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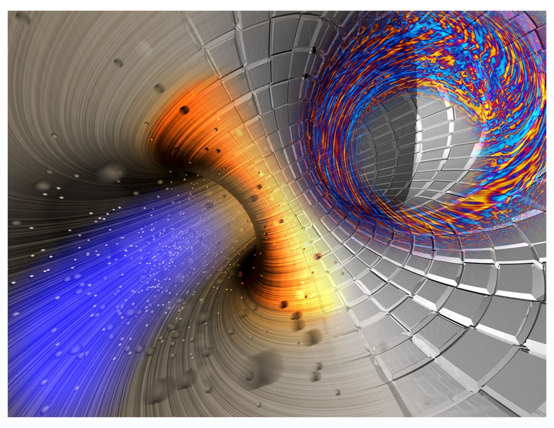
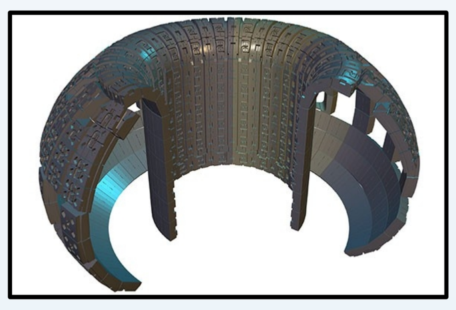
# Molecular Dynamics Simulations of the Sputtering Behavior of Mixed Be/C-Materials



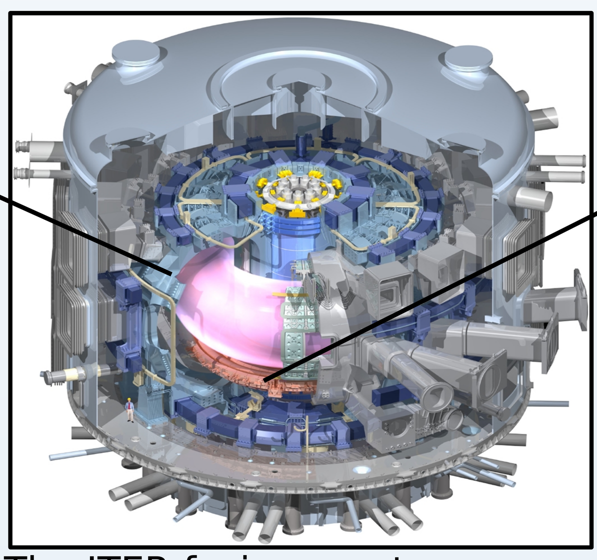
Association Euratom-Tekes

## Introduction

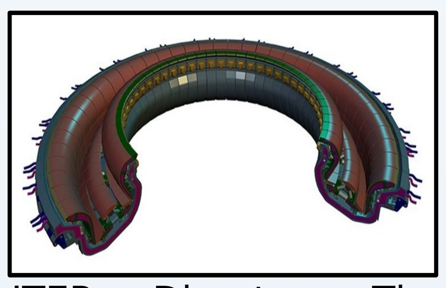
**Molecular dynamics (MD) computer simulations have shown that both carbon(C) and beryllium(Be) erosion at low impact energies can be explained by a special type of chemical sputtering, where the incoming energetic ion enters between two substrate atoms, forcing them apart if its kinetic energy is low enough that it spends a substantial amount of time between the atoms.**



ITER Blanket. The plasma-facing first wall will be covered with beryllium.



The ITER fusion reactor

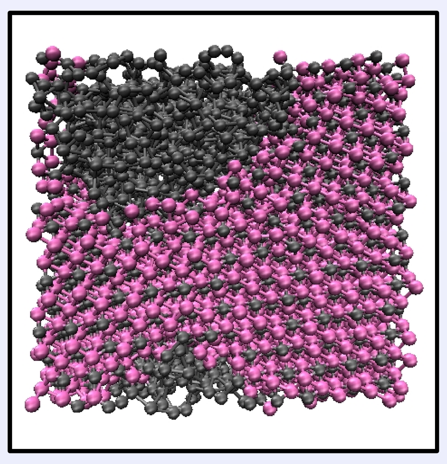


ITER Divertor. The strike points will be made of carbon composite.

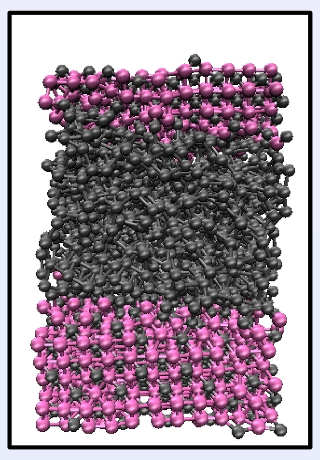
Erosion, and subsequent transport and redeposition, will cause wall materials to mix in the surface layers of the inner wall of fusion devices. Thus an understanding of the sputtering behavior of these mixtures is crucial.

## Simulations

- Simulation cells were created with different concentrations of Be and C.
- The cells were annealed by heating to 5000K and slowly cooling, which resulted in a separation of areas of amorphous C and crystalline $Be_2C$.
- Cells with periodic borders in x-, y-directions were bombarded perpendicularly with 10-100 eV D ions.
- After each consecutive impact the cell was allowed to cool, and was shifted randomly before the next event for an even flux over the whole surface.
- The MD code PARCAS was used for all simulations.

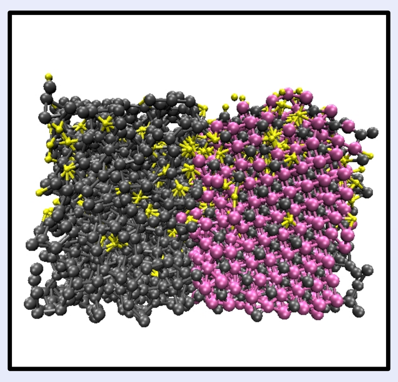


Annealed BeC cell with 4500 atoms, height of cell ~ 40 Å

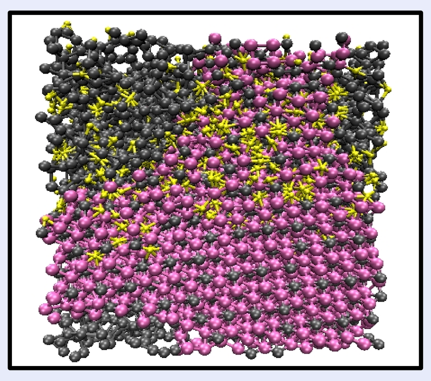


Annealed BeC2 cell with 3000 atoms and $Be_2C$ surface, height of cell ~ 40 Å

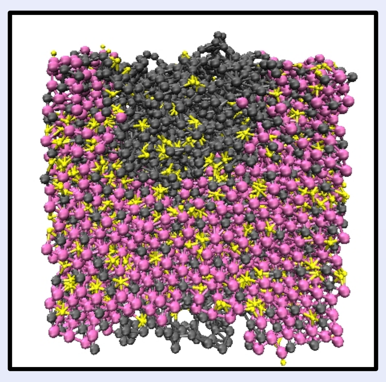
After 2000 D impacts (grey = C, pink = Be, yellow = D)



