DEVELOPMENT OF NANOSCALE VIRTUAL REALITY SIMULATIONS FOR THE TEACHING OF NANOTECHNOLOGY

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Abstract

This paper presents the development of 3D Virtual Reality (VR) based nano-simulations using the PowerWall System - a large scale VR System. The users can fully immerse themselves in the nano world and interact with various nano structures. Another objective of the work is to study how effectively and efficiently the VR simulations can enhance the students' understanding of nanoscale concepts. Three simulations have been presented, including "understanding the scale of nanotube", "understanding different structures of nanomaterials", and "understanding the chirality of nanotube". The nano-simulations have been integrated in the teaching of course ELEG4223 "Photonic and Electronic Materials and Devices". The student survey results are presented in the paper. Students' responses show that they believe that the VR simulations are very helpful in increasing their understanding of nanotechnology.

Introduction

The fields of nanoscience and nanotechnology have rapidly developed and received enormous amount of attention in recent decades[1]. The U.S. has long been playing the leadership role in research and development of emerging nano-technologies. To maintain its technological and economic leadership, there are emerging needs for U. S educators to change and enhance the infrastructure for nanotechnology education[2]. Rapid development in nanotechnology has now brought urgent challenges to undergraduate engineering education: How to integrate the emerging nanotechnologies into classroom teaching? How to prepare our students for tomorrow's highly competitive global job mar-

kets? And how to maintain the US's leadership and dominance in science and technology in an era of globalization?

Funded by the Department of Education, a project is carried out to integrate nanotechnology into the undergraduate science and engineering curricula through a sequential preparation approach from introductory freshman to the advanced senior level. The curricula are reinforced by innovative computer simulations and state-of-the-art nanomaterials laboratory experiments and demonstrations. The work presented in this paper is part of the project, which aims at utilizing Virtual Reality (VR) simulations to enhance the students' learning and understanding of nanotechnologies.

The phenomena in the nano world are very different than in the macro world. Most of the nanoscience concepts are abstract and invisible. Therefore, the concepts of nanotechnology are very difficult for students to understand and conceptualize[3]. Studies have shown that the use of computer-interaction simulations, especially three-dimensional simulations, can significantly improve the students' understanding of the concept in question[4]. The Virtual Reality environment is a high-end user interface that involves real-time simulation and interactions through multiple sensorial channels, such as visual, auditory, tactile, smell, taste, etc. It enables the user's immersion into a sensory-rich, interactive experience. In a Virtual Reality based nano-simulation, the users can fully immerse themselves in the nano world and interact with various nano structures which are impossible to see with bare human eyes. Students will play an active role in the virtual environment. Involving students in consciously choosing to

investigate the properties of a nanoscale object is a more effective way to maintain attention and motivation of students than passive types of learning, such as watching a science video[5, 6]. It has been demonstrated that VR techniques such as haptic is an efficient media to assist learning and teaching of undergraduate engineering students[7].

This paper presents the development of 3D VR based simulations to display nano structures using the PowerWall System. Currently three simulations have been developed, including "understanding the scale of nanotube", "understanding different structures of nanomaterials", and "understanding the chirality of nanotube". The simulations were implemented in the teaching of an undergraduate course. The student survey was conducted to study how effectively and efficiently the nano-simulations can enhance the users' understanding of nanoscale science and engineering concepts.

Related Work

Many related researches have been carried out to explore the effectiveness of VR simulations in the enhancement of students' understanding of complex nanoscience topics. Al-khalifah and McCrindle[8] conducted a study to determine what VR should contribute to the education process and to formulate the perceived advantages and limitations of using VR as an education tool. Jones et al.[7, 9] developed a tool called NanoManipulator which combined an atomic force microscope (AFM) with haptic device PHANToM. They investigated how this instructional tool influences students' learning at the nanoscale. Millet et al.[6] introduced a pedagogical tool using haptic feedback and visual analogy to improve perception and understanding of nanoscale phenomena. A virtual reality simulator with haptic feedback was developed by Gao and Lecuyer[10] for the purpose of education, training, and prototyping of nanotube manipulation. Pawluk et al.[3] developed a nanoscale virtual environment integrated with haptic feedback system. The system helped the visually impaired students in perception and conceptualization of nanoscale forces and objects. Most of the related work utilized desktop based VR system. In our work, the large scale VR system called PowerWall is utilized in the display of nano-simulations, which has a stereoscopic screen with dimension of 10 ft by 7.5 ft. It provides users more realistic and immersive experience than desktop based VR system.

