kinetic Monte Carlo Simulations (kMC)

Author: Jingyuan Liang — Electrical Engineering, SURF 2013, Purdue University
Faculty Mentor: R. Edwin Garcia
Graduate Mentor: Ding-Wen (Tony) Chung
Collaborator: David Ely

1. INTRODUCTION

kMC is a set of scientific libraries designed to deploy kinetic Monte Carlo simulations (kMC). kMC allows the user to intuitively generate single component crystal lattices to simulate, post process, and visualize the kinetic Monte Carlo-based dynamics of materials.

Philosophically, kMC was designed to directly interface with any kinetic Monte Carlo application and to provide a uniform, user friendly interface to rapidly deploy advanced simulations.

Organizationally, kMC is a virtual portal to couple and integrate multiple length scales computational materials science applications, such as OOF, FiPy, etc.

Specifically, kMC provides a very flexible Python application programming interface (API) that allows to rapidly program complex atomistic simulations, while simultaneously taking advantage of the speed of the C++ core infrastructure.

kMC provides an interface to a Kinetic Simulator and is specifically designed to simulate individual atomic deposition (**condensation**) and dissolution (**evaporation**) events, while simultaneously tracking the surface and bulk crystallographic anisotropic **diffusion**.

2. OBJECTIVES

The main goal of my project is to make Graphical User Interfaces for WulffShape and vapor deposition. We are trying to offer users an option to modify parameters which can influence the evolvements of materials. And at the end, users will see the corresponding results.

5. CONCLUSIONS

Users have the option to choose a material, specify the material and change environmental parameters.

Matplotlib displays evolved images of WulffShape and physical vapor deposition.
visIt creates three-dimensional images as you can see on the bottom right.

6. REFERENCES

David R. Ely and R. Edwin Garc´ıa. “kMC User Manual. ” Version 0.1. 20 May 2013

“VisIt Python Interface Manual.” *VisIt Visualization Tool.* UCRL-WEB-229972, 26 September 2012.
https://wci.llnl.gov/codes/visit/manuals.html

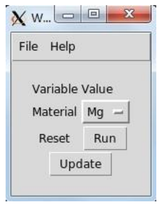
John Hunter, Darren Dale, Eric Firing, Michael Droettboom and the matplotlib development team. matplotlib: python plotting — Matplotlib 1.2.1 documentation, 29 May 29 2013.
http://matplotlib.org/

3. METHODOLOGY

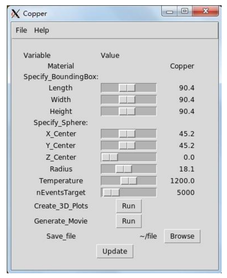
-python
-mpi4py
-numpy
-matplotlib
-raster3D
-visit

4. RESULTS

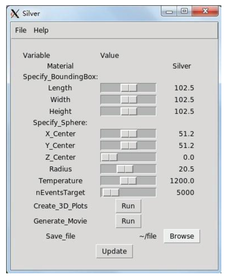
Part I: Graphical User Interfaces



GUI 01

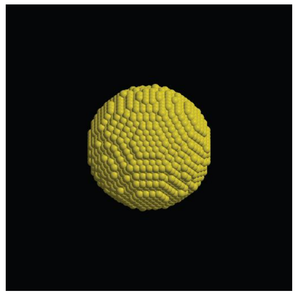


GUI 02

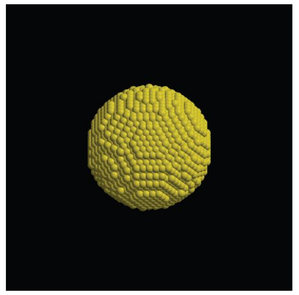


GUI 03

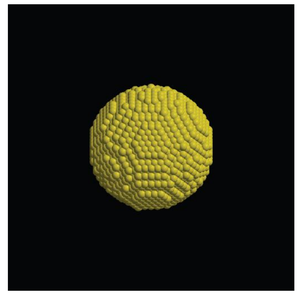
Part II: The top three images show WulShape of Copper
The bottom three images show WulShape of Magnesium



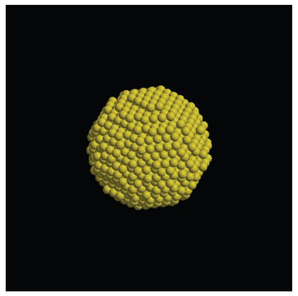
WulffShape 01



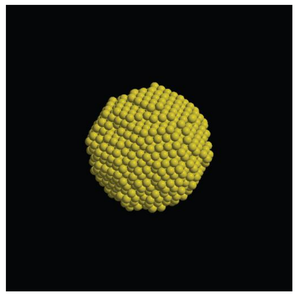
WulffShape 02



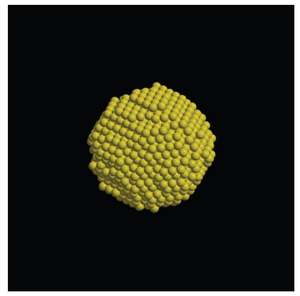
WulffShape 03



WulffShape 01

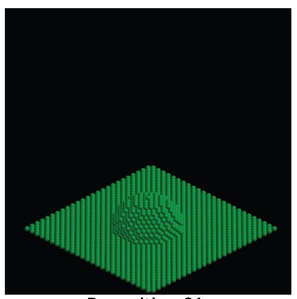


WulffShape 02

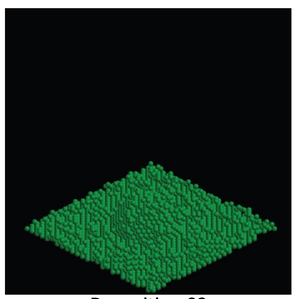


WulffShape 03

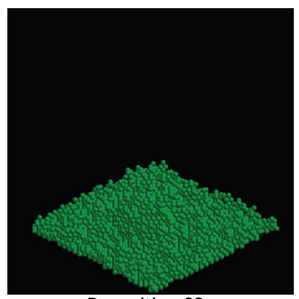
Part III: The top five images show Physical Vapor Deposition of Copper
The bottom six images show the same process in a three-dimensional view



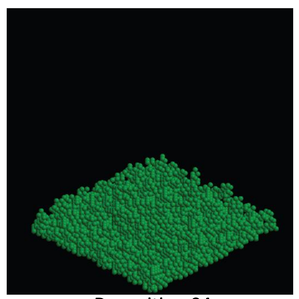
Deposition 01



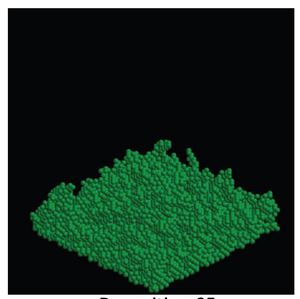
Deposition 02



Deposition 03

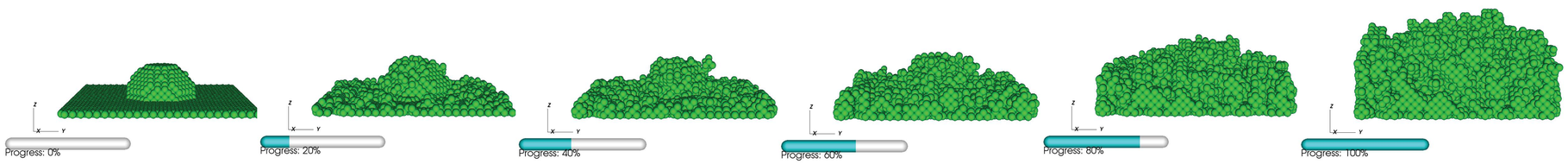


Deposition 04



Deposition 05

3D Images :



Acknowledgements:
Thank Professor Garcia for giving me a chance to do this research with you. Thank David Ely for your help with my understanding on previous code. Thank Alexander Bartol for your help with improving GUI. Thank the development team of nanoHUB for helping install our tool (kMC) online. Thank SURF staff for your contributions.