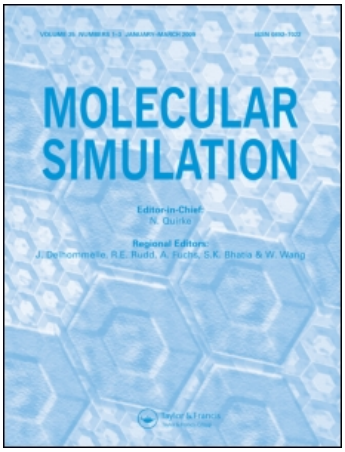

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Novel Simulation Tools for Materials Engineering Education

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NOVEL SIMULATION TOOLS FOR MATERIALS ENGINEERING EDUCATION

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A novel simulation interface is being developed as an educational tool to help students better understand fundamentals of materials science. This interface makes use of virtual reality (VR) technology consisting of PC-based graphics and a force-feedback haptic device. Visualization of atomistic processes with simultaneous tactile sensation *via* the haptic provides a powerful method for understanding complex phenomena that are otherwise difficult to comprehend. Modules are described that allow students to interactively explore interatomic bonding and single-atom diffusion through materials.

Keywords: Virtual reality; haptic

INTRODUCTION

Materials' engineers must have a detailed understanding of the fundamental principles of chemistry and physics as well as a practical knowledge of the processing, properties, and testing of materials. While most engineering students can master the latter, they often have trouble grasping what may seem like abstract physical principles. For example, fracture can be intuitively understood from everyday experience, while there is little 'hands-on' experience from which to understand the atomic-scale characteristics of different types of chemical bonding and how they influence fracture strengths.

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Instructors traditionally attempt to illustrate physical principles through two-dimensional graphs, sketches and illustrations. For example, interatomic forces are often discussed using graphs of energy and force *versus* atom separation. While useful knowledge can be conveyed this way, students often have trouble truly comprehending and especially retaining information from this approach. More recently, computer-based multimedia instructional tools have been developed that overcome many of the constraints inherent in traditional illustrations. Interactive CD-ROMs and web-based utilities that utilize computer visualization, for example, are powerful tools for helping to illustrate complex and often abstract concepts in ways that can be very understandable to students [1].

The next generation of multimedia educational tools will likely be virtual-reality (VR) interfaces that allow both visual and tactile interaction with an educational computer model. These will greatly facilitate learning compared to strictly visual interfaces because

- our environment is typically interpreted both visually and tactilely;
- the amount of information that can be assimilated is increased over strictly visual interfaces;
- they are natural platforms for hands-on active learning;
- they can enhance intuitive understanding of complex topics.

Effective VR technology had required expensive tactile interfaces and specialized graphics computers. This precluded the use of this technology for most educational purposes. Over the past few years, however, there have been significant breakthroughs in the cost of high-fidelity force-feedback haptic devices and PCs with powerful graphics capabilities. These have begun to make VR technology economically feasible for higher education.

In this paper, two software modules that illustrate atomistic principles of chemical bonding are described. These modules have been developed to take advantage of recent price and performance breakthroughs in PC-based graphics and a force feedback haptics. The first module demonstrates the energy and range of interaction for various types of bonding by allowing students to move one atom relative to a second stationary atom while simultaneously sensing the interatomic force between the atoms. The second module allows students to move a single atom in and around a lattice while simultaneously sensing the forces from the lattice acting on the atom. This module is designed for active learning of self-diffusion principles and the role of various kinds of defect structures in diffusion barriers.

A picture of the hardware for which the modules have been designed is shown in Figure 1. It is composed of a Pentium PC and a three-degree-of-freedom Phantom haptic. The PC is used for visualization, control of the haptic, and to store student responses to questions posed by the software. The haptic, visible in the bottom right of the figure, is a hand-held device that is used to manipulate virtual objects on the computer screen. Mechanical linkages within the device control forces on the haptic in response to the motion of the virtual objects. These forces can be a push or pull, or a resistance to motion. The device currently being used (pictured in Fig. 1) was manufactured by SensAble Technologies [2]. It has a maximum feedback rate with WindowsNT of 100 Hz, a nominal position resolution of 0.03 mm and a maximum exertable force of 8.5 N. This haptic provides a much higher response rate, more fluid motion, and a generally greater range of responses to virtual object motion than force feedback interfaces such as joy sticks and steering wheels that have recently been introduced for computer games. These are critical features for our effort, and combine to produce a natural intuitive interaction with the virtual environment on the computer screen.