Structure of the PowerWall Virtual Reality System

The PowerWall VR system consists of active stereo PowerWall, stereo eyewear and emitters, computer system, tracking system, and development software Vizard. The schematic of the VR system is depicted in Figure 1. The input devices, including PHANToM Omni, wand, and head tracker, gather the input information from the user and transmit it to the virtual world. The tracker is a sensor that provides the position and orientation of the object that the tracker is mounted on and maps it to the object's relative position in the virtual environment. The wand is an input device which allows the user to move, rotate, and manipulate the 3D scene in the virtual environment. Software integrates various hardware elements into a coherent system that enables the user to interact with the virtual environment. Output devices, including PowerWall and PHANToM Omni, are applied in the virtual environment to present the user with visual and haptic feedback about his or her actions. Currently the PHANToM is not used in the simulations. The major component of the system is the PowerWall which is a flat, large-scale stereoscopic visualization system with the dimension of 10 ft by 7.5 ft. It is illuminated from the rear by an active stereo projector. Figure 2 shows the set-up of the PowerWall system.

The following abilities make the PowerWall VR system distinguished educational tools: (1) Helping learners understand complex, abstract, and non-intuitive concepts and systems. Through the PowerWall VR system, learners can be immersed within any non-existing
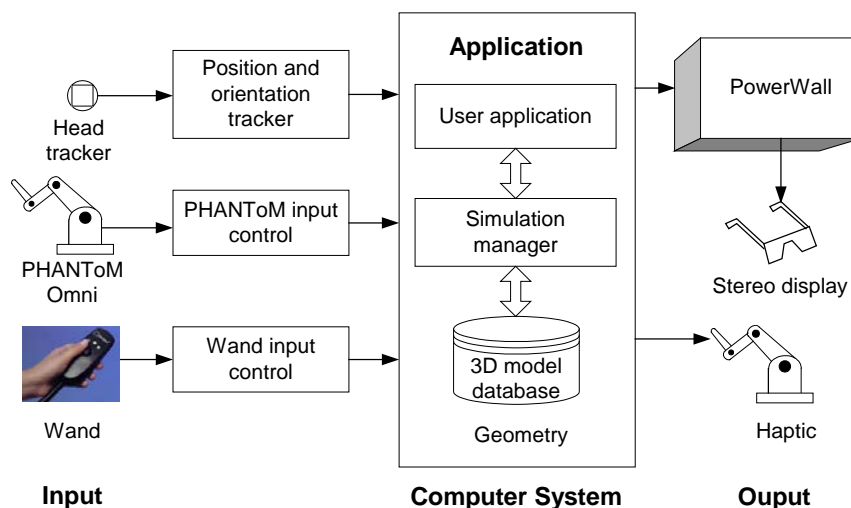
Figure 1. Schematic of the PowerWall virtual reality system.

Figure 2. The set-up of the PowerWall system.

phenomenon (visually, auditory, and haptically) thus helping them to comprehend the abstract data or concepts deeply and intuitively. (2) The PowerWall VR system is engaging, entertaining, attractive, and interactive. Students are better able to master and retain knowledge when they are actively involved in constructing the knowledge through learning-by-doing. (3) Allowing students to have learning experiences that are not possible within physical educational settings. For example, the learner could interact with and even step into atoms and electrons.

Development of Virtual Reality Nano-Simulations

In our nano-simulations, head tracker and wand are used as input devices. Vizard is used as an application development tool, which uses python as the programming language. The output devices are PowerWall where the simulations are displayed and manipulated. The 3D active mode is obtained by graphics card Nvidia Quadro FX 5800. The 3D simulations are visualized and manipulated in the PowerWall by the shutter glasses and wand.

Currently three simulations have been developed, including "understanding the scale of nanotube", "understanding different structures of nanomaterials", and "understanding the chirality of nanotube". The 3D models of nano structures were created using software Nanotube Modeler. The models were then imported into Vizard. The simulations were developed using Vizard so that the users can interact with the models.

