Open source software for visualization in condensed matter Physics

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Abstract

Research shows that effective college learning requires active learning involving active participation of students in the classroom [1]. This is especially true in introductory condensed matter physics which involves plenty of visual understanding to learn different types of crystal structures, crystal planes, reciprocal lattice, Brillouin zones, etc. In this article we discuss the possibility of classroom usage of an open source software called visual molecular dynamics (VMD) to interactively create and visualize crystal structures to aid student understanding of several concepts in condensed matter physics. A visualization example is shown with step-by-step guided instructions to visualize crystal structure of sodium chloride unit cell.

Keywords: Physics Education, Condensed Matter Physics, Visual Molecular Dynamics.

Resumen

Las investigaciones muestran que el aprendizaje eficaz en el colegio requiere un aprendizaje activo involucrando una participación activa de estudiantes en el salón de clases [1]. Esto es especialmente cierto en el curso introductorio de física de la materia condensada el cual incluye mucha comprensión visual para aprender diferentes tipos de estructuras cristalinas, planos de cristal, enrejado recíproco, zonas de Brillouin, etc. En este artículo discutimos la posibilidad de uso en el salón de clases de un software de código abierto llamado visual dinámico molecular (VMD) para crear de forma interactiva y visualización de estructuras cristalinas para ayudar a la comprensión del estudiante de los varios conceptos de la física de materia condensada. Un ejemplo de visualización se muestra con una guía de instrucciones paso-a-paso para visualizar la estructura cristalina de la unidad de celda de cloruro de sodio.

Palabras clave: Educación Física, Física de la Materia Condensada, Visualización Dinámica Molecular.

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I. INTRODUCTION

In all aspects of our interaction with the world, we come across materials in one form or the other. The computers make use of a class of materials based on Silicon. The atmosphere and the air we breathe is a mixture of several gases such as nitrogen, oxygen, argon, crbon dioxide, etc. Even our body is made of several kinds of organic materials. The Sun, Moon, and the Earth are made of matter in different phases such as solid, liquid, gas or plasma.

The branch of physics that deals with the physical properties of condensed phases of matter is called condensed matter physics [2]. This branch of Physics helps us understand various kinds of solids and their behavior. If one were to take an extremely powerful microscope and study different kinds of materials, one finds that they are all very similar – and yet they are unique. The similarity arises from the fact that all materials are fundamentally made up of atoms. The uniqueness comes from the fact that every element has its characteristic atomic configuration (arrangement). It is this interesting amalgamation of uniqueness and similarity that makes the world as colorful as it is.

In addition to the fact that different elements have varying atoms, an element (or molecule) can exist in several phases depending on its atomic (or molecular) arrangement. For example, a water molecule can exist with its molecules arranged in spectacular spatial regularity, forming ice. When heated, water molecules tend to drift away, causing ice to melt and become liquid water. When heated further, water molecules drift even further apart, thus vaporizing water into its gaseous phase called steam or water vapor.

Even in a given phase of matter, a substance can assume different atomic (or molecular) arrangement. For example, Carbon can exist with its atoms tightly packed close to each other, forming diamond. On the other hand, Carbon atoms can also be arranged in layered form, relatively loosely bound, forming graphite. It is this arrangement of atoms in the substance that often determines its physical properties.

From a physics perspective, these concepts are typically introduced in a condensed matter physics course which is often a mandatory class for a physics student in most countries. Understanding the basics of atomic arrangements in materials requires a three dimensional understanding and visualization of materials. Text books typically provide two dimensionally projected drawings of atomic arrangements which can be confusing to an average student. Getting a grasp of concepts in condensed matter physics typically requires students to actively engage themselves in imagining three dimensional structures. Although atomic and molecular models are available for students in many classrooms, they suffer from the following two serious drawbacks: (1) The students often don't have the option to manipulate the positions of the atoms in a structure, and (2) they don't have access to the models beyond their class hours.

In this article, we present a computer based method to create three dimensional models of atomic and molecular structures using a free of cost and open source molecular modeling and visualization computer software called Visual Molecular Dynamics (VMD) developed by University of Illinois at Urbana-Champaign, USA. Using VMD, the students can build the molecules with their own programs, and they can use it on their personal computers, solving the two drawbacks mentioned in the last paragraph.