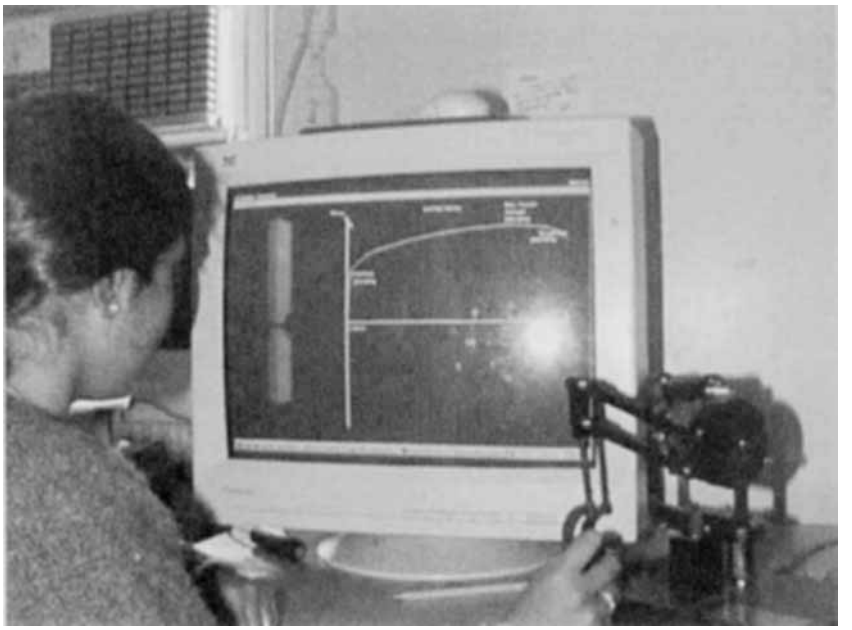

FIGURE 1 Hardware on which the software discussed here has been implemented.

MODULE 1: INTERATOMIC BONDING

Shown in Figure 2 is the software interface for the module on interatomic bonding. There are two purposes for this module. The first is to provide hands-on experience with interatomic forces by allowing students to feel repulsive and attractive interactions between atoms. The second purpose is to reinforce concepts such as relative bond strengths and distances for the different classes of bonding. The code was written using Microsoft Visual C++, with graphics written in open GL. The interface to the haptic uses the Ghost library from SensAble Technologies [2]. The virtual system is composed of an atom fixed in space and a second atom whose position is controlled by movement of the haptic. Two-dimensional graphs of energy and force *versus* distance are to the right of the window. Markers on the two plots reflect the force and energy for particular distances between the pair of atoms. By simultaneously moving the atom, viewing the positions of the markers on the graphs, and feeling the corresponding force, students are able to intuitively grasp the concept of interatomic forces and how they are related to the shapes of the graphs.

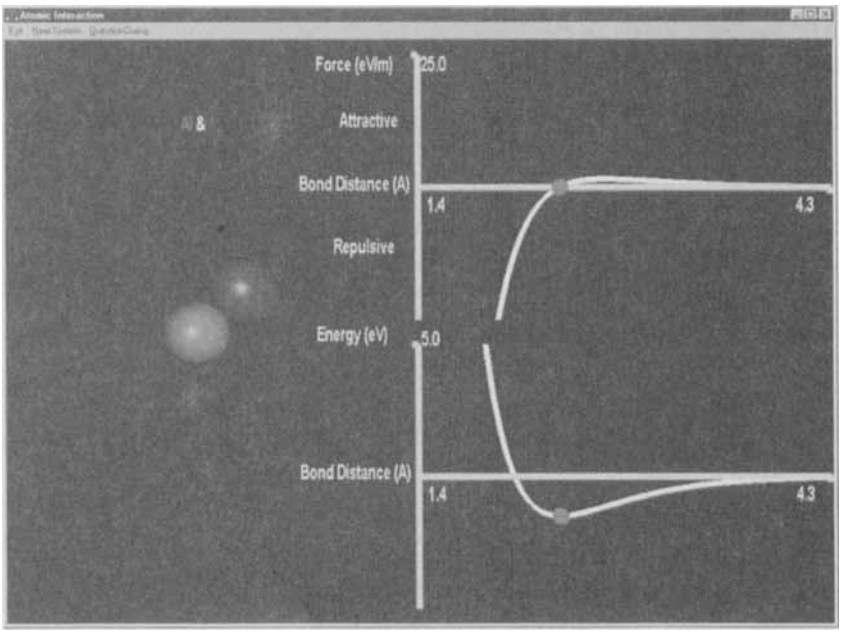

FIGURE 2 Interatomic bonding software interface.