The first simulation "understanding the scale of nanotube" is to help students understand the scale of nanometer. Students generally do not have a sense of how small a nanoscale object is. Nanoscale objects can only be "seen" under the electron microscopes or scanning probe microscopes. However, the use of these instruments is very costly and takes an extreme amount of training. Virtual Reality simulations can make the nanoscale object "visible" to students. It is done by comparing the objects in meter scale, millimeter scale (10^{-3} meter), micrometer scale (10^{-6} meter), and nanometer scale (10^{-9} meter). As shown in Figure 3, the three different scales of worlds represented by three rooms are created in 3D, including the real world, the microscale world, and the nanoscale world. The users can navigate through each world by pressing the buttons on the wand. In each world, two objects are displayed side by side so that the users can grasp the sense of scale of the objects.

As illustrated in Figure 4(a), a human body and a human hair are displayed in the real world. A human hair is generally 80 micrometers (0.08 millimeters) in diameter. It gives users the sense how small the millimeter scale object is compared to meter scale object. In the microscale world, the hair and the Fe-13Mn-1.3C alloy are displayed as shown in Figure 4(b). The alloy is represented as a box with a texture (jpg file) wrapped over it. It demonstrates that the alloy is much smaller even than a human hair. In the nanoscale world, the Fe-13Mn-1.3C alloy, a nanotube, and the DNA are displayed as shown in Figure 5(a). The DNA is 2.5 nm in width, which is about the same size as the nanotube. The users can comprehend how much smaller the nanotube is compared to the alloy material. By using the wand, the user can "move" himself/herself inside the nanotube and "look around" to explore how the nanotube is structured, as in Figure 5(b).

The second simulation "understanding the different structures of nanomaterials" displays the different types of nano-structures including nanocone, nanotube, and buckyball as shown in Figure 6. The different structures give nanomaterials different physical properties and applications. They are widely used in industries as semiconductors, conductors, and nanomachines, etc.[11] For instance, buckyball can be used in ball bearings in some mechanical
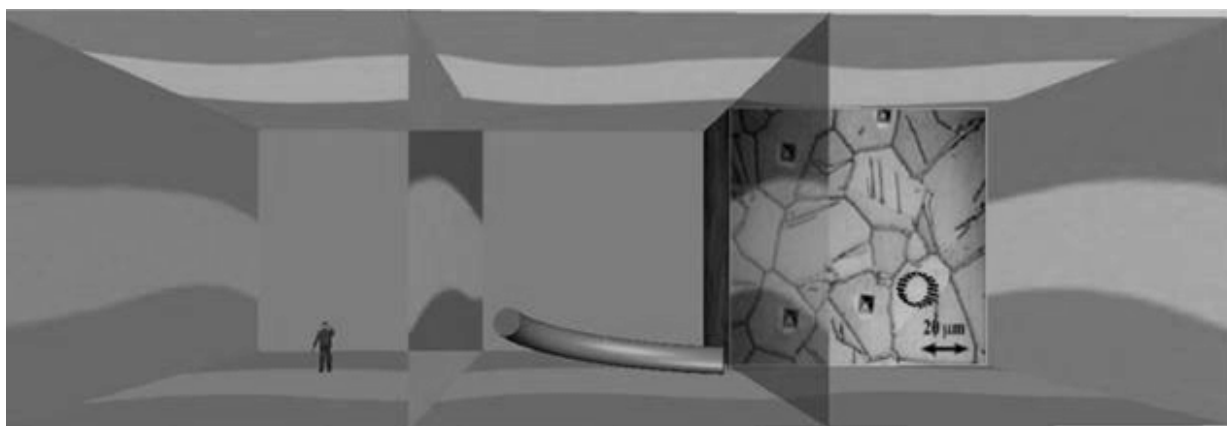

