Virtual Silicon Environment for Enhanced Visualization of the Silicon Crystal Structure

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Abstract

Many computers possess excellent graphic rendering capabilities, high speed projection of digital data, and hardware and software that allows physical interaction of users while viewing such data at comparably scaled sizes. Thus, these machines have precipitated a change in the philosophy of teaching introductory courses in semiconductor physics. Studies of introductory semiconductor courses have indicated that geometries, geometry-dependent properties of crystals, and an analysis of electrical, thermal, optical, or chemical energies in the electronics world, are among the common topics taught in introductory courses in semiconductor physics. A review of available software tools for teaching and learning semiconductor geometries indicates that there is a lack of highly effective visualization methodologies for commonly used semiconductor material structures. The purpose of this paper is to describe a virtual environment tutorial that has been developed to supplement a typical course in semiconductor physics.

Introduction

Traditionally, students of crystallography, semiconductor physics, and mechanics of crystalline materials, have struggled to visualize the complex geometries and structures associated with crystals. Pure and doped silicon, diamond, gallium arsenide and other materials, are commonly used and studied at electrical engineering departments in colleges and universities throughout the world. Several properties of these materials, especially semiconductors, are dependant on crystal orientation and the direction exposed to thermal, optical or chemical treatment. These crystal structures are comprised of atoms bonded together in a specific order.

Undergraduate students studying the crystallography of silicon are often faced with the task of visualizing specific planes and directions within the crystal in order to comprehensively study reaction rates, behaviors and various effects. For graduate students, this becomes even more important since electronics processing requires an understanding of the physics and chemistry behind the reactions associated with the semiconductor crystal. Because of their complex geometries, crystal structures can be extremely difficult to visualize. As a result, the learning process is severely hampered. For example, if a student in a semiconductor electronics or solid state physics course is studying the process of etching, it is important for him/her to understand how a compound like KOH is able to weaken and dissolve bonds quicker in one particular plane (e.g., the (100) plane) than another (e.g., the (111) plane). After receiving lectures on crystal structures and plane orientations, 8 students in a physics of semiconductor devices course participated in a survey to assess their understanding of this material. Results indicate that only 25% of the students claim to clearly understand the crystal structure of the atom. About 50% claimed that they could find directions, planes, and specific local points, in the crystal with some assistance. These alarming numbers suggest that a new method of teaching the crystal structure and crystal planes should be used.

In the past, one solution to the aforementioned problems in visualization was using solid 3D object models of crystals. These models have only produced a modest increase in learning or understanding. This strategy of teaching/learning suffers from design inflexibility when it becomes necessary to add or remove atoms in the crystal, or to be able to move seamlessly within a crystal in order to highlight certain areas of interest. Proposed in this study, is the construction of a virtual silicon crystal environment that solves all of the aforementioned problems and allows for clearer instruction and learning. This project enables students to "walk" through the crystal structure of silicon, and enables them to highlight specific planes, locations and directions. Not only does it allow them to view specific planes of interest within the crystal with a high degree of accuracy, but it allows for customized views of planes and directions.

Description of CAVE

A Computer Automated Virtual Environment (CAVE) with tracking devices is used for the purpose of visualization. The CAVE is used in conjunction with high-performance computing to project data from experiments or simulations onto the boundaries of a room, hence creating a realistic environment that enhances visualization and interpretation of data. Since engineers and scientists use CAVEs to understand and interpret results, these resources are available only at institutions where magnanimous amounts of data from research experiments need "illumination". Faculty and students can visually interact with their data in real time 3D by wearing stereo glasses and using interactive gloves while viewing data. Southern University is home of the only CAVE available in the state of Louisiana. Because the CAVE is such a unique facility, it is worth exploring the benefits that can be derived from use of the virtual reality technology.

Several successful attempts have been made in the past to use virtual reality in engineering education[1]. Such attempts have mainly employed software to generate three dimensional models on a regular computer monitor. This is a great asset in helping students to visualize complicated crystals[2]. The CAVE can be thought of as an extension of this philosophy. Besides providing a highly coordinated walk-in virtual environment, the CAVE also allows for interaction between a user and the computers that operate it, all in real time. A menu-driven computer program employed in the CAVE is much more than a tutorial; it is an experience.

