Understanding ice phases with virtual environments

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Understanding Ice Phases with Virtual Environments

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Abstract

Immersive virtual reality experiences have been considered a domain for games or military training. However, the use of three-dimensional environments became also essential in several scientific areas such as fluid dynamics, chemistry, etc. In science education, it is also becoming popular since it facilitates the development of correct scientific models.

"Virtual Water" is a virtual environment allowing the exploration of the molecular constituents of water as well as some of the macroscopic structures made up by them. Hydrogen bonding is the key feature for understanding the physical and chemical properties of water. Solid water has a rich phase diagram that is still not fully understood. We show how to explore some solid phases as well as clusters, which are intermediate structures between the molecule and the solid.

1. Introduction

Computer technologies may allow learners to visualize physical processes which would be otherwise difficult to see and, therefore, may allow them to construct better qualitative and quantitative understandings of natural phenomena. Ten years after virtual reality technologies emerged, an array of virtual worlds has been developed to help students to learn abstract and complex concepts. For instance, virtual reality applications allow students to see the effects of different physical laws and to observe events at microscopic and macroscopic scales.

An area where we are applying this kind of technology is the study of the structure of water, including the ice phases. Normal ice is a molecular solid in which the intermolecular binding is assured by the hydrogen bonds, a feature that accounts, among others, for the fact that ice floats in liquid water. The behavior of ice at high pressure is important for many problems in physics, chemistry and planetary sciences. For example, a newly discovered dense form of ice (ice XII) is expected to contribute to understanding the properties of the interiors of the outer planets in the solar systems, such as Saturn, Uranus and Neptune.

To aid pupils understanding the structure of water, the Physics and Mathematics Departments of the University of Coimbra, Portugal, the Exploratory Henry the Navigator and the High Education School for Technology and Management of Guarda, are developing the *Virtual Water* project. This consists in building and exploring a virtual environment devoted to learning the constitution and properties of water in its different phases. Within this environment, the simulation of the molecular dynamics of the solid, liquid and gaseous phases and phase transitions evolves in three-dimensional space, with the possibility of haptic interaction [1,2].

We aim at contributing to improve science education for students of the last year of secondary school and the first year of university. Our virtual environment is realistic enough and very comprehensive, allowing for exploring the microscopic constituents of water (we may "build" atoms and molecules, manipulate molecules and molecular clusters, etc.) and for studying some macroscopic properties.

2. Ice phases environments

We want to introduce students to molecular structures and chemical bonding, concepts which are not easy to learn from textbooks or traditional lectures. These aspects belong to the Chemistry curriculum ("structure and propriety of solids, liquids and gases") of the last year of Portuguese secondary school (12th grade). Our virtual environment is designed to illustrate specific scientific concepts. For example, students may catch and toss molecules, or break hydrogen bonds, to learn about, respectively, matter phases and chemical bonding. These possibilities are valuable teaching tools since all textbooks and almost all computer simulations which present these ideas restrict themselves to two-dimensional representations. Here we focus on ice structure. Fig. 1 is a snapshot from our virtual environment and showing the crystalline structure of normal ice.

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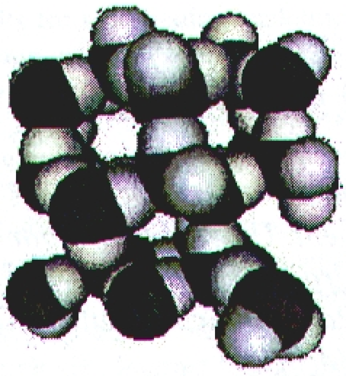

Fig. 1 - Crystalline structure of normal ice.

It is well known that a whole variety of clusters may exist in between a molecule and a solid. They usually have many isomers with similar energy. The cyclic isomer of the water hexamer (Fig. 2a) is studied in our virtual environment, as a representative of these clusters. It is the smallest piece of ice and it represents one of the newest and most important morphologies found in computer simulations of liquid water. At present, ice XII is the densest known phase of water. Figure 2b) shows its structure exhibiting the pentagonal rings which form channels along them.

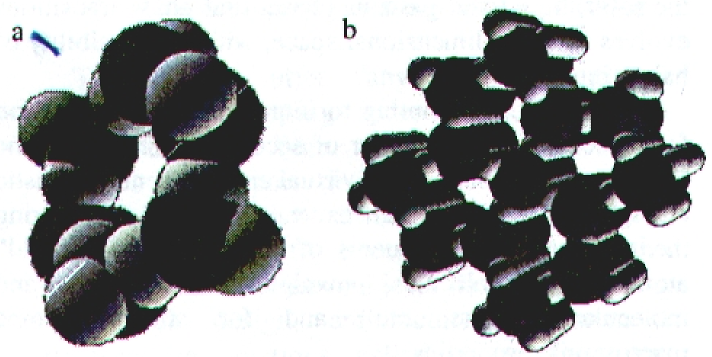

Fig. 2 - a) Cyclic isomer of the water hexamer; b) The structure of ice XII.

3. Conclusions

Enthusiasts crow that virtual reality is one of the most exciting tools that are now emerging for students and that it will revolutionize education. To skeptics virtual reality is just the latest overpriced, hyped-up educational fad. To many people the debate over virtual reality in education seems a replay of a similar debate twenty years ago about using computers in schools.

Clearly nothing can replace the contact with the real world that is, after all, the object of Physics and Chemistry. Nevertheless, it is remarkable that we can today, with the help of computers, create virtual worlds where we experience feelings of motion and action which are otherwise difficult or impossible to experience. We suggest that in the scientific-pedagogic community gets more involved this kind of projects.

Our project comprises the evaluation of the system's functionality, including the adaptation of the users to the virtual environment and the efficiency of its use in teaching and learning Physics and Chemistry. For that, the following goals were established:

- Analysis of some pedagogic difficulties in order to know whether they can be overcame through virtual scenarios.
- Visualization and interaction of students with virtual environments to develop analogies and contrasts with daily experience. Virtual reality should be useful to learn abstract objects as concepts since feeling or seeing an object mediates a mental representation.
- Comparison of learning progresses obtained with specific virtual reality hardware with other obtained with more traditional means.

The work is under way so that its evaluation is in a preliminary stage. Tests with students, which are planned, will give us information on the pedagogical value.

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