Figure 3. The three different scales of worlds: real world, microscale world, and nanoscale world.
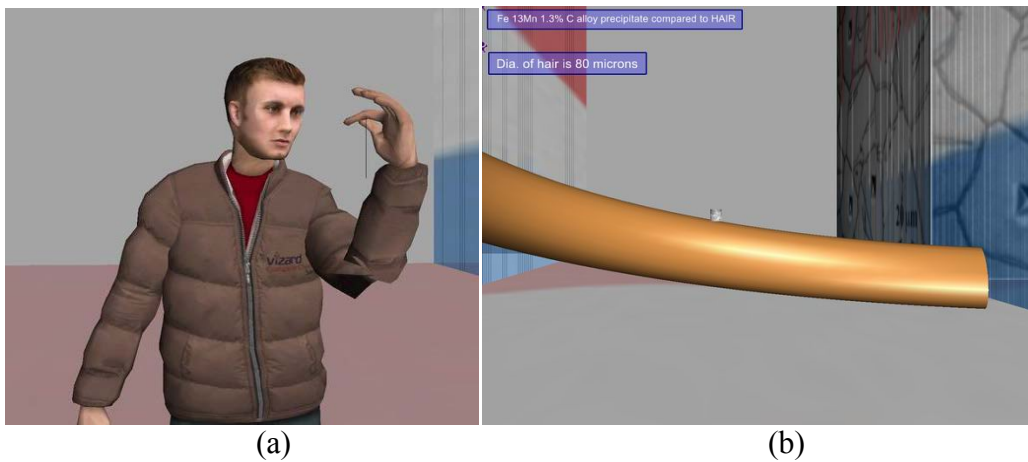
Figure 4. (a) A human body and his hair are displayed in the real world;
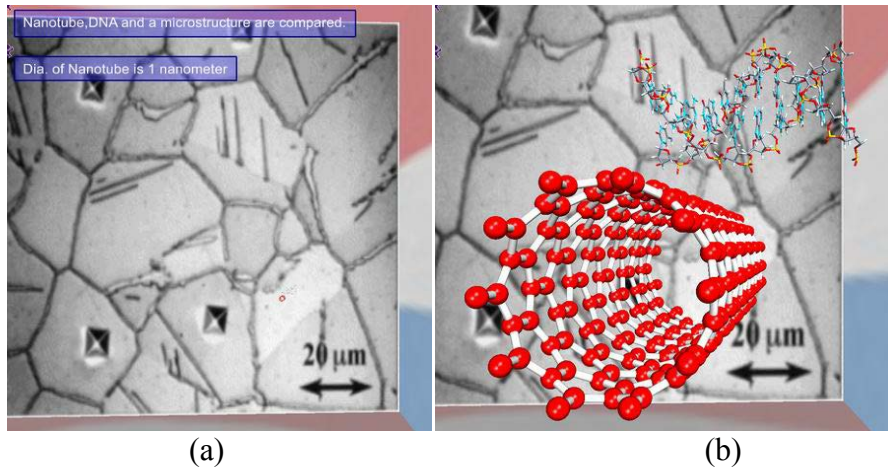(b) A hair and the Fe-13Mn-1.3C alloy are displayed in the microscale world.

Figure 5. (a) The Fe-13Mn-1.3C alloy, a nanotube, and the DNA are displayed
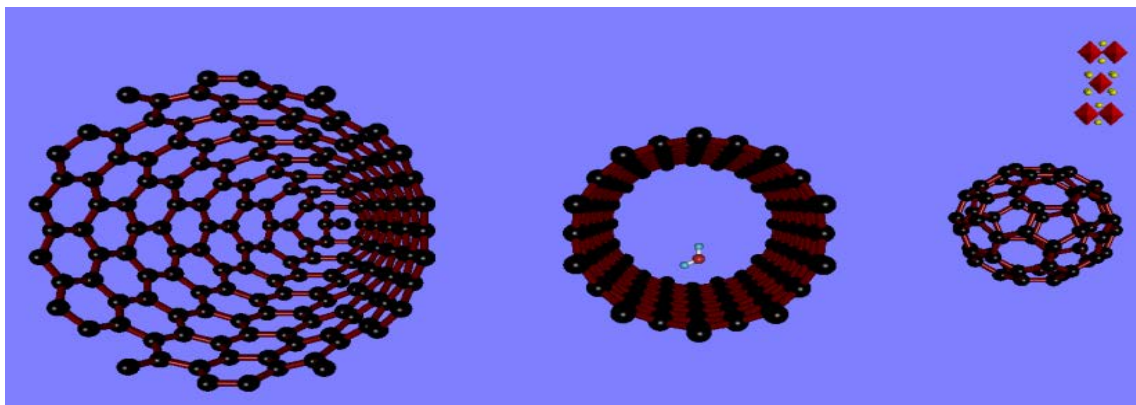in the nanoscale world; (b) The user can be immersed inside the nanotube.

