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Modelling of metal nanostructure growth

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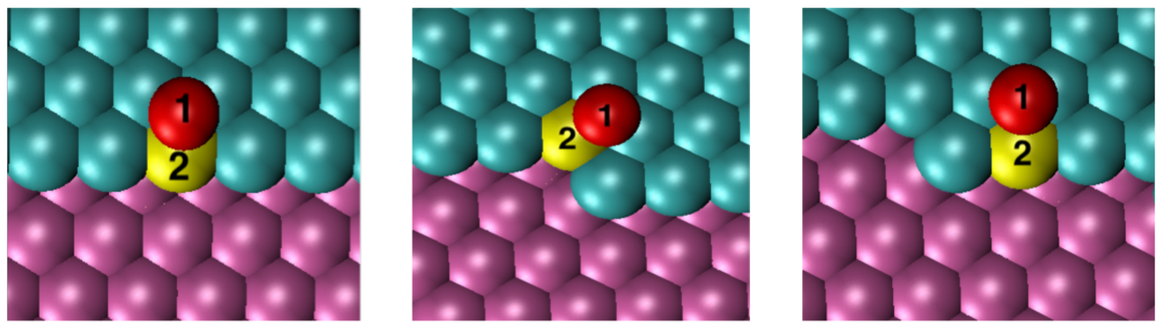
Introduction

- In the FEBID process, metal atoms are deposited on a substrate with the goal of forming a metal nanostructure with desired properties.
- My project involves simulations of the growth of nanostructure from the deposited metal atoms.
- The goal is to identify how the growth mode depends on the conditions such as temperature, growth rate, etc.
- This requires calculations of the mechanism and rate of the various atomic rearrangements that can take place.
- In the calculations carried out so far, the interaction between the atoms has been described using the effective medium theory (EMT) to describe the atomic interactions.
- We identify the mechanism by which an atom that lands on top of a metal island can descend to a lower layer. This is known to be a central issue determining whether the metal grows layer-by-layer or forms three dimensional islands.
- The down stepping of Au adatom on Au (111) via exchange mechanisms at straight step edges, near kinks and at kinks has been studies.
- The down stepping near (but not at) kinks has been shown to explain re-entrant layer-by-layer growth of Pt (111) [1].

Theoretical Methodology



(a) **(b)** **(c)**

Figure 1: Descent of adatom to lower layer on Au (111) island **(a)** at straight edge **(b)** at kink site **(c)** near kink

- We used kinked and stepped surfaces (of large enough size to get convergence) of **Au** for our studies .
- and determined the minimum energy paths for the descent of an adatom at straight B-edge, near a kink on B-edge and at kink on B-edge .
- In all processes Au adatom is starting from minimum to a high energy site bonded to the three ninefold coordinated atoms.
- The paths were calculated using the nudged elastic band (NEB) method.

Results and Discussions

- EMT results in **figure 2.** illustrate the down stepping of Au adatom at straight edge **(i)**, at kink **(ii)** and near kink **(iii).**
- The energy barriers for these processes were calculated to be **0.20 eV** for straight B-edge, **0.14 eV** for down stepping near a kink and **0.24** eV for down stepping at kink on the B-edge.
- This shows that down stepping near kinks **(ii)** is significantly faster than down stepping at kinks **(iii)** or at straight edges **(i)** at room temperature.
- Also, similar trend was found for A-type: **0.24 eV** for straight A-edge, **0.22 eV** for down stepping near kink and **0.26 eV** for down stepping at kink on the A-edge.

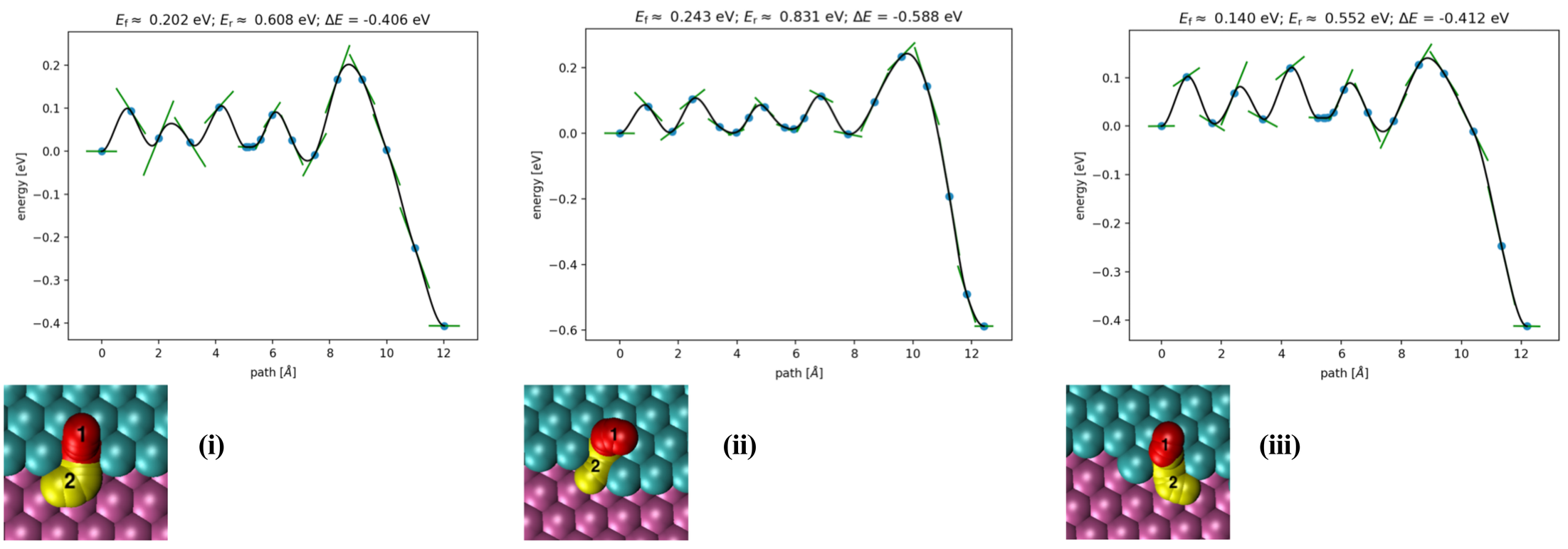


Figure (2). Down stepping of Au adatom at B-edge on Au(111) island **(i)** straight edge **(ii)** at kink **(iii)** near kink.

Future Plan

- In order to study these processes with high accuracy, we are moving towards DFT calculations. The results will be used in Kinetic Monte Carlo simulations of Au nanostructure growth.

References

[1] Jónsson H, Annu. Rev. Phys. Chem, **51**, 62-53 (2000)

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