited states. Observation of the Doppler shift of these excited atoms as they radiate gives a measure of the plasma temperature. If absolute cross sections of these processes are known, then spatial ion densities are measurable.

The absolute cross sections for the formation of the 2s and 3p states by electron capture, are known for energies greater than 3 keV. Needed are the cross sections for energies less than 3 keV and the cross sections and branching ratios for the formation of the n = 3 states.

4D. Heavy ion collision ionization probe

High-energy heavy-ion beam probes have been developed to determine the spatial plasma potential and relative particle densities. Absolute cross sections for the collisional ionization processes will provide absolute spatially resolved densities.

Needed are the absolute cross sections for the following collisions:

- in the energy range 10 eV to 10 keV

$$(Tl^+, Rb^+) + e \longrightarrow (Tl^{++}, Rb^{++}) + 2e$$

- in the energy range 0.05 MeV to 1 MeV

$$(Tl^+, K^+, Rb^+, Ba^+) + H^+ \longrightarrow (Tl^{++}, K^{++}, Rb^{++}, Ba^{++}) + H^+ + e$$

and

$$(Tl^+, K^+, Rb^+, Ba^+) + H^+ \longrightarrow (Tl^{++}, K^{++}, Rb^{++}, Ba^{++}) + H$$

4E. Photon Scattering

Thompson scattering of laser beams by free electrons is a well established diagnostic technique. Improvements in laser technology might extend the technique to scattering from free $(H)^+$. Another new application of laser scattering is resonance scattering from (H), which should provide information about the distribution of electromagnetic fields.

In resonance scattering from ground to excited states of atoms or ions, the absorption cross-section (or induced transition probability B_{21}) for several atomic systems needs to be known. (For example in hydrogen, mixing of 2s - 2p states in magnetic fields will alter the cross-section for resonance pumping from n = 1 to n = 2). This has some importance in resonance scattering from charge-exchange neutrals. The same argument holds for resonance scattering from complex and weakly ionized impurity ions.

PROBLEM AREAS | DATA NEEDS

4F. Other interaction process data of importance to emission spectroscopy

(i) In the case of collision cross-sections, values derived from swarm techniques (i.e. averaged over the electron velocity distribution) are of interest. A few experimental data points exist for bound-bound excitation rates in modest Z ions. From theory these rates are thought to be accurate within a factor of two. The problem is that there is no single good way of treating all classes of bound-bound transitions. For example, for some collisions, exchange terms or configuration mixing may have to be included in the theoretical treatment. Low energy processes are of particular relevance to wall-plasma interactions.

Availability of relevant numerical computer programmes to calculate wave functions are important in the calculation of impact cross-sections and oscillator strengths.

(ii) The same components apply to recombination rates. Calculation of dielectronic recombination and autoionizing rates are important in the assessment of likely populations of high Z ion impurities.

(iii) 2-photon decay cross sections from $1s2s\,^1S_1$ helium isoelectronic states are also important, as are oscillator strengths of metastable levels (e.g. $1s2s\,^3S_1$) in high Z ions.

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5. ADDITIONAL PROBLEM AREAS RELATED TO LASER-FUSION COMPRESSION.

At the ultrahigh plasma densities achieved in laser compressions there arise a number of areas which require additional experimental data and theoretical understanding. They include: accurate description of the microexplosion physics, diagnostics, target design, current laser needs, development of new lasers, and reactor design.

5A. Microexplosion Physics

The mechanisms and magnitudes of energy release from a D-T pellet microexplosion are estimated to be as follows:

Mechanism	Energy Release	Particles per pulse	Average Energy per particle
X-rays	1 MJ	-	4 keV peak
Alphas escaping plasma	7 MJ	2.2×10^{19}	? MeV
Plasma Kinetic energy	15 MJ		
Alpha's	76 MJ (total for Alpha's, Deuterons, Tritons, Neutrons)	1.3×10^{19}	0.6 MeV
Deuterons		1.2×10^{20}	0.3 MeV
Tritons		1.2×10^{20}	0.4 MeV
Neutrons		3.3×10^{19}	14.1 MeV

(i) Equation of state (EOS) data is needed for a variety of materials (elements, compounds, and mixtures) at densities from 10^{-5} gm/cm^3 and at temperatures from about 0.1 eV to 10 keV. Calculations may be possible which include finite temperature and the presence of neighboring ions.