20 eV

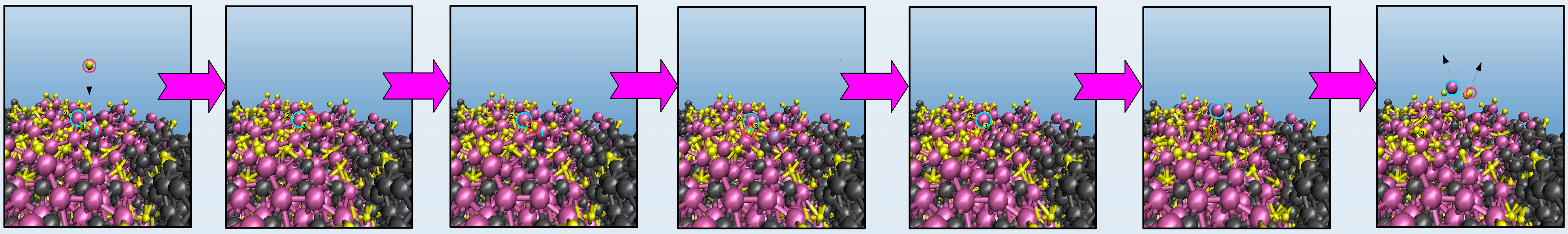


50 eV



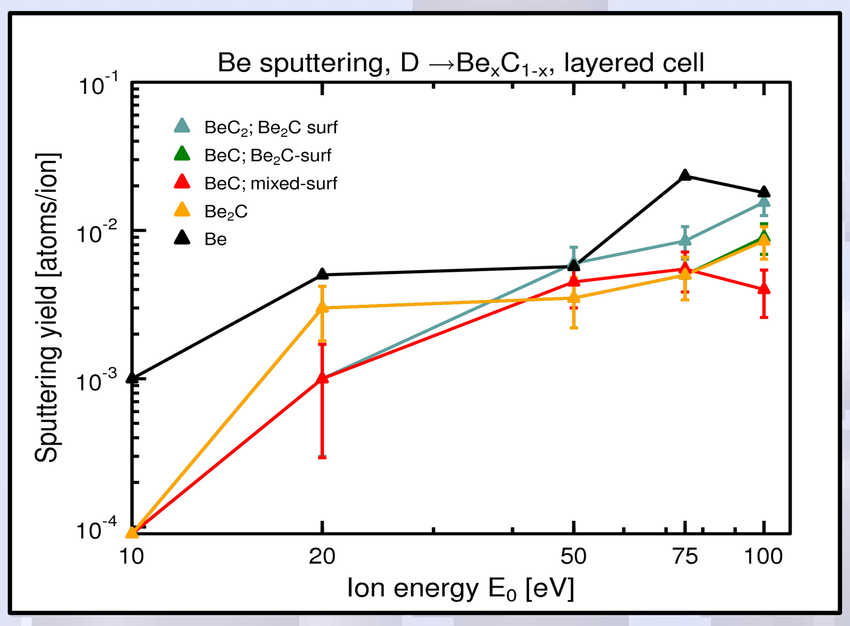
100 eV

## Swift chemical sputtering

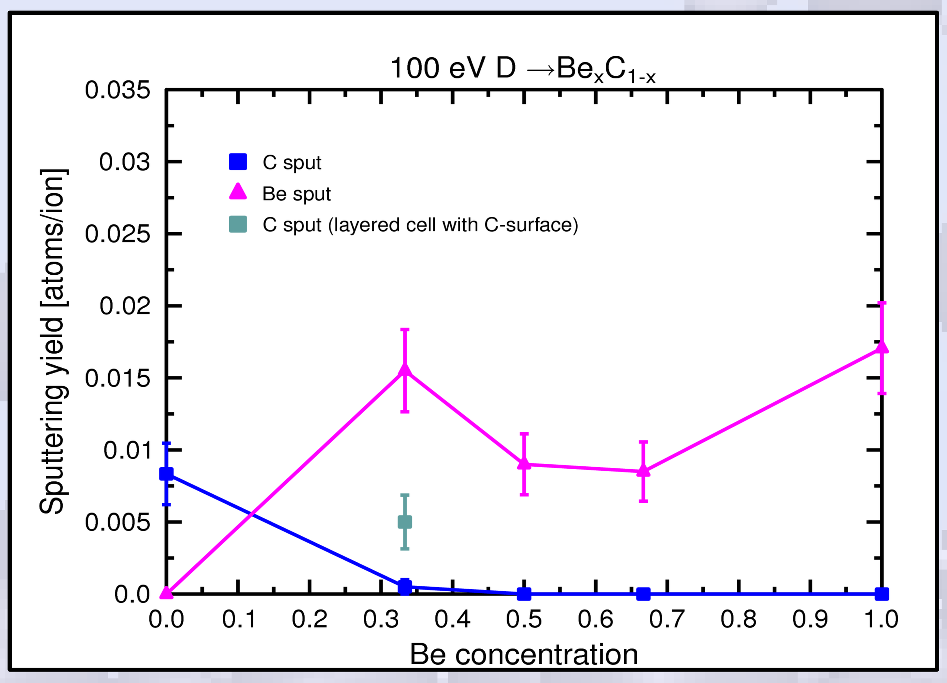


- A recently discovered method of erosion is swift chemical sputtering (SCS), which can occur when low-energy ions enter between two surface atoms, breaking their bond and allowing the freed atom or group of atoms to escape. SCS has been experimentally observed from hydrogenated carbon surfaces.
- The picture series shows impact of a 20 eV D ion, and subsequent sputtering of a BeD molecule and a $D_2$ molecule.

## Results




Be sputtering yield at different energies and surface compositions

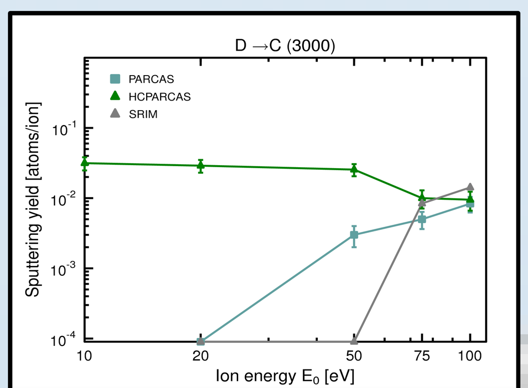



Sputtering at 100 eV for different concentrations of Be, where the mixed cells had a $Be_2C$ surface, and one test case with a C-surface in a cell with 33% Be

- The level of sputtering depended on whether the surface layer was Be, $Be_2C$ or C, regardless of what the concentration of Be was in the whole cell.
- $Be_2C$ sputters slightly less than pure Be, due to the stronger carbide binding.
- The relatively high Be sputtering from surfaces with 50% C and 50% $Be_2C$ indicates a high tendency to sputter from grain boundaries.

## Future work

- Simulations of C sputtering with different MD methods show variation in results:




- The code HCPARCAS uses a more detailed calculation method, and is ideally suited to treating the bonding behavior of hydrocarbons.
- HCPARCAS will in the future be extended to include elements such as Be, and the effect of this on sputtering yields for $Be_2C$ will be investigated.

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