Crystal Viewer Tool v2.0 Using NEMO5

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INTRODUCTION:

What is the Crystal Viewer Tool?

Crystal Viewer Tool is an interactive educational tool on nanohub that provides insight about the crystalline structure of various materials. NanoHub is a "cyberinfrastructure where researchers, educators, and professionals collaborate, share resources, and solve real nanotechnology problems"

The Crystal Viewer Tool visualizes Bravais lattices, Miller planes, and crystal structures off various materials needed for various reasons using NEMO5.
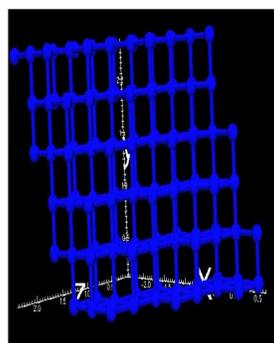
What is NEMO5?

NEMO5 is the 5th edition of the multipurpose, multiscale, highly parallelized NanoElectronics Modeling tool of the Klimeck group in the Network for Computational Nanotechnology (NCN) at Purdue University. NEMO5 is compatible with many external software (both for output and input) and can either be used as a tool or a as a library.
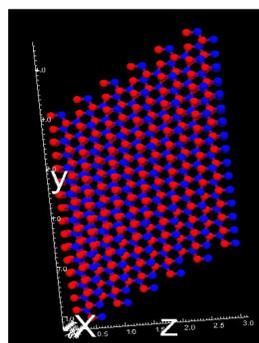
OBJECTIVE:

Despite the surge in technology, it is difficult to find a web-based, user friendly tool to view and investigate the crystalline structure of different semiconductor materials.

Due to the complex characteristics of materials, a tool that enables users to manipulate the crystalline structure of different materials will be beneficial in the research and education fields. The goal of this project is to provide a tool that is novice friendly and improves the capabilities of the old Crystal Viewer tool.
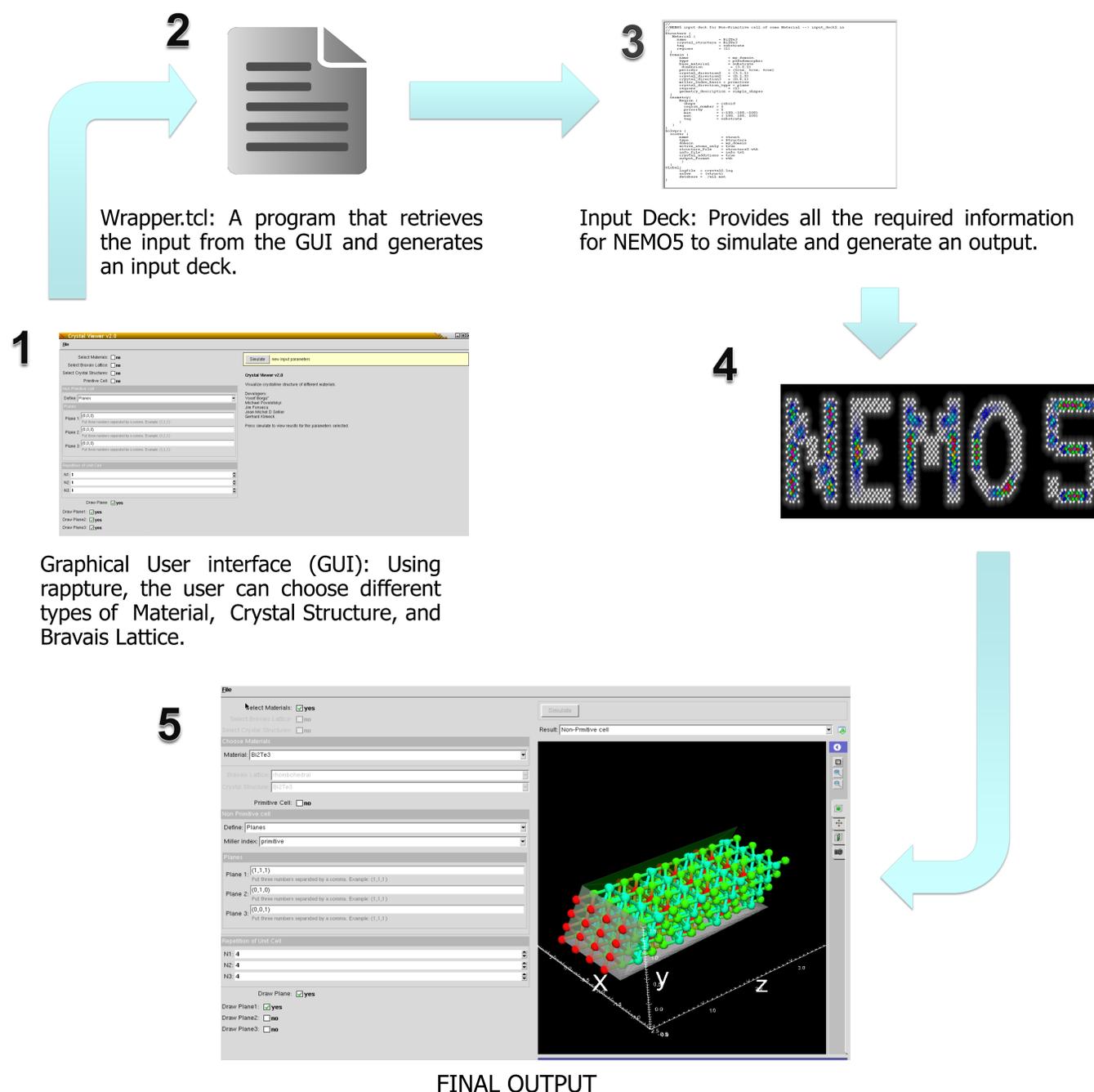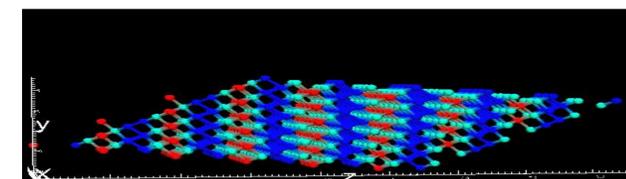
Magnesium Oxide   Gallium Arsenide