II. VISUAL MOLECULAR DYANMICS

Visual Molecular Dynamics (VMD) is visualization software intended for use with molecular dynamics simulations. VMD is available open source, and can be downloaded on the internet free of cost, for computers running MacOS X, UNIX or Windows. Although it is broadly used for modeling polymers and biomolecules, it can very well be used for modeling crystal structures. VMD can be downloaded from the website http://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD.

Creating and visualizing a molecule in VMD requires us to input the atomic coordinates of the constituent atoms of its unit cell [3]. In the next section we present an example structure to visualize the structure of sodium chloride (NaCl) molecule.

III. SODIUM CHLORIDE STRUCTURE

The atomic coordinates of a NaCl molecule are given in Reference [4]. The NaCl unit cell has a face centered cubic crystal structure with each sodium ion surrounded by 6 chloride ions as nearest neighbors, and each chlorine ion surrounded by 6 sodium ions as their nearest neighbors. The structure of NaCl can be thought of as two interpenetrating face centered cubic lattices [5]. NaCl has a lattice parameter of 5.64×10^{-10} m, which means every edge of its cubic unit cell is 5.64×10^{-10} m.

In order to visualize NaCl structure, we first create an ASCII file listing the total number of ions in NaCl unit cell (27 in this case) and the *x*, *y*, and *z* positions of all atoms of the unit cell cube. The sample file for creating NaCl structure would look like this:

```
27

Na    2.82  2.82  2.82
Na    2.82  0     0
Na    0     2.82  0
Na    0     0     2.82
Na    5.64  2.82  0
Na    0     5.64  2.82
Na    0     2.82  5.64
Na    5.64  2.82  5.64
Na    2.82  5.64  5.64
Na    2.82  5.64  5.64
Na    5.64  5.64  2.82
Na    5.64  2.82  2.82
Na    5.64  2.82  2.82
Cl    0     0     0
Cl    0     2.82  2.82
Cl    2.82  0     2.82
Cl    2.82  2.82  0
Cl    5.64  0     0
Cl    0     5.64  0
Cl    0     0     5.64
Cl    5.64  5.64  5.64
Cl    0     5.64  5.64
Cl    5.64  0     5.64
Cl    5.64  5.64  0
Cl    5.64  2.82  2.82
Cl    2.82  5.64  2.82
Cl    2.82  2.82  5.64
```

Note carefully that the first line of the file contains the total number of ions (27), followed by an empty newline. The name and three dimensional position coordinates of the ions start on the next line.

The data mentioned in the above format needs to be stored in a file named with an extension of ".xyz". For example, we could name this file as "NaCl.xyz". When this molecule is loaded and rendered using VMD, the visualization screen renders the three dimensional structure of NaCl as shown in Fig. 1.

IV. CONCLUSIONS

In conclusion, we have introduced the readers to freely available open source software called Visual Molecular Dynamics. Since visualization is an important aspect of teaching and learning physics, we think this will be a promising student aid in learning condensed matter physics. In addition to being open source, VMD is also easy to use, and low on memory consumption for static visualization of crystal structures. The students can interact with the crystal structures they create, making the process of learning more

independent, student-oriented, active and, fun. This software is also very helpful in visualizing crystal structures, crystal planes, distances between atoms, etc. Although usually to be used for research purposes, VMD can be very useful when used for introductory condensed matter physics courses.

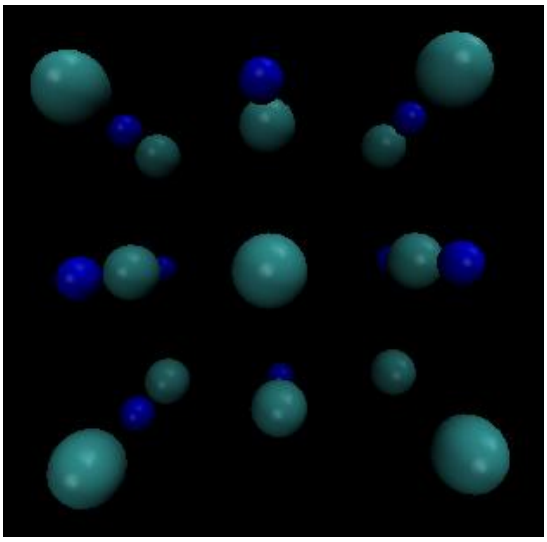

FIGURE 1. The cubic structure of sodium chloride rendered by VMD. This is a view from the *z* axis picture rendered by VMD. The bigger ions represent Chlorine (Cl^-) and smaller ions represent Sodium (Na^+). The crystal can be rotated in 3D to obtain other perspectives.

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