Figure 1. The CAVE, visualization equipment, and a user interacting with data inside the running CAVE.

Contents of the Program

The Virtual Silicon Environment (VISIEN) program has been written using the MS Visual C++ programming language. The menu-driven program uses several GUIs (Graphical User Interfaces) and runs simultaneously to produce four images based on user-position and input (These are the images that are projected on screens that make the walls of the CAVE). A "wand" with buttons serves as the student's input device. The CAVE and some hardware devices are pictured in figure 1. The student also uses stereo glasses to converge the images that are available to the eye. All of the above is furnished using a readymade API (Application Programming Interface), programmed for use with the CAVE and ported in a library called CAVELib™, available from VRCO®. CAVELib™ provides the cornerstone for creating robust interactive three-dimensional environments with inherent functions that use OpenGL as the basis of its programming[3].

Program Objective

The main objective of the program is to present the three dimensional crystal structure of silicon[4] to undergraduate students. There are several secondary objectives that the program serves, and can be divided into three sections: a section to ensure that undergraduate students grasp concepts that are not immediately related to crystal structure, an advanced concepts section to allow graduate students to visualize detail associated with silicon processing, and a section for researchers to visualize complex geometries involved with crystals and complex molecules. Regardless of student classification and background, the crystal structure of silicon, along with basic functionality is available via this computer program.

Program Modules and Functionality

Basic Concepts for Undergraduates

Once the student has familiarized himself/herself with the structure, additional options are available. The student can choose to view a particular direction in a unit cell of the crystal, or the student can choose to view specific planes. Families of directions and planes are also available to view (although it is recommended that student first attempt to find these planes before referring to the CAVE program display). For example, an assignment can be given to calculate the area of a non-trivial plane within the unit cell. This is where using a CAVE has a vast advantage over a thought experiment. Planes can be visualized inside the CAVE free of interpolation and disruption from atoms, bonds, edges, vertices, corners, and directions, which might interrupt mental visualization after reading a textbook. Such geometric entities that are irrelevant to the question at hand can be avoided altogether inside the CAVE, by several methods including dimming their radiance, changing their color, or removing them completely for the view of the original entity. Visualization of these entities can help students to derive accurate numbers when doing homework after using the CAVE. Motivation for answering such questions, however, needs to be provided by the instructor. For example, the student should know why the calculation of a plane area is done, or why the number of atoms in a plane needs to be evaluated.

As an example of the usefulness of the CAVE, consider the example of an undergraduate student given an assignment to calculate the density of atoms in a non-trivial plane (e.g., the (313) plane) within the unit cell. To answer such a question, the student will need to visualize the plane using more than one unit cell, and then remove the portion of the plane outside of the unit cell. A resulting plane within a unit cell will have the form of a quadrilateral (in most cases), a trapezoid, or a triangle (in rare cases). The student will also need to count the number of atoms that sit on this plane, which can be very confusing if the student tries to mentally picture this, but it reduces to mere counting when using the CAVE. Error free visualization of the plane will then be accomplished, but that would be just half the task. Finding the area of the plane will enable the student to calculate the density. Innovative examples can be employed to let students realize that the best mechanical and electrical properties can be derived only if proper crystal geometries are used. (Future references to this example within this paper will be given as the 313 example).

Advanced Concepts for Graduate Students

For graduate students with some processing and fabrication knowledge/experience, the CAVE has plenty to offer. The CAVE can be used to visualize simulations that are made for evaluating the changes that a specific processing step will bring. CAVEs using Windows 2000 offer more migration flexibility for data than the other platforms do. They possess drag and drop functionality and hence, much shorter learning curves for the instructors/programmers who write and maintain CAVE programs. Therefore, programs written to simulate processing and fabrication steps can be migrated to the CAVE with a fair amount of ease. The CAVE can be used, for example to analyze the geometries of a hole that would be drilled into a wafer by double-side etching. Several simulation software programs can do this task, but only a few if any, can show exactly how atoms and bonds would react to chemical treatment in real time.