PROCEDURE:

2

Wrapper.tcl: A program that retrieves the input from the GUI and generates an input deck.

3

Input Deck: Provides all the required information for NEMO5 to simulate and generate an output.

1

Graphical User interface (GUI): Using rappture, the user can choose different types of Material, Crystal Structure, and Bravais Lattice.

4

5

FINAL OUTPUT

SAMPLE SIMULATION:

Bismuth Telluride

CONCLUSION AND FUTURE WORK:

- This project improves upon the capabilities of the Crystal Viewer tool with a completely redesigned interface. This tool should aid beginners in visualizing the standard basic structures of semiconductor materials. Crystal Viewer Tool will be vital for wide range of students, researchers as well as professors in various fields of pertaining to materials studies.
- Expand the library: Add more Materials, Crystal Structure and Bravais Lattice.
- Allow the plane to slice the atoms in the unit cell and remove one side, so that the remaining structure, with the sliced atoms, can be rotated and viewed from different angles.

RESOURCES:

1. Klimeck, G., Lundstrom, M. S., Adams, G. B., Brophy, S. P., & McLennan, M. (2008). nanoHUB.org: Advancing Education and Research in Nanotechnology. 17-23.
2. Saumitra Raj Mehrotra; Michael Povolotskyi; Sebastian Steiger; Tillmann Christoph Kubis; Abhijeet Paul; Xingshu Sun; Victoria Savikhin; Gerhard Klimeck (2012), "Crystal Viewer Tool,"http://nanohub.org/resources/crystal_viewer. (DOI: 10.4231/D3VX0627Z).
3. Tillmann Christoph Kubis; Michael Povolotskyi; Jean Michel D Sellier; James Fonseca; Gerhard Klimeck (2012), "NEMO5 overview presentation," http://nanohub.org/resources/14701.

ACKNOWLDGEMENT: