

Python-Based Kinetic Monte Carlo Simulation Tool

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Nowadays, scholars are working on nanoscale more and more frequently. At that scale, descriptions could be hard to make since most of nano materials cannot be seen at normal life. Therefore, program simulation of nanoscaled materials are more and more needed.

Project Goals:

My research project is developing a simulation tool for the diffusion reactions in different types of materials. My main responsibility is to create a Graphic User Interface of the tool and generate graphical results so that users can have more understanding on the output. Therefore, my research interests mainly focused on Graphic User Interface design, Computation Optimizing, or Human-Machine Interfacing.

Research Methods:

To create the Graphic User Interface, I used the Virtual Kinetics of Materials Laboratory created by Prof.Garcia, Alex Bartol and David R. Ely from School of Materials Engineering at Purdue University. The software is python-based and is used to get input simulation data from the user. However, there are no methods to display graphical outputs by using the Virtual Kinetics of Materials Laboratory software. Therefore, GTK+ toolkit has been used to create another graphic user interface to display the graphical outputs. GTK+ is an open-source software specialized in creating Graphic User Interface.

For the diffusion simulation between different materials, material properties need to be defined first so that the program can create the corresponding lattice and proceed the simulation. Therefore, I create a menu for the program, and if clicking the menu buttons in the pull-down menu, there is a separate window for each menu. In the first window, there will be slider bars or pull-down menu to get input information from user. All the required input in the first window are what needed to create the lattice according to the input material property. In the second window, there will be controls to get the information of the simulation environment, such as temperature and number of steps of the simulation. User will be able to start the simulation and generate all the outputs in the second window. By doing this, user can be informed with the order of the simulation step, and have a much clearer sense of how the simulation will be running. Also, there will be less potential errors done by users by doing that. Since the simulation may take a long time, the output image will be updated as new simulation results arrived. To get a real-time-updated plot, GTK+ toolkit has been used to create the output frame and to create the main loop to continue the simulation.

Key Results:

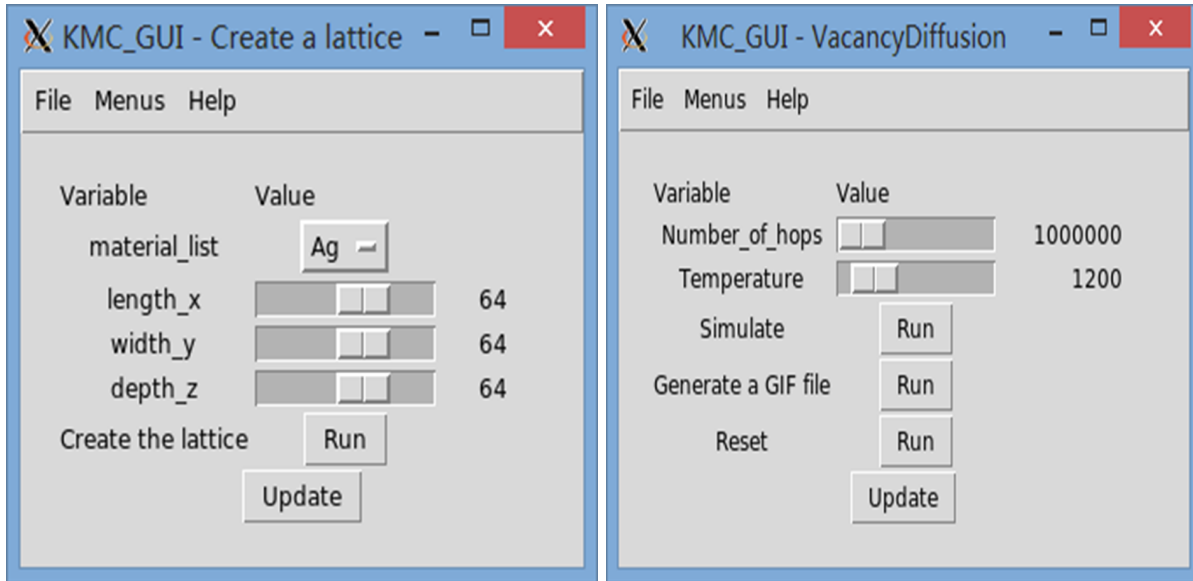


Figure 1. Graphic User Interface of the simulation tool

The two windows above is the Graphic User Interface of the simulation tool. The first window is the first output window of the first option in the pull-down menu, while the second window is the second output window of the second option in the pull-down menu. As seen above, the input controls in the first window are mainly related to the size of the lattice and materials used. Those information will be used to create the lattice. However, the input controls in the second window are mainly related to the simulation environment. Those information are used in simulating the experiment. There is an option in the second window used to generate a GIF file of all the output pictures. By looking at the GIF movie, the simulation results will be more clearer and persuasive.