(ii) Electron thermal conductivity data is also needed over the same range as (i) with degenerate and bound electrons correctly treated. Collective anomalies which reduce conductivity must be better treated.

(iii) Atomic cross sections for electron and x-ray excitation for rate equation calculation of non-LTE evolution are required. Energy-loss measurements (MeV/g/cm^2) are required for: 2.0 → 4.0 MeV α-particles, 1.0 → 3.0 MeV protons, 0.3 → 1.0 MeV in hot (0.2 → 5 keV) SiO_2 and in hot D,T plasmas.

(iv) There is, at present, no reliable practical computational scheme for predicting inoization rates in intense fields from arbitrary excited states of atoms. Possible theoretical models for strong field ionization should be developed and validated by comparison with carefully controlled experiments.

PROBLEM AREAS

DATA NEEDS

A considerable fraction ($\sim 22\%$) of the energy released is in plasma kinetic energy and escaping particles. The microexplosion described above is typical of low ρr microexplosion. For intermediate ρ (i.e., reaction in the pellet) large α and x-ray yields are predicted; 50% neutrons, 40% charged particles and 10% x-rays.

(v) Calculations are also possible for radiative emission rates involving distortions due to finite temperature and pressure.

5B. Diagnostic Needs

Hydrogen- and helium-like spectra of ionized atoms have been studied and are used as diagnostic handles in plasma studies.

(i) With progress toward hotter plasmas the line spectra from highly stripped atomic species will play an important role in the diagnostics and analysis of plasma heating dynamics. Emission, absorption, opacities, and scattering cross-sections are among quantities necessary for the interpretation of pinhole photography.

(ii) Spectral-line profiles offer potential plasma-diagnostic tools, with further theoretical and experimental development, although it is likely that line ratios will be of more value for diagnostics, profile measurements require high resolution and the interpretation is made difficult in the presence of hydrodynamic motion (expansion) and multiple scattering.

(iii) The properties of photon scattering off surfaces at grazing angles should be explored at 1 keV - 100 keV to assist in improvement of pinhole and reflective optics for both laser and e-beam pellet diagnostics.

(iv) There is a need for improved quantum efficiency stable photocathodes for image tubes operating in the near infrared. Also photocathodes suitable for x-ray imaging cameras need development with regard to efficiency and keeping the energy spectrum of emitted electrons narrow.

5C. Data Required for Microtarget Design

(i) The emission-line needs (5B) are also required to determine optimum atomic species to incorporate as target impurities for diagnostics.

(ii) EOS (Equation of State) data is required for target-material elements from liquid helium temperatures ($\sim 3 \times 10^{-4}$ eV) to 10^5 °K.

(iii) Thermodynamic, mechanical, optical and electrical parameters in the same (ii) temperature range.

Isotopic mixes of D and T may influence some of these properties, and such effects should be determined.

5D. Data Required for Current Laser Systems

(i) Focusable laser power for fusion experiments is limited by beam breakup caused by the intensity-dependent refractive index (n_2) of the transparent media in the laser system. This includes optical materials used for lenses, windows, substrates for transmission polarizers, and Faraday rotators for isolation. Reduction in n_2 can be achieved by developing lower index, low dispersion glasses and crystals.

Accurate measurements of the non-linear refractive index of transmissive optical components is needed for the design of lasers with known beam propagation characteristics. Additional studies of the dispersion of n_2 and the cross section for multiphoton absorption in solids are needed to guide the selection of materials for new lasers operating at other wavelengths.

PROBLEM AREAS

DATA NEEDS

(ii) Breakdown of thin-film coatings used for AR-coated lenses, mirrors, polarizers and beam splitters are frequently the limiting element for the propagation of high-intensity laser beams. Improvements in the technology and characterization of coatings are required to develop more damage resistant thin films.

Measurements of the laser induced damage for thin-film coatings are needed for various design criteria. The dependence of damage thresholds on the laser pulse duration and wavelength also needs further study. The meaningfulness and usefulness of these measurements requires improvements of technology and processing to yield reproducible coatings.

(iii) Current gas lasers (CO_2 and HF) for fusion require additional information.

Details of beam propagation and energy extraction in multiline systems are needed. (For further information, see 5E).

5E. Laser Development

(i) Many promising high-power laser devices are initiated with electron beams. The interaction of the secondary electrons with atomic and molecular species is poorly understood (the primary electrons give rise to ionization and electronic excitation).