The module currently contains a pop-up window, shown in Figure 3, from which 11 different pairs of atoms can be chosen, each of which illustrates characteristics of one of the different classes of bonding (metallic, covalent, ionic, and weak secondary bonding). For example, students can compare bonding between pairs of Kr atoms, C atoms, and Li^+Cl^- ions to probe differences in bond strengths and interaction ranges for weak, covalent and ionic bonding.

To enhance active learning capabilities of the VR interface, a series of leading questions are included in a pop-up window (Fig. 4). These questions are designed to guide students through the learning process. The students are given a choice of answers, and they submit what they believe to be the correct answer. If the answer is incorrect, they are given an appropriate open-ended answer such as look again at a particular curve or compare bonding between two pairs of atoms. For example, if they do not choose Van der Waals bonding as being weaker than covalent bonding, they are instructed to compare Kr_2 to C_2.

While difficult to convey without using the interface, the effect of moving an atom and sensing the force is remarkable, and has lead to new insights, even for experienced researchers. It becomes immediately clear, for example, that interatomic forces are dominated primarily by the repulsive part of the potential, and the attraction essentially just holds that atoms together. This intuitive result is largely independent of the type of bonding.

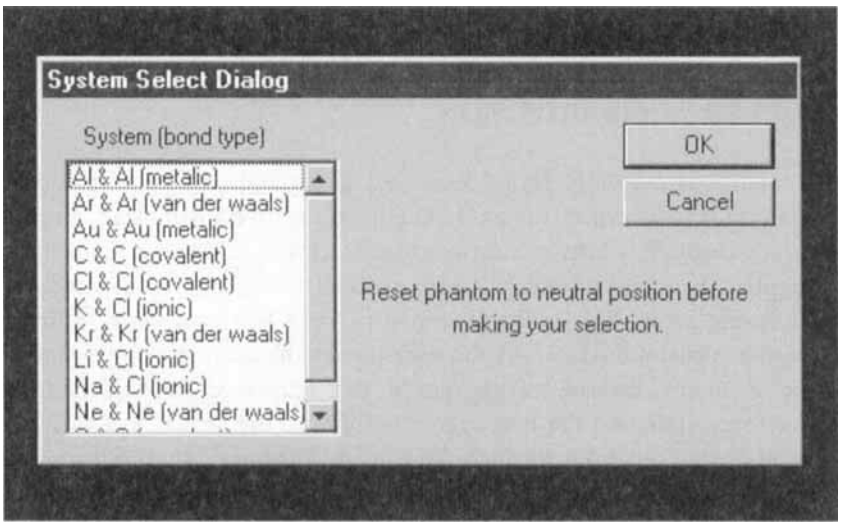

FIGURE 3 Pop-up window from which different pairs of atoms can be chosen.

