Visualizing Nanodiamond and Nanotubes with AViz

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Abstract. Carbon atoms form a surprising variety of geometrical structures with a wide range of geometrical, physical and chemical properties. Our AViz atomistic visualization software enables visualization of the results of atomistic simulations of carbon allotropes. Techniques to aid in the perception of the three-dimensional structural specifics of different carbon nanosystems, both alone and in interaction with hydrocarbons are discussed in this chapter.

1 Introduction

Visualization is very helpful for atomistic simulations, and the AViz package developed [1] [2][3] by the Computational Physics Group at the Technion is an easy way to implement visualization with true three dimensional quality on simple LINUX boxes. It is useful for both teaching and research applications.

AViz is simple to apply. A file of the x, y and z coordinates of atoms is prepared, either from a simulation or by construction, and then interactively enhanced by adding bonds of varying lengths. The visualization can be updated during a simulation, sliced to show the sample interior, or animated to show time development. We zoom in and out or rotate the sample in order to get a feeling about that third dimension out of a two dimensional screen. In recent years we have been concentrating on extending AViz' applications to general situations where three dimensional visualization can help us deduce what is going on inside samples. Some of these extensions have required new programming but most just require deducing how to utilize features that already exist.

Carbon poses a special challenge to visualization because the different hybridizations lead to different numbers of neighbours, including two (e.g. linear chains or carbyne phase), three (e.g. graphite) and four (e.g. diamond). The projects from which the visualization issues relating to carbon have been extracted and will be described below all have been/will be described in separate publications and presentations together with the physical issues, as well as qualitative results. Here we concentrate on visualization issues in greater depth than might be appropriate elsewhere. We note that all projects have in common the use of visualization to debug, deduce at which coordinates detailed measurement is needed, show experimental partners what is happening, and finally make presentations.

Our simulations are made with a range of techniques - Molecular Dynamics (MD), Monte Carlo (simulated annealing and simulated tempering), (both with Tersoff/Brenner [4] [5] potentials), tight-binding MD (Oxon [6] and Plato [7]), abinitio (Abinit [8]) as suited (and possible). We collaborate extensively with experimentalists at the Technion, and the visualizations form the basis for discussing results with them. In general, our visualizations do not tap directly into the electronic stucture to decide about the hybridization, but rely purely on geometric information. The geometric information of how many nearest neighbours are present largely gives the correct hybridization and certainly enables us to gather useful information because we are, after all, trying to visualize geometric structure.

If carbon only took the two forms of diamond and graphite, that would be enough to make it special. However, as well as carbon being one of the building blocks of organic molecules, pure carbon takes the form of buckyballs, nanotubes etc. And if that were not sufficient, in addition to cubic diamond, there is another, hexagonal solid known as londsdaleite, whose distinction from the cubic form makes most other carbon visualization issues trivial. (The above ode may be sung to the tune of "dayenu" from the Passover seder, if desired.)

We now describe some specific issues. Because we indeed wish to view samples in color and undergoing animation, we refer the reader to the webpage [9] where these are so presented.

2 Red, blue and yellow

The first steps in attacking carbon specific visualization issues in our Computational Physics group were made by David Segev (Saada) when studying damage in diamond [10]. He also developed our first OpenGL codes for atomistic visualization. The simple idea of using different colors for threefold and fourfold coordinated carbon and in particular of using different colors to indicate bonds of different lengths enabled us to find defects and graphitic structures hiding in 5000 atom samples. We originally used red/blue for threefold and fourfold coordinated atoms, as well as yellow for fourfold coordinated atoms that are neighbours of threefold coordinated ones, and later switched to yellow/blue for three/fourfold coordinated atoms so that the images were understandable in greyscale. More recently some of the graphics was restyled, using colored bonds to join threefold coordinated atoms, leading to a clearer view of graphitic damage in diamond [9].