Low-energy electron scattering cross-sections and the effects of intense fields on the atomic and molecular species are required.

(ii) After initiation, by electron beams, flash lamps, electrical discharge, etc., a complex sequence of chemical reactions funnels the energy into the appropriate upper laser states.

Kinetic models describing large numbers of consecutive chemical reactions, in turn requiring detailed rate constants, scattering cross sections, etc. are required. In many cases the quantities are not experimentally available, hence, theoretical calculations must be used to determine the required microproperties.

(iii) In addition to understanding, modeling, and optimizing the basic lasing process, loss mechanisms must be properly treated.

Population inversions can be destroyed by a number of radiative processes: inter-molecular energy transfer (V-T, V-V, E-V, etc. relaxation), intra-molecular energy transfer (intersystem crossing, etc.), collisions with secondary electrons (super-inelastic scattering), photoionization, (particularly rare gas systems), Penning ionization and/or dissociative electron attachment.

Extraction of energy from lasers depends on the cross sections for stimulated emission and absorption; they should be obtained and catalogued.

Development of new laser candidate systems requires considerable spectroscopic and dynamic data which should be collected, evaluated and catalogued (computerized data base).

5F. Reactor Design Needs

Equation of state data is required for first-wall materials. These materials are likely to be under high tension.

The photoionization cross sections (mainly due to inner-shell ionization) for incident photons of about 10 keV and ionization cross sections by electron beams with energies of approximately 100 keV are required for these materials. Materials include refractory materials; lithium, stainless steel, pyrolytic graphite, etc.

B. CURRENT STATUS OF ATOMIC AND MOLECULAR DATA COMPILATION

This section and the Appendix summarize the status of continuing data compilation activities in which bibliographical or numerical data of interest to fusion are collected and disseminated (and, in same cases, evaluated) on an organized basis. In addition to these continuing activities many individual compilations have been published or are otherwise known to exist.

The following general conclusions can be drawn on the basis of the present survey:

a) Bibliographical data:

- A significant amount of bibliographical/reference compilation is being done, almost all of which is computerized.

b) Numerical data:

- Individual compilations are extensively published in the literature, primarily in the form of tabulations.
- Hardly any computerization of numeric A+M data compilation has been done; there has been no coordination between centers or unification of format.

Known A+M data activities are summarized by country in the following pages. More detailed information about some of these activities is presented in the Appendix.

Activities in France

1. Laboratoire de Physique des Plasmas Université de Paris-Sud.

The "GAPHYOR" (Gaz-Physique-Orsay) system consists of a computerized bibliographic and numerical data bank which forms the basis of this data center's activities. The system stores the basic properties of single atoms or molecules (energy levels, lifetimes of excited states, etc.), the properties of interactions between such particles (collision cross-sections, etc.) and certain basic macroscopic properties (transport coefficients, etc.) which are the fundamental data of the physics of gases. The approach has been to select and classify data from the standpoint of a specific group of users - physicists, physical chemists and engineers concerned with the physics of inert or ionized gases under conditions of high temperature and pressure.

Conceived in broad outline at the beginning of 1972, GAPHYOR was initially tried out at the laboratory level. Early in 1973, it was proposed as a specialized documentation service for potential users in France. In 1974, the service was extended to cover users in other countries. The service provided by this group is not cost-free, and has aspirations of becoming self-supporting.

2. CEN, Fontenay aux Roses

Dr. Drawin compiles bibliographic and numerical data of interest for plasma diagnostics.

Activities in the Federal Republic of Germany

1. Institut f. Plasma Physik, Garching

- R. Behrisch compiles lists of references and keywords on sputtering work; this information is periodically published by ZAED at the Kernforschungszentrum Karlsruhe.

- W. Lotz tabulation of calculated ionization cross section.

2. Zentralstelle für Atomkernenergie-Dokumentation (ZAED), Leopoldshafen

- surface physics and thin layers:
  - absorption properties of gases at surfaces
  - work functions of metals
  - sputtering data due to ion bombardment

- atomic data
  - lifetime of excited states
  - isotopic shifting
  - g-factors
  - polarization
  - excitation and ionization cross-sections for electron collisions
  - hyperfine structure data

- molecular data
  - dipole moments
  - excitation and ionization cross-sections
  - reaction cross-sections
  - interatomic potentials
  - electron affinity
  - dissociation energy

- plasma physics
  - spectral line broadening in plasmas
  - excitation and ionization cross-section of gases

- ion mobilities
- transport coefficients

3. Physikalisch-Technische Bundesanstalt, Institut Berlin

- measurement and compilation of data on
  - transition probabilities
  - line broadening
  - continuum emission

4. Kernforschungsanlage Jülich, Institut für Chemie (Nuklear-Chemie)

- measurement of data on
  - tritium permeation through metals
  - lithium diffusion in metals
  - chemical reactions of hydrogen and oxygen atoms resp. ions with metals
  - energy distribution of sputtering products resulting from ion bombardment

Activities in Japan

The two A+M data activities which stand out in Japan are Prof. K. Takayanagi's individual effort (at the Institute of Space and Aeronautical Science, University of Tokyo) to compile bibliographic references in the field of atomic collision data, and the study group on atomic data at the Institute of Plasma Physics, Nagoya University, currently under the leadership of Prof. H. Suzuki.

Prof. Takayanagi's effort is based on his personal collection of references which he has accumulated during the past twenty five years. Because of time limitation, his bibliographies are not complete, particularly for the most recent periods. The list of bibliographies published by Prof. Takayanagi is given in the Appendix. The publications are in English.

The Institute of Plasma Physics (Nagoya University) study group which started its work in 1973, performs compilations of cross section data for atomic processes of pertinence to plasma physics and fusion research. The group consists of 10 physicists involved in atomic collision research or molecular spectroscopy, and of 10 plasma/fusion scientists who serve primarily as advisors to this group.

The group is in the process of publishing a data compendium, the first volume of which Data Compilation of Cross Sections on Atomic Processes, Vol. 1, Processes Involving Hydrogen Isotopes, their Ions, Electrons and Photons" (in Japanese) was edited by Prof. Takayanagi and published in May 1975 as report IPPJ-DT-48. The second volume of this compendium which is to include radiative and collisional processes between hydrogen, helium and their ions, and electrons and photons, is in preparation. A third volume, which will include other cross section data of importance to fusion research, particularly plasma diagnostics, is planned to be published still within the current fiscal year. The data in these publications is presented in graphical form annotated in Japanese. The activities of the atomic data study are planned to be incorporated into a Research Information centre scheduled to be established next fiscal year at Nagoya University.

Activities in the UK

1. AWRE; Aldermaston

- Mass spectrometry data compilation by Mr. Daly.

2. Universities

- Polytechnic of North London, UK.
  M. Outred compiles infrared atomic wave numbers.

3. The Institute of Electrical Engineers in their periodical publication Physics Abstracts provides an abstract service which covers the most important international journals and includes subject classifications of interest for fusion.

Activities in the US

1. Controlled Fusion Data Center
(Oak Ridge National Laboratory, Oak Ridge)

The US Energy Research and Development Administration (ERDA) established the Controlled Fusion Data Center at the Oak Ridge National Laboratory, to replace the Atomic and Molecular Processes Information Center which until 1974 was jointly sponsored by the U.S.A.E.C. and the Office of Standard Reference Data at the National Bureau of Standards.

This Center serves fusion scientists and technicians by collecting, storing, evaluating and disseminating atomic and molecular data of interest to plasma research and fusion technology. The center has published a set of comprehensive annotated bibliographies for the years 1950 - 1970, as part of the ORNL-AMPIC report series. Interrupted because of limited funds and manpower, the publication of this bibliographic compilation is planned to be resumed in 1975. Information for the bibliographic data base is collected by the Center personnel by searching the literature for atomic and molecular collision data, and making a preliminary evaluation of the papers. Key information, such as collision energy range, whether the work is experimental or theoretical, the collision reactants, and names of authors, is recorded and entered into the bibliography data base to serve as indexing variables.

The bibliographic data base is now fully computerized, and the center is exploring the feasibility of storing data in the large CTR computer located at the Lawrence Livermore Laboratory. This would permit on-line retrieval of atomic data by all US laboratories engaged in fusion research.

Regarding numerical data, the center has been revising an earlier data compilation, "Atomic Cross Section of Interest to Controlled Fusion Research", published as ORNL-3113 in 1964. The updated version of this report, containing data in both graphical and tabular form, is to be published shortly after June 1975. The next compilation, is to be published in 1976.

More recently, this center, in cooperation with the National Bureau of Standards, has initiated a bimonthly newsletter on Atomic Data for Fusion in order to provide interested fusion researchers with the most recent atomic data applicable to fusion work, prior to journal publication.

2. National Bureau of Standards (NBS)

The following is an excerpt from NBS Technical Note 747 (June 1972):

The National Standard Reference Data System program for Atomic and Molecular Data places major emphasis on two elements. The first element is timely completion of data compilations on atomic and molecular spectroscopy, collision and ionization processes and related subjects. NBS staff scientists are deeply involved in many of these projects. The second element is cooperative development and application of data standards, evaluation criteria, and compilation planning for several of the specific fields of molecular spectroscopy. Panels of outside advisors, including representatives of appropriate professional societies, are features of these latter efforts, which seek more to coordinate and assist actual data compilation activities than to operate them. In its support of both elements, the Office of Standard Reference Data follows the priority list which evolved during two meetings (in 1965 and 1967) of the Advisory Panel on Atomic and Molecular Properties.

The data evaluation projects in this area continue to emphasize atomic and molecular spectra, collision cross-sections and certain other molecular properties. Publications have been issued which deal with atomic data derived from optical spectra, ionization of atoms by electron impact, ultraviolet photoabsorption cross-sections, the absorption spectrum of carbon monoxide, molecular vibrational frequencies, and the spectrum of molecular oxygen. Small efforts have begun on a revision of the fundamental constants and an exploration of the value of high quality infrared molecular spectral data. Planning has been completed for a project on interatomic distances, and compilation work has started at an informal level.

The charter of the standard reference data program recognizes the appropriateness of support of experimental determination of data to which a particularly high importance is attached. Such "benchmark" data can include measurements aimed at either (a) clearing up major discrepancies in key physical properties; or (b) providing a reliable value of a quantity to which a large number of relative measurements can be tied.

A list of NBS data centers which have direct bearing on A+M data for fusion is given in the Appendix.

3. Argonne National Laboratory (ANL)

A Surface Science Center for CTR programs, headed by Dr. M. Kaminsky, has been set up at ANL.

LIST OF KNOWN COMPILATION EFFORTS

Title: GAPHYOR Data Centre

Director: J.L. Delcroix

Address: Laboratoire de Physique des Plasmas
Université de Paris-Sud
91405 Orsay
France

Total staff:

Data type: atomic and molecular properties (e.g. energy levels, lifetimes, etc.) interactions between particles (e.g. collision cross sections, ...) and macroscopic properties (e.g. transport coefficients,...) basic to gas and plasma physics.

Compilation type: bibliographic, computerized
numeric, computerized

Publication/Product: data centre service for both selected bibliographic and numerical data retrievals. Service is not free.

Title: (Individual effort)

Compiler: Professor Kazuo Takayanagi

Address: Department of Space Science
Institute of Space and Aeronautical Science
University of Tokyo
Komaba, Meguro-ku
Tokyo, Japan

Total staff: 1

Data type: Atomic collisions

Compilation type: bibliographical, not computerized

Publication/Product: The following reports have been published (in English)

1. Rotational and vibrational transitions in molecular collisions (experimental, 1927-1964) (1966)

2. Ionic impact (experimental, 1923-1965) (1967)

3. Ionic impact (experimental, 1966, 1967) (1968)

4. Heavy particle collisions with electronic transitions (theoretical, 1964-1967) (1969)

5. Electron collisions with atoms and molecules (experimental, 1921-1960) (1969)

6. Electron collisions with atoms and molecules (theoretical, 1924-1963) (1971)

7. Electron collisions with atoms and molecules (experimental, 1961-1967) (1973)

8. Electron collisions with atoms and molecules (theoretical, 1964-1967) (1974)

9. Electron collisions with atoms and molecules (theoretical, 1968-1970) (1975)

Title:	Atomic data study group
Group leader:	Prof. H. Suzuki *
Address:	Institute of Plasma Physics Nagoya University/Furoo-cho, Chigusa-ku Nagoya 464, Japan
Others on staff:	Professor Kazuo Takayanagi Professor Junji Fujita Dr. Shunsuke Ohtani
Total Staff:	10 physicists (part-time) 10 scientists (part-time/advisors)
Data type:	atomic collision and atomic and molecular spectroscopic data
Compilation type:	numerical data, not computerized
Publications/Product:	"Data Compilation of Cross Sections on Atomic Processes", Vol. 1 (May 1975) IPPJ-DT-48. Editor: Prof. K. Takayanagi (Institute of Space and Aeronautical Science, University of Tokyo). Content: radiative and collision processes involving hydrogen isotopes, their ions and electrons.