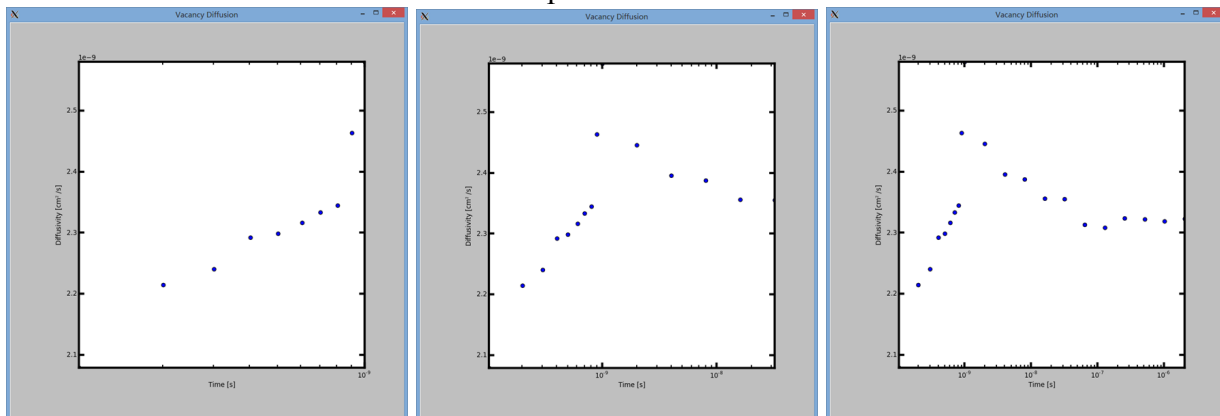


Figure 2. Snap shots of the output image during the simulation

The three images above are three phases during the simulation. The first image is the output in the beginning of the simulation, the second image is the output in the middle of the simulation and the third image is the output in the end of the simulation. As seen above, the output image is updated during the simulation.

Analysis and Interpretation:

The outputs shown in the results section has successfully displayed the diffusivity property of the silver material. It has shown a proper result of the silver self diffusion.

Appendices

Appendix 1:

The program, which contains the physical engine of vacancy diffusion mechanism, has already been programmed by Prof. Garcia and Dave R. Ely in MSE department at Purdue. However, users cannot observe the changing numbers of diffusivities during Vacancy Diffusion simulations between different materials. Also, there is no Graphic User Interface for the simulation tools. To solve the problem, the Virtual Kinetics of Materials Laboratory program is used to create the Graphic User Interface. Also, GTK+ toolkit has been used to create a pop-up window displaying updated diffusivities during the simulation. For user purpose, the pop-up window has been set to display a plot of diffusivity versus simulation time. During the programming process, several problems were found and solved by using GTK+ main loop and functions in Matplotlib plotting library.

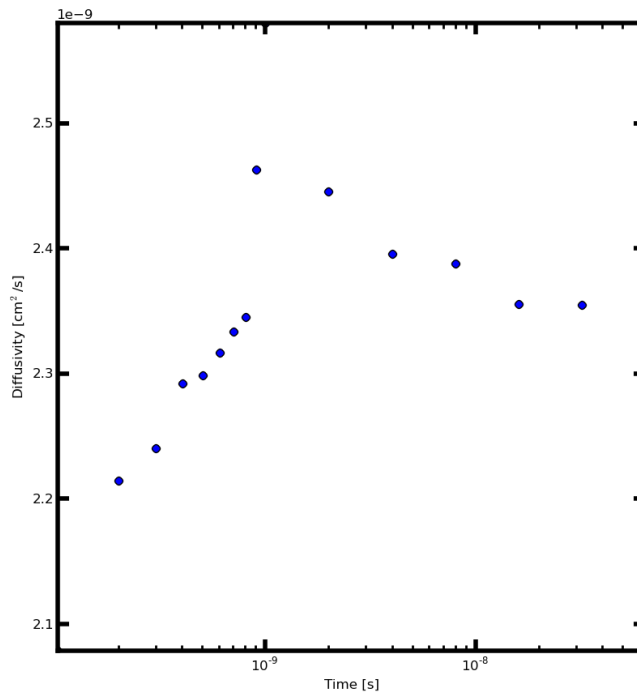
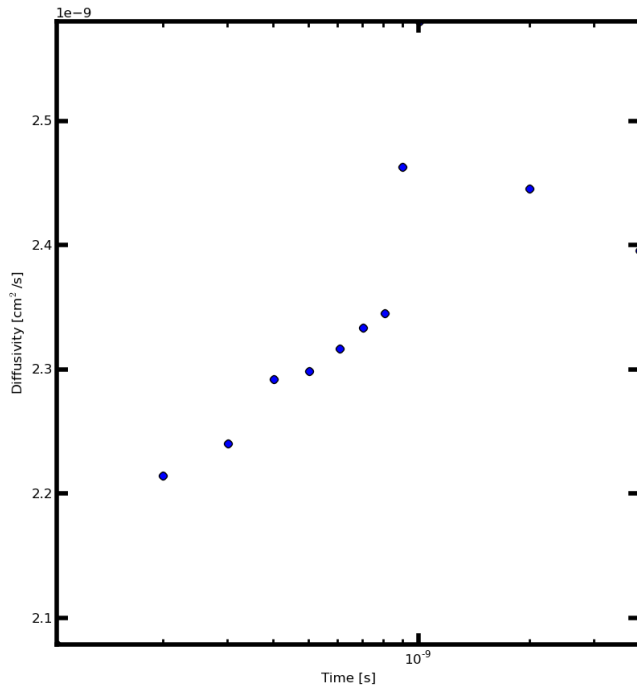
The main challenge, which is create an updated image with the real-time-updated information, was solved by using the GTK+ main loop. By doing that, the function pointer of the simulation function in the program has been passed to the GTK+ main loop. The GTK+ engine will run the function automatically until there is a False value returned. As long as the function is running, the `set_data` function will be used to update the new line of data in the plotting function. The plotting function is using the matplotlib library. The matplotlib returns an object reference after each plotting function being called, which allows me to control the line object. By doing that, I am able to update the line drawn to reflect the new values.