The (313) Example Revisited For Graduate Students

Apart from the research application referred to above, the CAVE can be used for classroom calculations. Error calculations are often important parts of engineering problems. Commercial vendors specify the quantity of error that can exist in the orientation of the crystal. With the advent of nanotechnology, it has become even more important to be able to calculate exactly what one could expect from an error in the orientation of a crystalline wafer. The CAVE can be used to “tilt” the (313) plane by a pre-specified miniscule angle. By doing so, one can see how many atoms fall out-of-plane every n-unit cells. By obtaining this number, it would then be possible for the graduate student to calculate how much longer or shorter a wafer should be exposed to chemical treatment, radiation etc. Such calculations represent common assignments in an advanced IC processing courses.

Program Structure

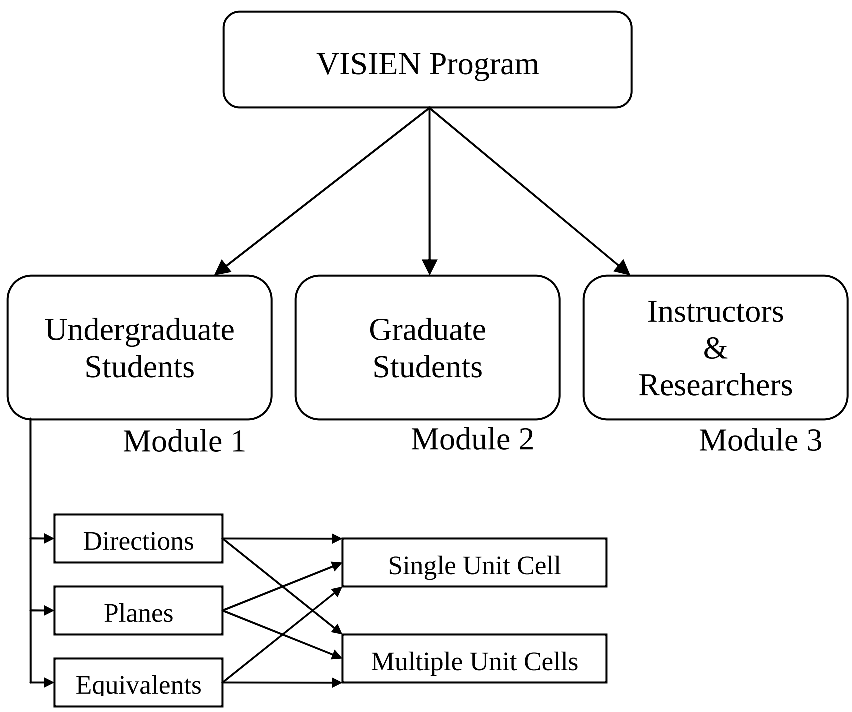

Figure 2. Functional Structure of the *VI*rtual *SI*licon *EN*vironment Program (VISIEN).

As discussed above, the VISIEN program has been divided into three modules based on its functionality (Figure 2). The remainder of this paper presents Module 1, its implementation, and discusses results achieved from it. It is planned that upon successful completion of Module 1, Modules 2 and 3, which are separate projects in their entirety, will be undertaken.

VISIEN Design and Program Flow

Module 1 is driven by the underlying objective to serve undergraduate students and increase their comprehension. Hence no complicated simulation or functionality has been implemented, but the visualization of the three dimensional crystal structure of silicon, with atoms and bonds, has been enabled. The menus available to the user are outlined below.

1. Introduction to VISIEN
2. Main Menu
    - 2.1. Basic Concepts
        - 2.1.1. Lattice Display (Single Unit Cell)
            1. With Grid (Cell Outline)
            2. Without Grid
        - 2.1.2. Single Unit Cell Displays
            1. View Directions
            2. View Planes
            3. View Equivalent Directions
            4. View Equivalent Planes
        - 2.1.3. Multiple Unit Cell Displays
            1. 8-Cell Displays with functionality from 2.1.2
            2. Semi-finite (256)-Cell Displays with functionality from 2.1.2
    - 2.2. Advanced Concepts (Modules 2 and 3)
3. How to use Wand
4. Exit

The program flow with functionality detailed above is considered sufficient for the purposes of an undergraduate class. Minor modifications of the above, can lead to the reconstruction of the program to incorporate a tutorial of the silicon crystal, which will open the program to every student of solid state electronics. Eight students were surveyed before and three students were surveyed after a CAVE tutorial session.

