The IAEA database for Chemical Erosion, Physical Sputtering and Radiation-Enhanced Sublimation: History, Current Status and Future Directions

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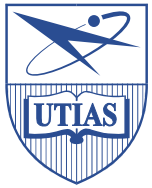


IAEA Technical Meeting on "Improving the Database for Physical and Chemical Sputtering"

Mon-Tue 12-13 December 2011

Outline

- History, and the objectives of APID 7A & 7B
- Current status
- Improvements and additions to the database

History

- Coordinated Research Program (CRP) on:

  "Plasma-Interaction Induced Erosion of Fusion Reactor Materials"

- 1992 – 1997
- Participants: Tony Haasz (Toronto)
  Egon vietzke (Juelich)
  Wolfgang Eckstein (Garching)
  Yoshi Hirooka (UCSD)
  Maria Guseva (Moscow)
  Kenji Morita (Nagoya)
  Luo Zhengming (Chengdu)

History

- 1-D physical sputtering calculations, and accelerator-based erosion measurements were perceived as a mature field
- Decision was made to compile data, particularly for Be, C and W

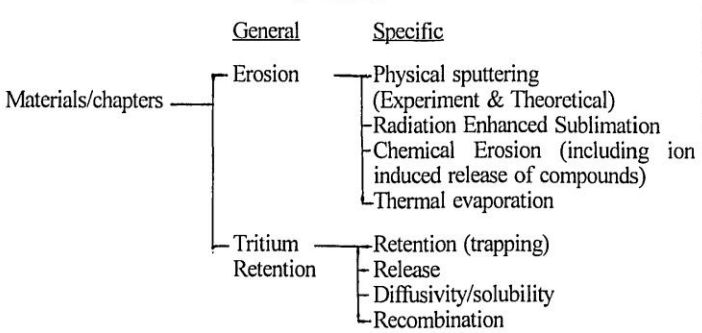
Table 2. Publication Plan for Final Document of CRP

1. Schedule
   Meeting for final discussion of publication
   (Summer 1996)

2. Format
   Data - handbook presentation for ITER (or equivalent) designers; similar to Nucl. Fusion Supplement, Vol. 4 (1993)

3. Contents (general)
   a) Erosion yield data
   b) Retention data (including diffusivity and solubility); materials to be included: Be, C, W and their compounds

4. Report structure



5. Content (detailed/chapters)
   (contributors, *=lead contributors)

5.1 Be	*	Y. Hirooka	5.1.1	Pure Be including HIP and LPPS
		W. Eckstein	5.1.2	BeO
		M. Guseva	5.1.3	BeC
		R. Langley	5.1.4	Other
5.2 C	*	A. Haasz	5.2.1	Pure C including pyrolytic, isotopic, films
	*	E. Vietzke	5.2.2	Doped C including B-, Ti-, Si- doped
		M. Guseva	5.2.3	Redeposited C
		W. Eckstein	5.2.4	Other
		R. Langley		
5.3 W	*	W. Eckstein	5.3.1	Pure W including LPPs, CVD, HIP
		K. Morita	5.3.2	WO
		Y. Hirooka	5.3.3	WC
			5.3.4	Other

   5.4 Back-up materials; e.g. Li, V5Cr5Ti, other

6. Responsibilities for chapter contributors
   6.1 Collection of data
   6.2 Formulation of comments/remarks with statement of completeness
   6.3 Critical assessment of data
   6.4 Consideration of uncertainty (accuracy)

Objectives of APID 7A & 7B

- To provide a comprehensive database of erosion data for other members of the fusion community
  - ➢ Specifically for modelling
- Essentially, we compiled all of the data we could find.
  - ➢ Data extracted from papers as necessary
  - ➢ Analytic or Empirical fits created for all data sets

Data Presentation

- All data sets are displayed along with the empirical fitting equations
  - Equation coefficients given in tables
- Various experimental parameters were identified:
  - Incident species/target materials
  - Energy, temperature, etc.
  - Author, research lab

IAEA Website

- All data were subsequently made available on the IAEA website
- Allows searches by species, authors, etc.

Problems with Database 1

Too Much Information

Problems with Database 1

Too Much Information

- The database is not as useful to non-experts as we would like.
- Problems primarily with Chemical Erosion section.
  - Non-experts need a simpler way to access simpler information
  - Current practice is to use specific papers, rather than the IAEA database.

Problems with Database 2

- We previously considered ignoring certain data sets, promoting others, or displaying bands on graphs.
  - ➢ Significant drawbacks to each

- In the end, the APID reports have a front section with chosen “characteristic results”, but we did not provide “endorsed” data sets.
  - ➢ Hard to see how this could be done

Physical Sputtering 1

- Generally good agreement between experimental and computational results.
  - Data compiled by Eckstein
  - Limited number of labs involved (Garching)

- Fitting equations are based on physics, and have some predictive capability.
  - This is very useful for modellers

Physical Sputtering 2

- This data is fairly accessible, and there are several other locations where this data is available.
- Dataset was recently updated by Eckstein (2009)
- Add data for other target materials?
- We may not wish to do anything here.

Radiation-Enhanced Sublimation 1

- This section is very comprehensive
  - Little experimental data obtained since (any?)
  - Reasonable consistency amongst different labs (few involved)
- Fitting equations (exponentials) also have physical meaning and predictive capability.
- Unfortunately, not currently a high-profile topic.

Radiation-Enhanced Sublimation 2

- Suggestions:
  - Reduce data available on website to 3-4 graphs
  - Temperature dependence for different incident species
  - energy dependence
  - Flux dependence
  - Leave out mixed materials
- Consider adding high temperature erosion of Be, etc.?

Chemical Erosion 1

- This is where an accessible database is most needed, but where our current database has not been very effective.
- Different experimental techniques, and small differences in experimental conditions lead to very large differences in results
  - Experiments are challenging
  - Many complicating factors
- In particular, small concentrations of elements other than carbon have a large effect on chemistry.

Chemical Erosion 2

- Can we be more selective?
- Is it better not to ?

Summary of Current Database

- Heroic efforts were required to prepare the current database.
  - Jeff Stephens, Wolfgang Eckstein and myself each contributed 100's of hours to this project
- This has produced a comprehensive data compilation which I find very useful and consult frequently, but this was not the objective.
- We must be more clear in setting objectives for any extensions.

Future Directions

- Main areas of advancement in the fusion materials erosion field are:
  - Plasma erosion experiments
  - Plasma deposition/material mixing experiments
  - MD calculations
  - Dynamic and multi-dimensional calculations
- There has also been more experimental work done on doped materials.

Plasma Experiments 1

- Erosion database greatly extended.
  - ➢ low energies
  - ➢ high fluxes
- Results highly relevant to fusion reactors.
- Results largely complementary to Accelerator measurements.
- Not a mature field.

Plasma Experiments 2

Questions:

- What aspects of this work would make sense to include on the IAEA database?
  - Should retention be included?
  - Material modification?
- Who would the audience be?

Molecular Dynamics Calculations

- Quite different from current database.
- New field.

Questions:

- What would go in a database?
- Who would be the audience?
  - ➢ Possibly a database primarily for the MD community?

Dynamic Modelling

- Extensions to current physical sputtering database.
- More mature field.
- Systems extremely complex

Questions:

- Can we come up with general rules associated with:
  - The effect of surface roughness
  - Timescales for compositional changes
  - Timescales for geometric changes

Summary

- Having an open database providing general results on various plasma-surface interaction processes is very useful, but requires a lot of effort.

- There are a number of things we can do to improve the current database, and perhaps, we are at the point where it makes sense to add new topics.