Figure 6. Different nanomaterials: nanocone, nanotube, and buckyball.

devices[12]. The wand can be used to manipulate the nanomaterials for better understanding of the structures. By pressing wand buttons, each structure gets rotated. The structures can be zoomed in and out by using the joystick on the wand.

The third simulation "understanding the chirality of nanotube" is developed to help students understand the concept of nanotube chirality. The chirality is a very important concept to study nanotube. It is a difficult concept for students to grasp as it is very abstract. As explained in the textbook[13], nanotubes are created by rolling up a hexagonal lattice of carbon (graphite). As shown in Figure 7, if the two vectors $\bar{m}$ and $\bar{n}$ are equal then armchair nanotube is formed. If the vector $\bar{m}$ is zero, then zigzag nanotube is formed. If the vectors $\bar{m}$ and $\bar{n}$ are unequal, then chiral nanotube is formed. The nanotubes are formed by rolling them in the resultant axis. The nanotube's chirality determines its electrical properties. The armchair structure has metallic characteristics. Both zigzag and chiral structures produce band gaps, making these nanotubes semiconductors.

Three different nanotubes with different chirality are modeled and simulated in the PowerWall as illustrated in Figure 8. They can be manipulated using the wand. The students can also navigate inside the nanotubes as shown in Figure 9 so that they are able to visualize and compare how the armchair, zigzag, and chiral nanotubes are formed.
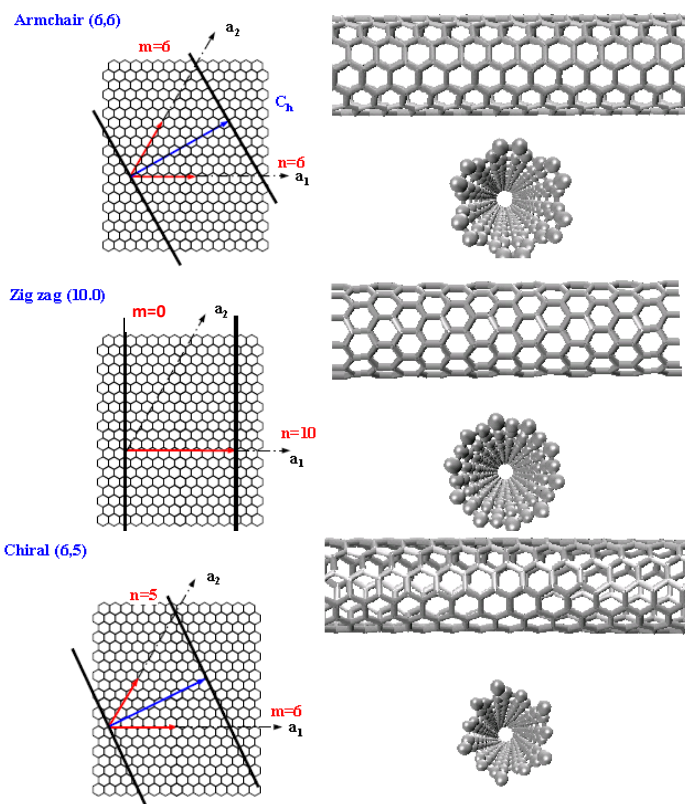

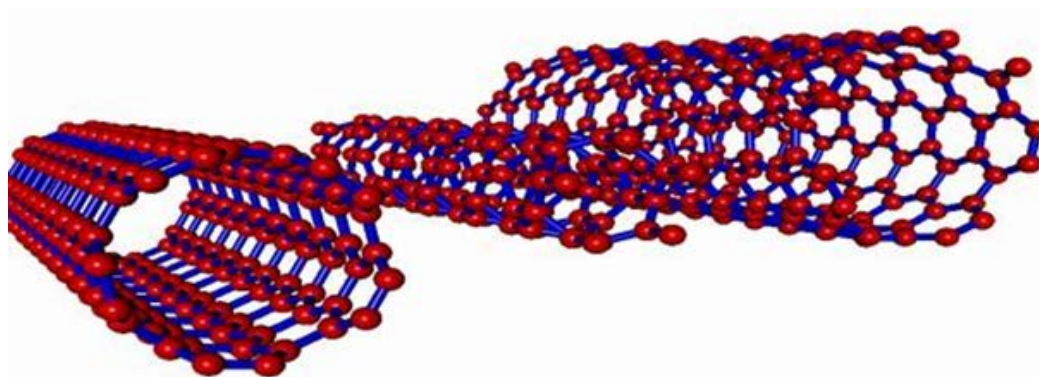Figure 7. Rolling the graphene in specific directions to obrain armchair, zigzag and chiral nanotubes[14].

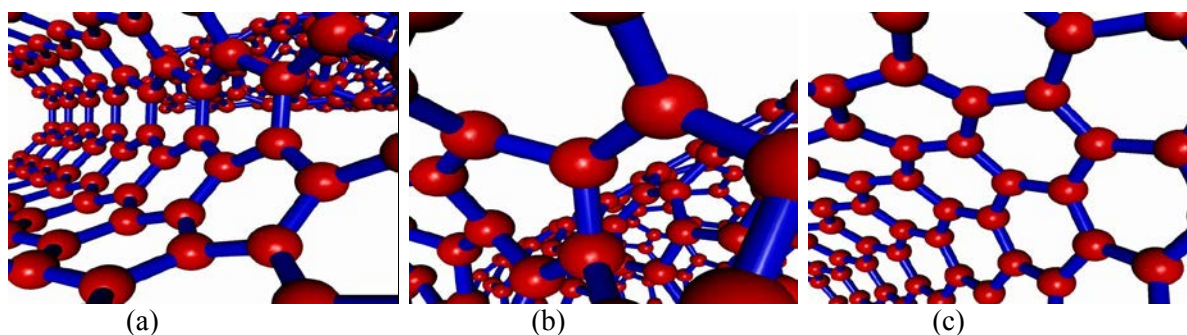Figure 8. Armchair, zigzag and chiral nanotubes visualized in PowerWall.

<center>(a)   (b)   (c)</center>

Figure 9. The close look at the armchair, zigzag, and chiral nanotubes.

Results

The nano-simulations have been integrated in the teaching of course ELEG4223 "Photonic and Electronic Materials and Devices". Twenty one (21) students participated in the nanotechnology VR simulations as part of their class (as shown in Fig. 10). The students then completed a quiz and a survey about the simulations. Information from this survey allows us to monitor the effectiveness of our efforts to integrate nanotechnology into undergraduate science and engineering curricula. The survey results were analyzed by external project evaluator.

Figure 10. Nano-simulations demonstrated to students.

21 students completed the survey about the simulations. The survey questions are listed in Table 1. The students responded to the questions in the scale of 0 to 4 (0 as "Not at all", 1 as "A little", 2 as "Somewhat", 3 as "A lot", 4 as "A great deal"). The average responses and standard deviations of each question are also given in Table 1. The results are graphed in Fig. 11. The following provides a summary of survey data collected from the students.

Students were asked how much the virtual reality simulations added to their understanding of three concepts. (1) How much did the VR simulation add to their understanding of nanoscale? 61.9% of students indicated "a great deal" and 38.1% indicated "a lot". (2) How much did the VR simulation add to their understanding of different nano structures? 52.4% of students answered "a great deal" and 28.6% of the students answered "a lot". 19% of the students answered "somewhat". (3) How much did the VR simulation add to their understanding of chirality of nanotubes? 61.9% of the students indicated "a great deal". 19% indicated "a lot". 9.5% indicated "somewhat". 9.5% indicated "not at all". Most of the students agreed that the virtual reality simulations added to their understanding of nanotechnology. The second and third simulations are not as effective as the first simulation since some students chose "somewhat" and "not at all" as their responses. These two simulations need to be improved.

Students were asked how interesting the virtual reality simulations are. 81% of the students indicated "very interesting". 4.8% of the students indicated "interesting". 14.3% of the students indicated "somewhat interesting". It is evident that the students agreed that the VR simulations are very interesting to them.