Results

A new survey was conducted at the end of the implementation of the project. It re-evaluated the students and instructors' learning and teaching experience respectively. It is anticipated that this new system will be permanently implanted in the curriculum of courses that teach crystal structure.

Future Work

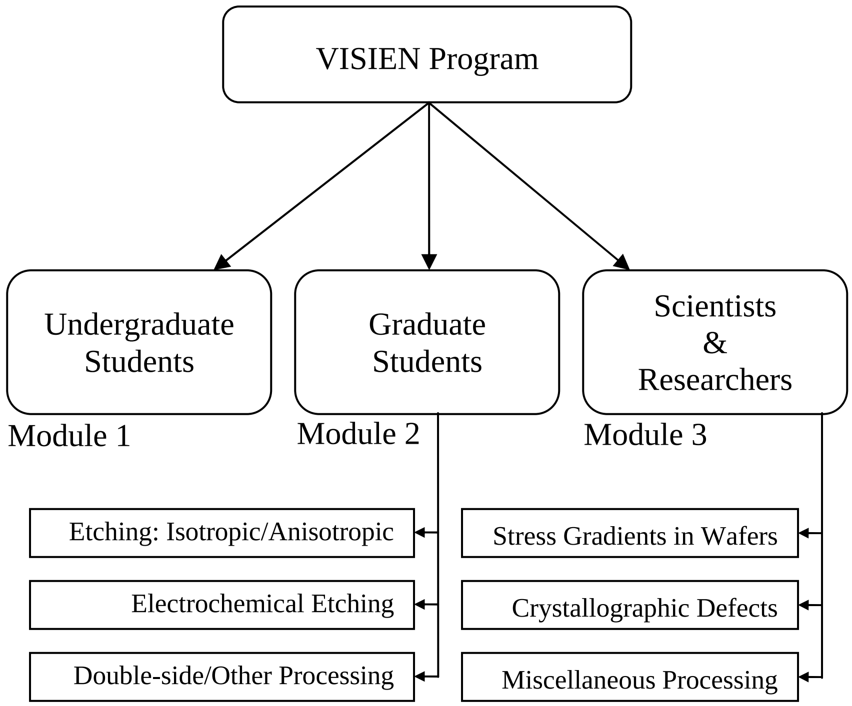

Figure 3. Examples of visualizations useful to graduate students and researchers; VISIEN can be programmed to accept externally generated data from foreign programs in the future

The items below include work that would enhance the learning experience in the CAVE:

1. Form tutorial within CAVE incorporating audio (voice) with access of sub-modules within the program – requires simple additions/modifications to current program code
2. Integrate with other software programs, so that results from simulations can be viewed easily
3. Allow for doping effects into the crystal where atoms can be replaced and stresses can be visualized.
4. Modify the geometry for other crystals (other than Si).

Summary and Conclusion

In conclusion, the CAVE represents a valuable learning tool that many schools don't have access to. This facility will enhance the educational experience of science and engineering students by allowing undergraduate and graduate students to gain a tremendous understanding of crystallography, and materials processing.

The project undertaken targeted undergraduate students who used a popular book in the Solid State Physics area, and surveyed their understanding of the silicon crystal. From results obtained at the end of this survey, it was concluded that a better learning tool of the crystal structure was required. A virtual reality tool, the CAVE, available at Southern University College of Engineering, was employed in addressing this issue. Software was written that generated a virtual model of the silicon crystal, and was presented to students. Enhancement of student learning and comprehension was achieved. The tool presents opportunities of enhanced visualization to graduate students and researchers, and is being developed to serve these sections of the academia.

References

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