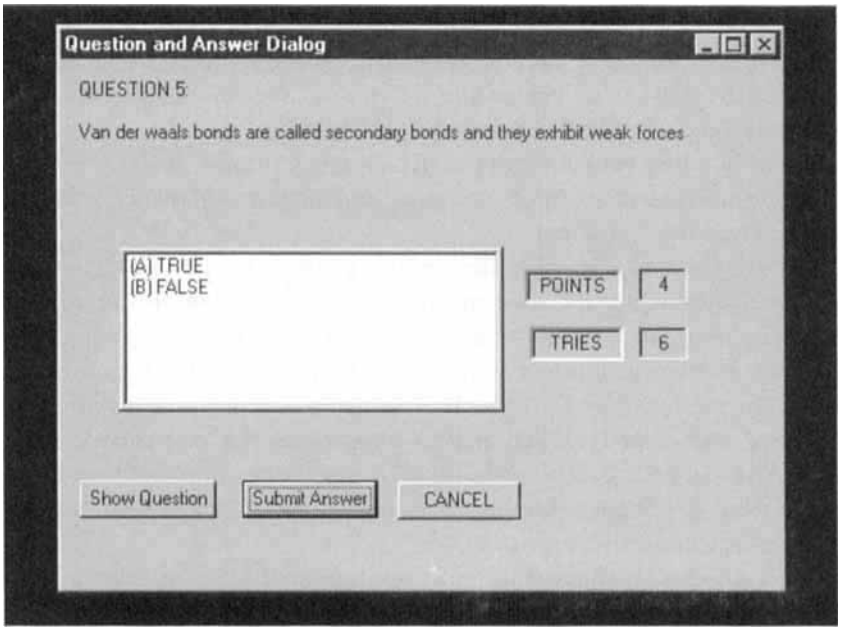

FIGURE 4 Question-Answer dialog box.

This is consistent with general theories of the liquid state that attribute structure to repulsion, and assume that interatomic attraction acts essentially like a glue to hold the system together [3].

MODULE 2: SOLID DIFFUSION

This module is currently being developed to simulate diffusion in a solid. The interface is shown in Figure 5. The haptic is used to translate a diffusing atom through a lattice. As the atom is moved, a force is returned to the haptic, the value of which is proportional to the interatomic force on the diffusing atom. The example shown is for a hydrogen atom diffusing through a nickel substrate. As the user moves the atom by motion of the haptic, a force is returned to the haptic that is proportional to the interatomic force acting on the hydrogen atom due to the lattice. For this case, the module demonstrates through the force to the haptic that diffusion occurs more easily (*i.e.*, with a lower barrier) along the surface than through the bulk nickel, and that there are preferred diffusion pathways through the substrate.

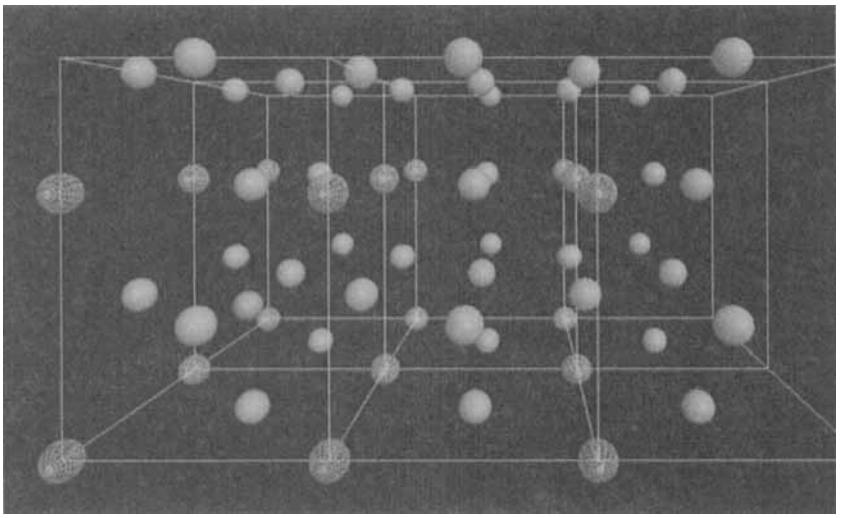

FIGURE 5 Diffusion interface illustrating motion of hydrogen in nickel.

The interatomic forces acting on the hydrogen atom were calculated using the embedded atom method [4]. Based on effective medium theory [5], this is a relatively simple analytic interatomic force model that provides a reasonably accurate description of bulk and surface properties of a variety of metals. As above, the module was written in visual C++, and uses OpenGL and Ghost software for graphics rendering and controlling the haptic, respectively. Despite the relative efficiency of using the embedded-atom method to calculate forces, the PC platform is not fast enough to simultaneously calculate forces, render the spheres representing the atoms, and control the haptic with a sufficiently fast response rate. Therefore the forces on the hydrogen atom were first calculated for a three-dimensional grid of points within a single unit cell using a high-performance workstation, and the values transferred to the PC. The only computing performed on the PC in addition to rendering and controlling the force on the haptic is to look up forces for a grid point corresponding to the position of the hydrogen atom within the unit cell. The drawback to this approach is that it requires lattice positions that do not respond to the hydrogen motion. While this can influence diffusion barriers, it does not significantly change the qualitative features of pathways and relative barriers for diffusion that are being presented to the user.

