Strathprints Institutional Repository

Bell, Andrew M and Brown, Richard E and Mulheran, Paul A (2015) Multi-scale chemistry modelling for spacecraft atmospheric re-entry. In: Faculty of Engineering Research Presentation Day 2015, 2015-06-24 - 2015-06-24. (Unpublished) ,

This version is available at http://strathprints.strath.ac.uk/57260/

Multi-scale Chemistry Modelling for Spacecraft Atmospheric Re-Entry

Andrew M Bell[1], Richard E Brown[2] and Paul A Mulheran[1]

1- Chemical and Process Engineering, University of Strathclyde, Glasgow (a.bell@strath.ac.uk)
2- Mechanical and Aerospace Engineering, University of Strathclyde, Glasgow

Project Overview

We aim to develop a model capable of simulating the surface chemistry and material erosion involved when a re-entry vehicle descends through the atmosphere. Our starting point is to simulate the erosion of a fcc crystal slab due to cluster bombardment, using the model Lennard-Jones potential. From this, we plan to scale up towards Direct Simulation Monte Carlo approaches for the gas dynamics above the surface.

Image Credit: cFASTT
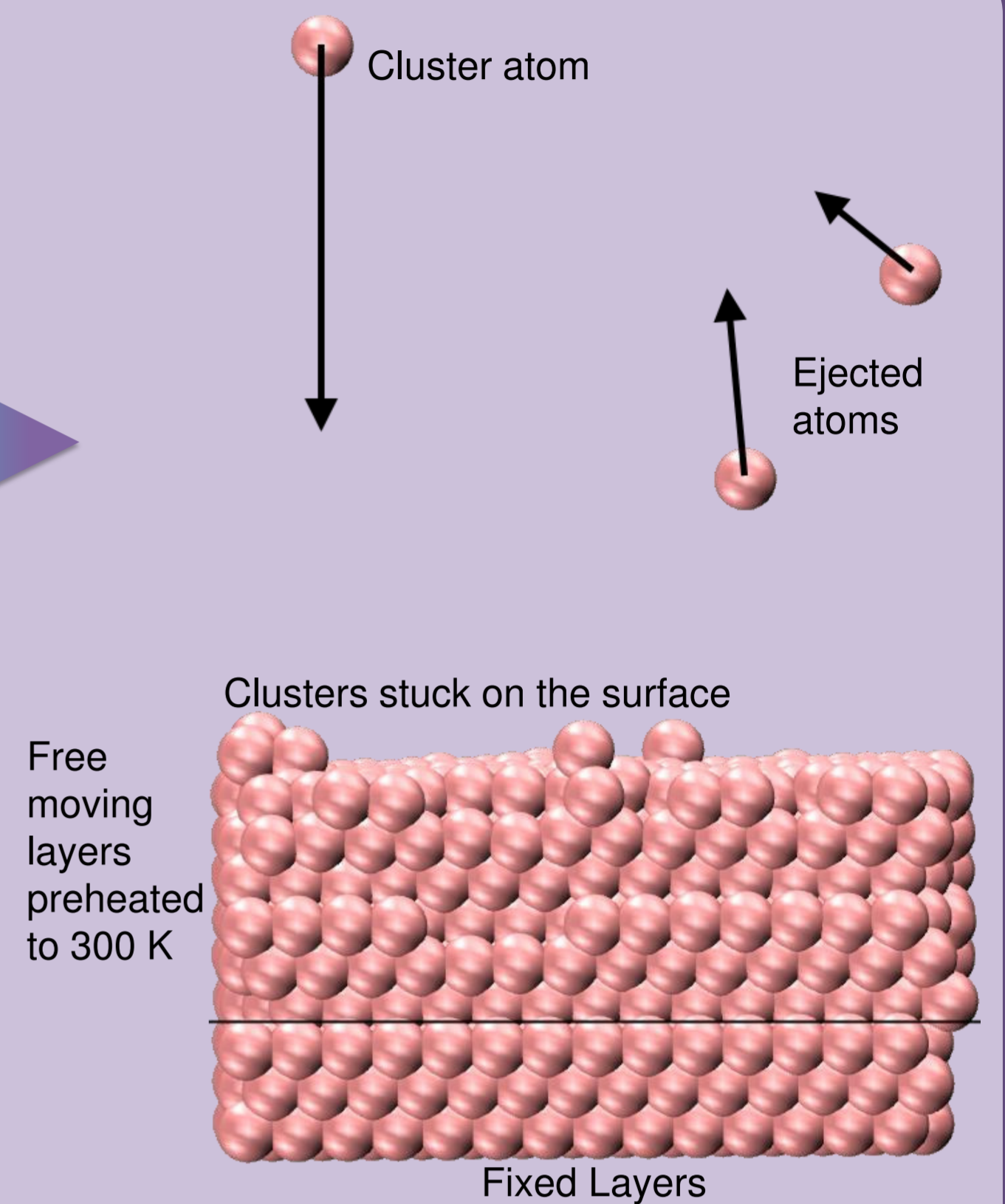
Simulation

A slab generator was created to build slabs, which will be used to represent the surface of a spacecraft, with the specified dimensions and the correct crystallographic surface on the top of the slab. The slab was then forced to relax with a slab minimizer, reducing the slab's potential energy to its minimum. From there, the free layers were allowed to move but the slab's temperature was controlled with a thermostat, scaling the energy of the slab's movements until it reached 300K.