* Guest staff from Faculty of Science and Technology, Sophia University, Japan

Title:	(Individual Effort (?))
Compiler:	M. Outred
Address:	Department of Physics The Polytechnic of North London London, England
Total staff:	1 (?)
Data type:	Infrared atomic wave numbers
Compilation type:	numerical, computerized
Publication/Product:	"Infrared Atomic Wavenumber Library" described in Infrared Physics, Vol. 13, pp. 131-133 (1973) - (Free service for IR spectroscopists)

Title: Controlled Fusion Data Center (of the Holifield National Laboratory)

Director: Dr. C.F. Barnett

Address: Holifield National Laboratory
P.O. Box X, Bldg. 6000
Oak Ridge, Tennessee 37830
USA

Total staff: 1 full-time professional
3-4 part-time professionals
2 non-professionals

Data type: Atomic and molecular collision processes

Compilation type: bibliographic: computerized
numerical: not computerized

Publications: Bibliographic Series, ORNL-AMPIC

Atomic Cross Sections of Interest to Controlled Fusion Research (to be published) (revision of earlier publication). Earlier compilation published as ORNL-3113.

Four books in the Wiley-Interscience series in atomic and molecular collisional processes have been published as part of this center's activities:

- Ion-molecule Reactions, E.W. McDaniel et al,
- Theory of Charge Exchange, R.A. Mapleton,
- Dissociation in Heavy Particle Collision, G.W. McClure and J.M. Peek,
- Excitations in Heavy Particle Collisions, E.W. Thomas.

Title:	Data Center for Atomic Transition Probabilities and Atomic Line Shapes and Shifts
Director:	Dr. W.L. Wiese
Address:	Optical Physics Division National Bureau of Standards Washington, DC 20234 USA
Total staff:	
Data type:	radiative transition probabilities of atoms and atomic ions in the gas phase
Compilation type:	bibliographic; computerized numerical; not computerized
Publications:	Bibliography on Atomic Transition Probabilities NBS special publication 320 + supplements Numerical Tables of Critically Evaluated Transition Probabilities NBS reports + others

Title:	Atomic Energy Levels Data Center
Principal Investigator:	Dr. W.C. Martin
Address:	Optical Physics Division National Bureau of Standards Washington, DC 20234 USA
Total staff:	
Data type:	Atomic energy levels and spectra
Compilation type:	bibliographic; computerized numerical; not computerized
Publications:	"Bibliography on Atomic Energy Levels and Spectra - July 1968 through June 1971". NBS special publication 363 (June 1972) "Selected Tables of Atomic Spectra", additional sections of NSRDS-NBS-3

Title:	Data Center for Atomic and Molecular Ionization Processes
Principal Investigator:	Dr. H.M. Rosenstock
Address:	Physical Chemistry Division National Bureau of Standards Washington, D.C. 20234 USA
Total staff:	
Data type:	atomic and molecular ionization and appearance potentials
Compilation type:	bibliographic, not computerized numerical, not computerized
Publications:	"Ionization Potentials, Appearance Potentials and Heats of Formation of Gaseous Positive Ions", NSRDS-NBS 26

Title: X-ray and Ionizing Radiation Data Center

Director: Dr. J.H. Hubbell

Address: Center for Radiation Research
National Bureau of Standards
Washington, DC 20234
USA

Total staff:

Data type: attenuation coefficients for high-energy photons

Compilation type: bibliographic, not computerized
numerical, not computerized

Publications: Photon Cross Sections, Attenuation Coefficients and Energy Absorption Coefficients from 10 keV to 100 GeV. NSRDS-NBS 29.

Title: Atomic Collision Cross Section Information Center

Director: Dr. E.C. Beaty

Address: Joint Institute for Laboratory Astrophysics
University of Colorado
Boulder, Colorado 80302
USA

Total staff:

Data type: low energy atomic collision cross section data needed in astrophysics

Compilation type: bibliographic, computerized
numerical, computerized

Publications: "Bibliography of Low Energy Electron Collision Cross Section Data".
(User service ?)

Title:	Surface Science Center, CTR Programmes
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