

PMI Issues for A+M Data Unit

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PMI Key Issues

Primarily

- Erosion (mainly physical and chemical sputtering)
- Hydrogen (tritium) retention and exhaust

But related to that one must be able to model

- Surface composition dynamics
- Surface structure modifications

Due to

- Plasma exposure (hydrogen and impurities, including molecules)
- Radiation
- Thermal history
- Both routine and non-routine exposure

Fundamental Modelling Tools

- Time-dependent DFT, DFT-TB Molecular Dynamics
- Classical Molecular Dynamics
- Binary Collision Approximation dynamics
- Kinetic Monte Carlo

Always need for parameterizations, e.g. of DFT-TB parameters or of MD potentials.

How to parameterize?

Output of basic modelling

Models at fine scale provide data for models at larger scales.

- Nicest case: results of fine scale calculations can be parameterized; e.g. PMI reduced to sticking coefficients, reflection coefficients, sputtering coefficients.
- Also good case: Results of fine scale calculations can be used to optimize reduced models; they provide coefficients to be used in some coarse-grained transport model that can be coupled to other calculations. Coefficients can depend on other parameters defined at the larger scale.