To simulate the erosion effects on the slab, monatomic clusters, which will be used to represent the air in the upper atmosphere, were added above the slab's surface. These were given random positions above the slab's surface and were impacted with a pre-set energy at a fixed angle to the surface. If the cluster atom fails to attach to the surface or a surface atom is ejected from the surface, details of the atom are recorded to provide an insight into the behaviour of the slab.
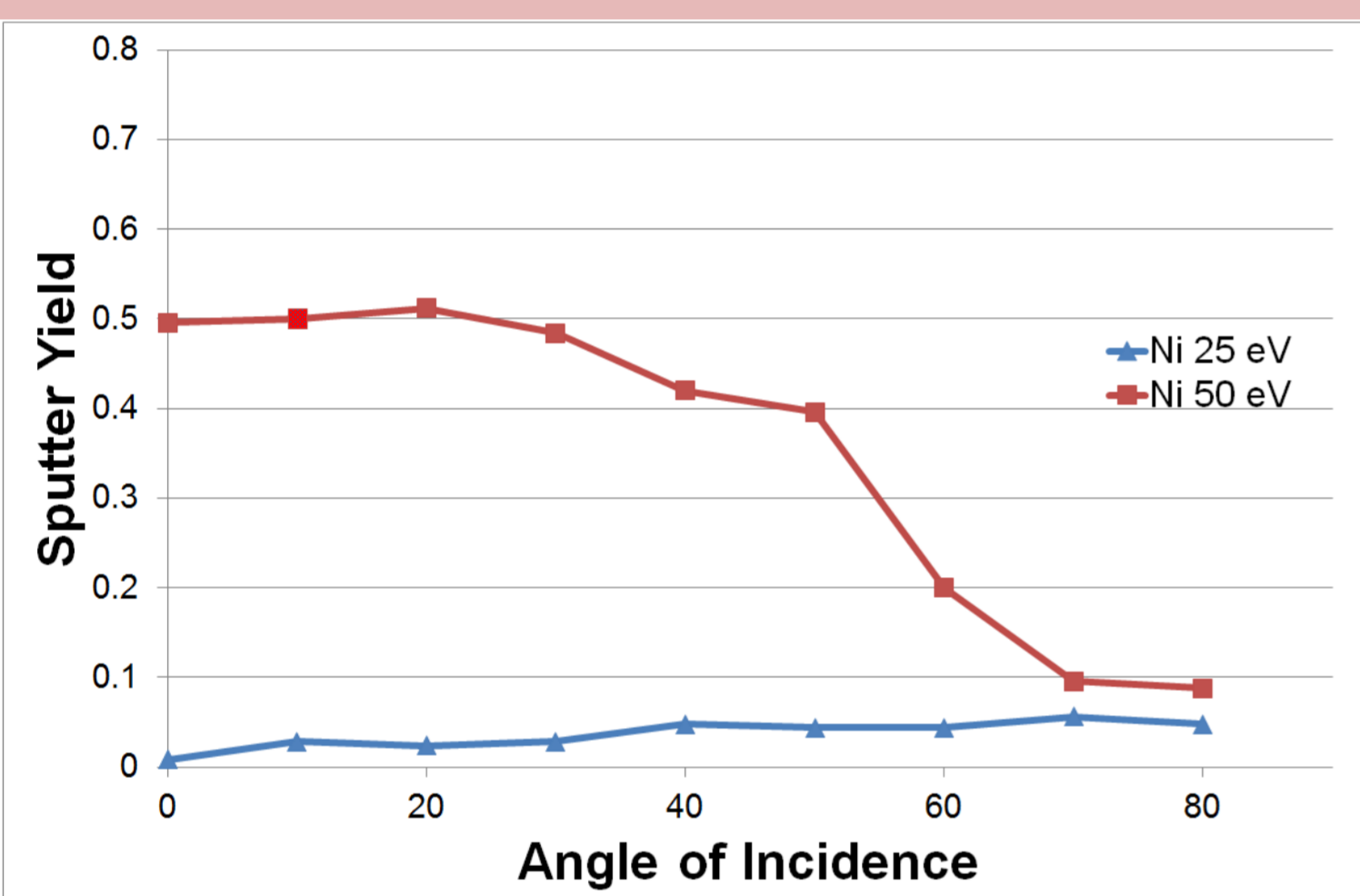
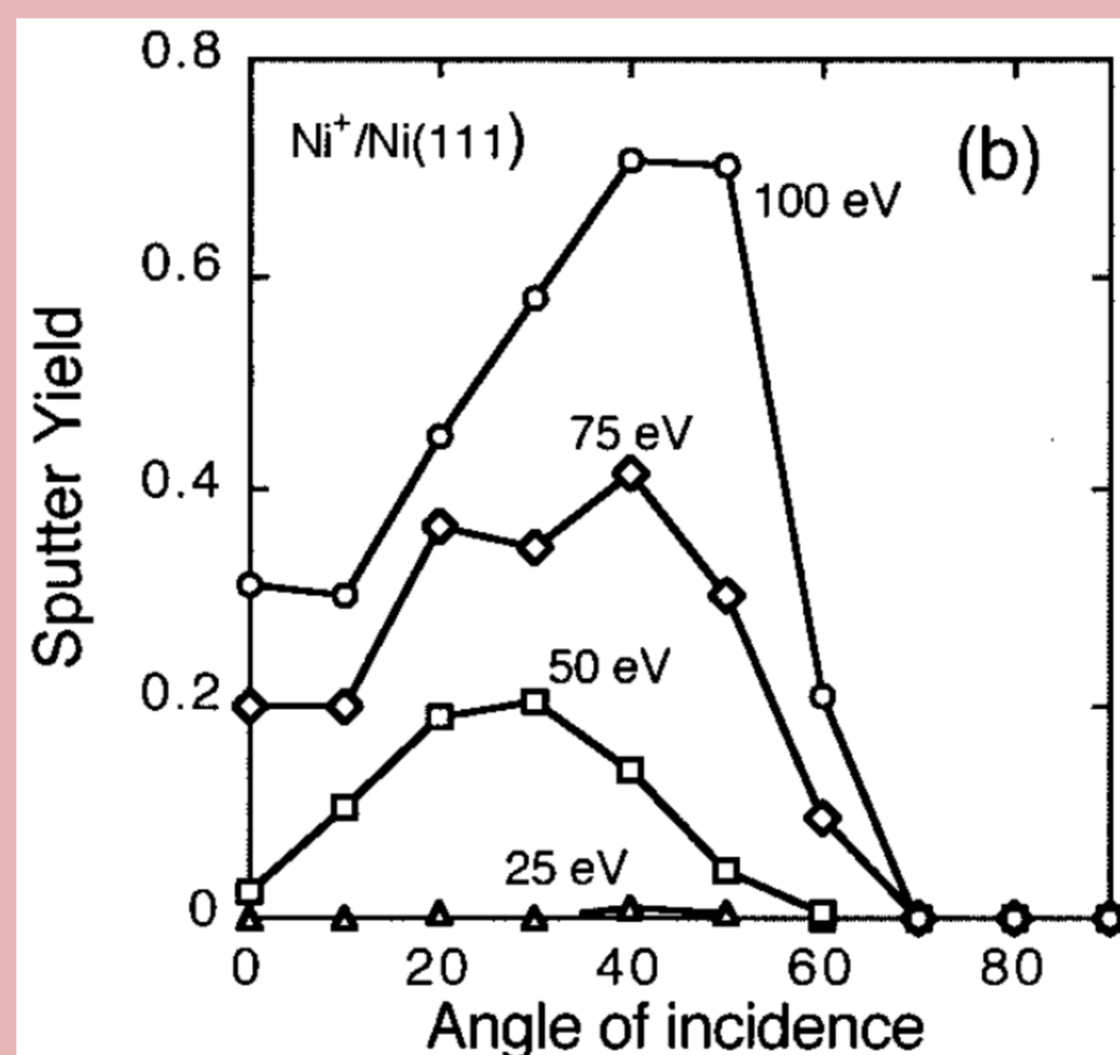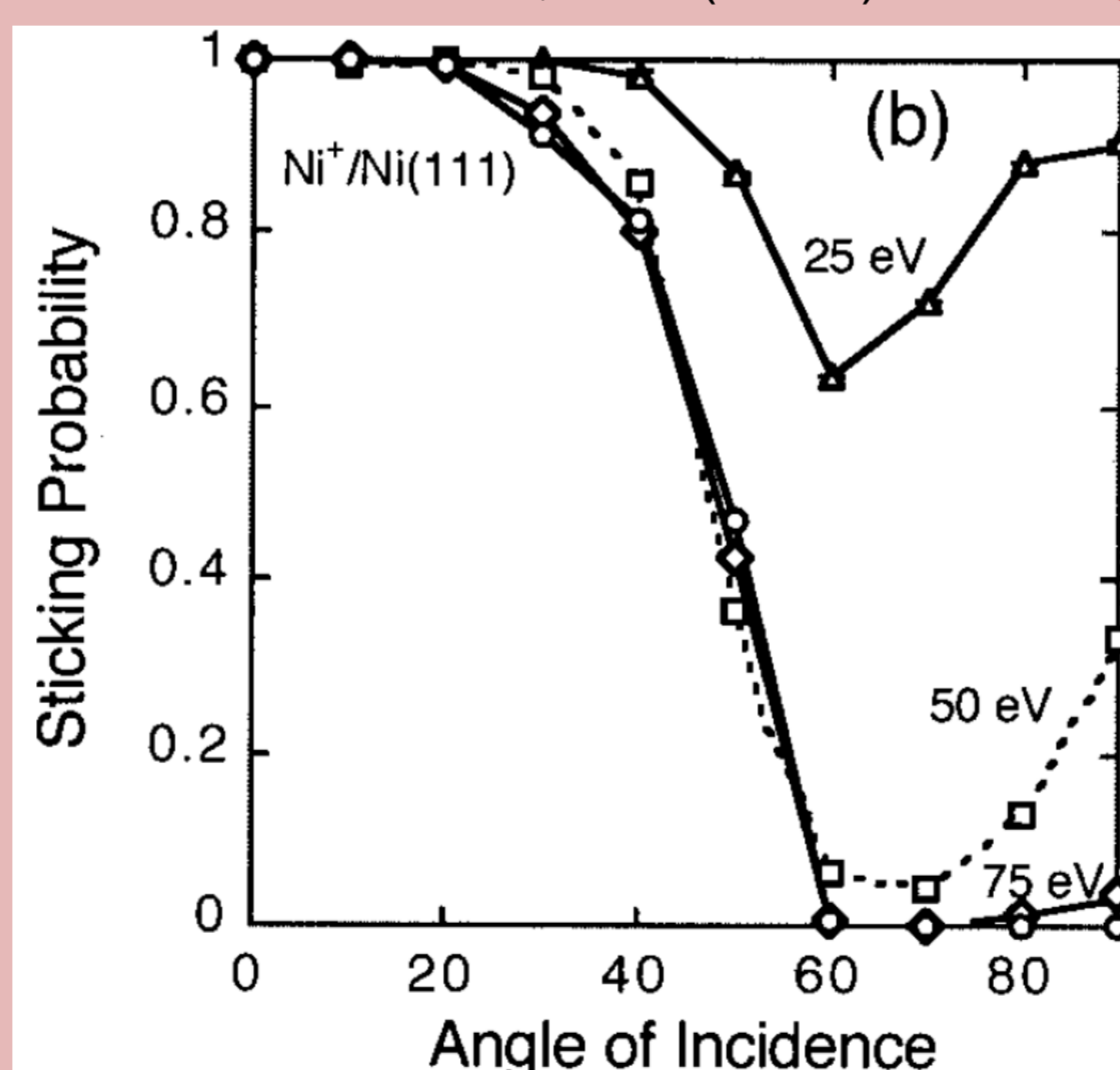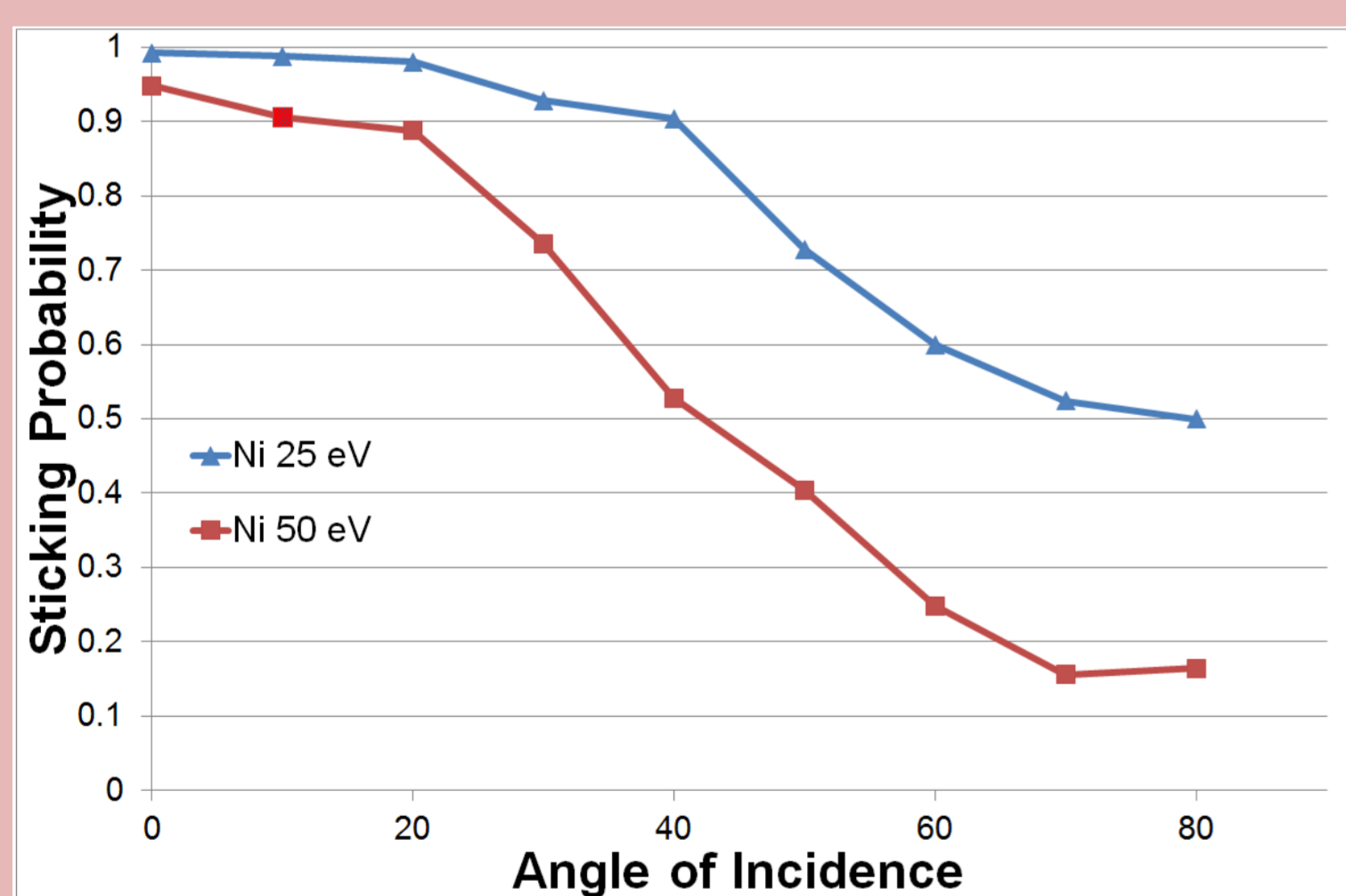Results obtained from simulations performed with the code created during the project

Image Credit: Hanson et al; J. Vac. Sci. Technol. A 19, 820 (2001)

Results

There is a poor correlation between datasets for the sputter yields especially for more energetic impacts at low incident angles.

The sticking probabilities didn't recover as expected above 60 degrees and didn't decrease as rapidly as expected for 50 eV between 30 degrees and 60 degrees.

From this, it can be concluded that Lennard-Jones potential can't capture the behaviour of the metal slabs accurately so a new model is needed.

Future Work

Retry comparison using the Sutton-Chen model

Move on to gas molecule impacts

Include reaction chemistry on the surface

Scale the model up towards DSMC scale