Summary of the IAEA Technical Meeting on Improving the Database for Physical and Chemical Sputtering, December 12-13, 2011

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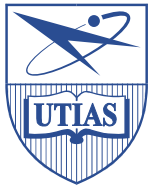

IAEA Technical Meeting on “Ab Initio Methods for Plasma-material Interactions in Fusion Devices"

Wed-Thur14-15 December 2011

Outline

- History, and the objectives of APID 7A & 7B
- Improvements to current database
- Additions and Extensions
  - MD calculations
  - Non-MD calculations
  - Experiments

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

Objectives of APID 7A & 7B

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

IAEA Website

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

Problems with Database

- Significant advances since 1995
- The database is not as useful to non-experts as we would like.
- Problems primarily with Chemical Erosion section.
  - Wide range of data

Physical Sputtering

- 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

Radiation-Enhanced Sublimation

- 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.

Chemical Erosion

- 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.
- New data available from plasma devices

Improvements to current database

- Firstly, we agreed that data evaluations and recommendation should be the focus of improving the current database, however, it was acknowledged that it would be very difficult to do so at the present time.

- We recommend that the IAEA identifies this as a key action for all new activities.

Additions and Extensions: MD calculations

1) Compile from available publications MD calculations (reflection, sticking, erosion) for:

   i) H, CH, CH_2, CH_3, CH_4 → C, a-C:H

   ii) H → Be, W

   iii) H → mixtures of Be, C, W (ie., BeC, W_2C)

- H plus isotopes (D,T)
- preference for validated data
- For the process (H → any) MD calculations would be needed to provide rates for the production of H_2. Information about production of vibrationally (ro-vibrationally) excited H_2 is completely absent from the database.

Additions and Extensions: MD calculations

2) MD calculations providing input for retention calculations:

- low-energy hydrogen implant data
- input data for models dealing with longer time-scales (reaction rates, Kinetic Monte-Carlo, ...)
- calculations of probability rates, eg., diffusion coefficients

Additions and Extensions: MD calculations

3) MD calculations of surface chemistry

- including atomistic microstructure changes, amorphization

4) Database of MD methods, procedures and technical parameters

- eg., temperature control, surface preparation strategy
- suitable for Wiki pages? largely for internal use by MD community

Additions and Extensions: Non-MD calculations

5) Time (fluence) scaling for macroscopic surface morphology changes

- removal (growth) of surface structures as a function of size
- No data available, requires a new study by Ralf

Additions and Extensions: Non-MD calculations

6) Organization of simple models or codes for erosion, sticking, etc.

- Simple inputs/add-ons for boundary plasma codes
- One-dimensional codes based on diffusion model and reaction rates could easily be coupled to edge plasma codes.
- Need to inventorize what is already available and used as part of larger code packages such as UEDGE and SOLPS; note also the work by C. Björkas at FZJ.

Additions and Extensions: Non-MD calculations

7) Mixed material sputtering

- Extend current physical sputtering database to include (specific) mixed materials and compounds, eg., BeW, etc.
- Identify the microstructures to be studied following Kai Nordlund
- Largely involves future work, but database could be started

Additions and Extensions: Experiments

8) Plasma material modifications

- general parametric expressions (and data) for Be/C mixing, Be/W mixing, codeposition D/Be ratio, etc.
- results available in publications; need to be collected

9) Mixed material preferential sputtering

- some papers available

Additions and Extensions: Experiments

10) High temperature erosion

- Similar to RES, but for metals
- Data available for Be, W, etc.

Summary

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

- The focus will be more to extend the database, than to improve the accessibility of the current material content.