This module can be utilized for illustrating systems and related concepts other than that shown in Figure 5 by inputting alternate force grids and

atomic positions. For example, a metal surface containing a step with a movable atom can be used to illustrate how diffusing atoms on a surface will tend to stick to steps and other defects. This concept in turn can be used to effectively teach students common growth mechanisms of vapor deposition. A second example is using a substrate containing a grain boundary around which a diffusing atom can be moved with the haptic. Sensing lower barriers for diffusion through the substrate defect would illustrate the principle of rapid grain boundary diffusion in bulk materials.

An interface similar in spirit to that in Figure 5 has been developed by Levit and Henze at NASA-Ames [6]. In their system, virtual carbon and/or hydrogen atoms are moved with a haptic while the feedback forces are simultaneously calculated from an analytic potential. Their system, which uses a four-processor Silicon Graphics high-performance workstation for the rendering and computation and a Phantom haptic like that in Figure 1, can currently maintain a reasonable rendering and force feedback update rate for up to about 60 carbon and hydrogen atoms. The hardware for this system, while powerful, is currently too expensive for the type of educational goals being addressed here.

TECHNICAL INSIGHTS AND CHALLENGES

Two unanticipated technical issues have so far arisen from this project: The first is related to graphing forces and energies *versus* distance for strong and weak (secondary) bonding. The general shapes of these curves are similar for covalent and Van der Waals bonding. If these curves are graphed on a common scale, however, it is not obvious that they have the same shape due to the large differences in bond strengths. On the other hand, using different force and energy scales, while making the curves appear similar, does not easily convey the differences in bonding properties. With tactile stimulation there is no need to plot these properties on the same scales for the two types of bonding because the relative bond strengths are easily sensed by the tactile sensation of the haptic.

While the graphing issue is neatly resolved, a second technical difficulty was encountered with the haptic. When moving the atoms past deep energy wells into the repulsive region of the potential in the first module, the haptic pushes the atoms apart. Depending on the force, the moving atom (and hence the haptic arm) can be thrown back into the attractive part of the potential. If the potential is steep enough around the well, this motion can result in a 'chatter' of the haptic as the atom is bounced around the bottom

of the well. A similar effect occurs for the second module when the atom is moved into a region of the system in which the force rapidly changes with atom motion.

Two solutions to the chatter issue are currently being explored. The simplest of the two is to reduce the proportionality between the haptic response and the interatomic force. However, if this is reduced too much, it becomes impossible to sense bonding associated with weak secondary forces in the first module, or to sense all of the relevant diffusion barriers in the second module. Assuming a different proportionality between interatomic and haptic forces for weak and strong bonding results in the same sorts of issues as in plotting graphs of energies and forces discussed above. At present, the module compromises between reducing (but not yet eliminating) chatter while still retaining an apparent attraction for weak bonding and sensing important barriers for diffusion.

A solution to the chatter problem that has been incorporated in the NASA interface mentioned above is to have a damped spring connecting the haptic and the mobile atom [6]. By adjusting the value of the spring constant and the mass of the atoms, the chatter can apparently be reduced without severely compromising the fidelity of the haptic. This feature is currently being implemented into the software described here.

FUTURE PROSPECTS

The cost of the hardware for which the software was implemented, while significantly less than had been required for this type of system just a few years ago, is still prohibitively large for wide spread undergraduate educational use (the station shown in Fig. 1 costs about $25,000). However, if current trends in cost reduction continue, this type of technology will be well within reach of most universities within the next decade. The haptic manufacturer, for example, has introduced a desktop version of their haptic that costs less than $10,000 [2], about a 1/3 reduction from the device shown in Figure 1. Furthermore, this company has predicted that the cost can be brought down to as low as $500 within a few years. At the other end of the scale, the performance of the low-fidelity force feedback devices recently introduced for computer games (which typically cost around $100) will undoubtedly improve, making these devices potentially useful for educational purposes. With the rapid enhancements in PC-based graphics capabilities, it is anticipated that it will be possible to fill an entire room with these types of stations so that students may actively explore physical

principles with VR technology without time constraints inherent to usage of a few, expensive stations.

Acknowledgements

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