Table 1. Survey questions and student responses.

| Survey questions	Average	Standard deviation
How much did the virtual reality simulation add to your understanding of nanoscale?	3.62	0.485621
How much did the virtual reality simulation add to your understanding of different nano structures?	3.33	0.776643
How much did the virtual reality simulation add to your understanding of chirality of nanotubes?	3.24	1.230747
How interesting were virtual reality simulations?	3.67	0.712697
How much did the virtual reality simulations increase your interest in nanotechnology?	3	1.023533
Do simulations like this need to be more interactive?	3.81	0.392677
Do you believe other virtual reality simulations would be helpful in increasing your understanding of nanotechnology?	4	0
Would you like to use more virtual reality simulations?	3.71	0.699854
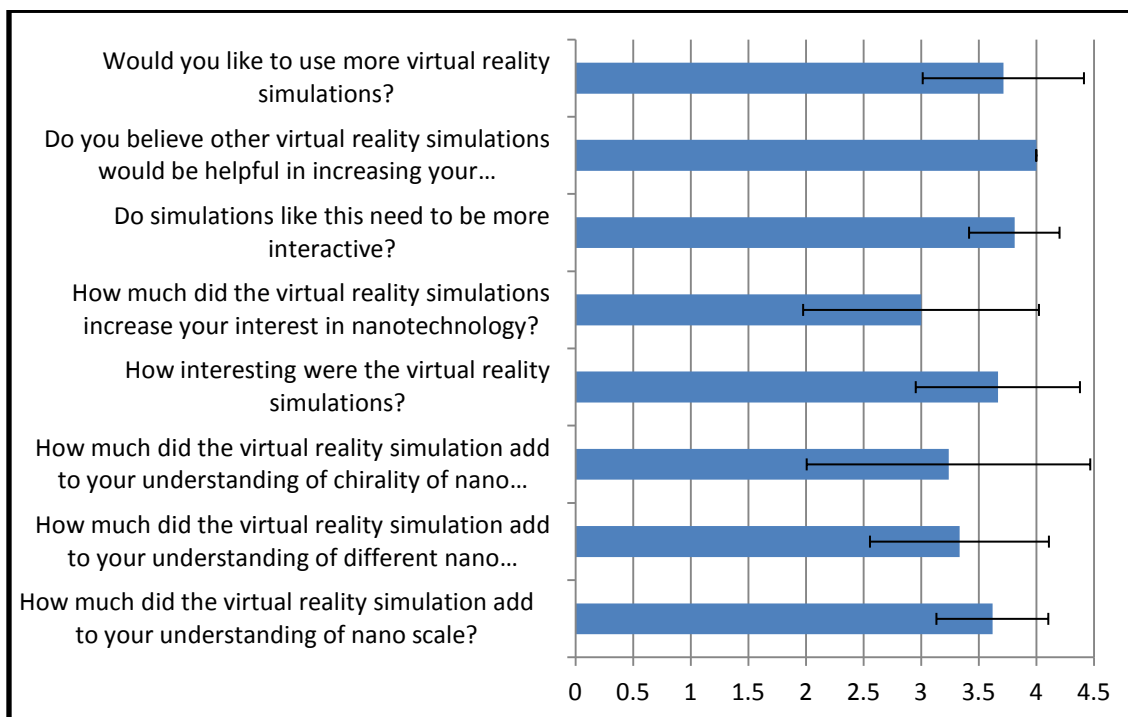
Figure 11. Summary of Students' responses on three simulations.

Students were asked how much the VR simulations increase their interests in nanotechnology. 38.1% of the students indicated "a great deal". 33.3% of the students indicated "a lot". 23.8% of the students indicated "somewhat". Students found that the VR simulations increased their interests in nanotechnology. The survey also asked students if the simulations could be more interactive. 81% of the students answered "yes". 19% of the students answered "no". Students like to see the simulations to be more interactive.

The survey asked the students "do you believe other virtual reality simulations would be helpful in increasing your understanding of nano-

technology?". 100% of the students answered "yes". Students were asked if they like to use more virtual reality simulations. 85.7% of the students indicated "yes". 0% of the students indicated "no". 14.3% of the students indicated "not sure".

Students' responses are very positive. They believe that the VR simulations are very helpful in increasing their understanding of nanotechnology. They want to use more simulations.

Conclusions

This paper presents the development of VR nano-simulations. The simulations are intended to enhance students' understanding of basic nano science concepts, including the nano scale, the structures of nanomaterials, and the chirality. With the help of virtual reality technology, the simulations can engage students in the 3D VR environment and convey the abstract nano concepts in a touchable way. The students can play an active role in the simulations to explore the nano world. The student survey results show that the VR nano-simulations are very helpful in increasing their understanding of nanotechnology. The feedback from students also calls for future work to make the simulations more interactive. More simulations will be developed in the future and they will be used in more courses.

Acknowledgements

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