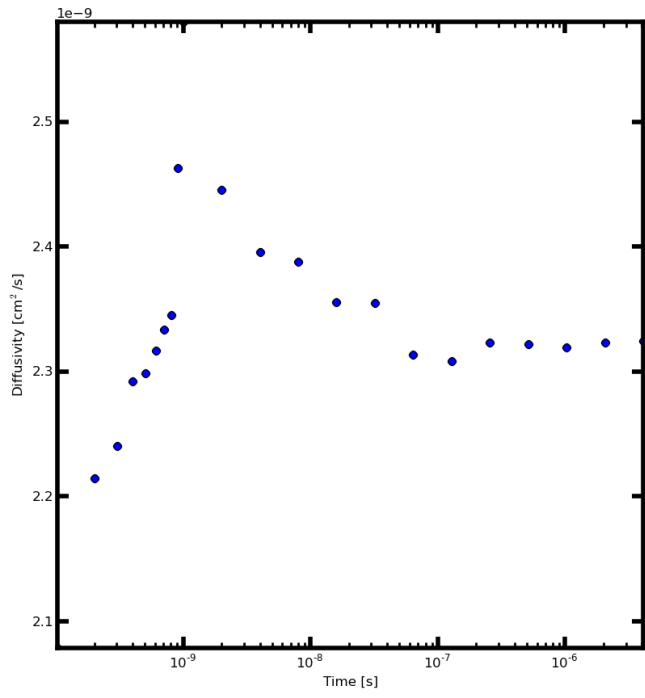
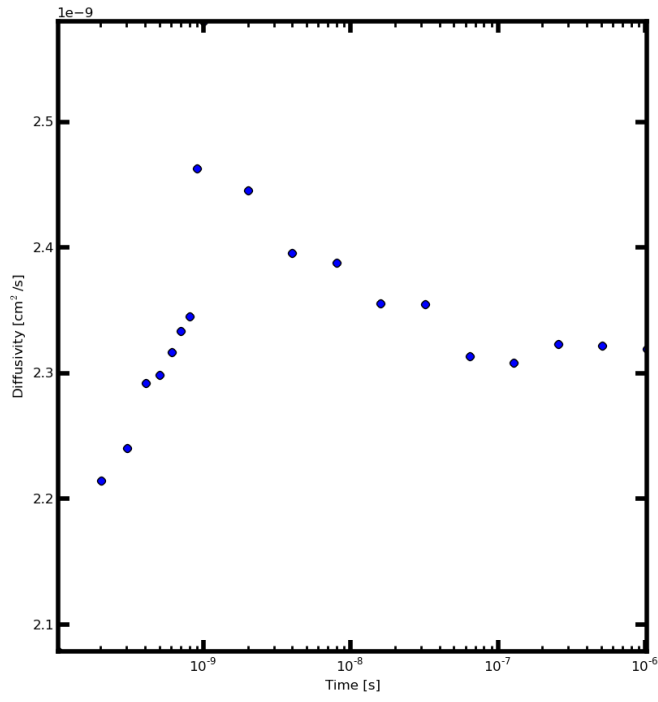
Appendix 2:

The figure 1 has shown the final Graphical User Interface. The program has the following main features:

- Be able to generate a model for a cubic lattice with the three dimensional measurements entered by users and the material chosen by users
- Simulation temperature is controlled by users
- Number of hops during the simulation is controlled by users
- Be able to generate a GIF file based on all the pictures generated during the simulation
- Users can clear all the materials generated during the simulation by click the Run button beside the Reset Tag
- Simulation results will be displayed graphically during the run-time simulation

Also, as shown above, the figure 2 is the main output of the simulation tool. It's a real time plot simulation. The following pictures are some output pictures generated by the simulation tool.





Appendix 3 (References):

1.Ely, D. R., & Garcia, E. R.(2013). KMC User Manual Version 0.1.

2.Tosi, S (2009). *Matplotlib for Python Developers*. Birmingham, UK: Packt Publishing Ltd.