Differentiating between cubic diamond and graphite is easy if there are large samples of perfectly ordered material. In disordered or amorphous samples this is much less clear and has been an ongoing challenge for us. Recent results from a study [11] of diamond nucleation under high pressure were possible mainly because the atoms were color coded for coordination number

and then the diamond nanocrystals became visible within the amorphous matrix.

Possibly the hardest challenge has been differentiating visually between cubic and hexagonal diamond. This is hard even with large ordered samples, because the structures are different only in a subtle way. (It is also hard from an experimental viewpoint.) This is harder when searching for nanocrystals embedded in an amorphous matrix, but the possibility to extract the nanocrystals and then rotate them and compare with reference cubic and hexagonal crystals can result in unambiguous identification of the correct form.

3 Transporting, vibrating and bending nanotubes

Static nanotubes can be drawn in many ways, and there are lots of nice pictures on the web. Their vibrations and distortions are less easy to illustrate and visualizing their interactions with other molecules even less so. The issue of transport of hydrocarbons in nanotubes is of interest for applications to the chemical and pharmaceutical industries. The nanotube (which is the flow region) is bounded by two control volumes (CV) with fixed atomic concentrations at the edges to study chemical-gradient driven diffusion. The chemical potential in each CV is fixed by inserting and deleting particles according to the Grand Canonical Monte Carlo (GCMC phase), and the dynamic motion is described by Molecular Dynamics. The particles diffuse through the tube and the parameters of the flow are calculated. In order to show both the tube and the particles passing through it is necessary to find a way to show the tube atoms and bonds being almost transparent so that the diffusing particles can be seen. In order to ensure that they really pass through they are drawn in a different color as they exit, to confirm they have indeed done so. Figure 1 shows methane molecules in detail, including bonds for perspective. (with Brenner potentials used for both the tube and the methane) entering a tube. For more etensive runs, we used Brenner potentials for short range and Lennard-Jones potentials for long range interactions, and in Figure 2 where the full experiment is shown, for the case of a rigid (6,6) carbon nanotube, of radius 4.07 and length 100 angstroms. The densities of the control volumes in reduced units are CV1 on the right = 0.006, and CV2 on the left=0.0003. Here we illustrate methane by the larger single spheres, and do not show the bonds of the nanotube explicitly to aid in the transparency. A full characterization of this diffusion will be provided in the future [12].

An experimental group of systems of current interest are nanoscale systems in which there is a coupling between the mechanical and the electrical degrees of freedom. For example, Nano-Electro-Mechanical Systems (NEMS) are being studied in order to realize ultra-sensitive mass resonators, with the aim of achieving the ultimate single molecule detection limit. There are technical limitations to manufacturing smaller nanomechanical beams with

Fig. 1. Nanotube with methane molecules

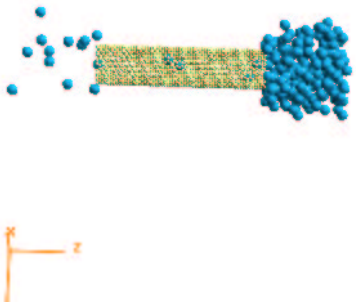

Fig. 2. Nanotube with methane molecules diffusing between two control volumes

conventional photo or e-beam lithography techniques, and degradation is expected in the quality factor as the surface-to-volume ratio increases. An alternative approach is to use carbon nanotubes as the mechanical resonators.

To model this it is necessary to study nanotube vibrations, so we began this by clamping a nanotube at both ends and allowing it to move under a downward force [13]. We studied the best way to visualize the three dimensional tube and found that by indicating the coordinates of each atom as a dot and drawing bonds of a specific length in each case one could clearly see how the tube bends by contacting bonds at the top center and lower ends and

lengthening bonds at the top ends and lower center. When the tube vibrates again upward the extended bonds contract.

4 Zoom

Another topic of interest is the visualization of different carbon structures such as bucky balls, C240 etc. A two dimenional straight-on picture fails to do justice to their extreme symmetry. Simple rotation of an image does a better job, but successive zooms with a cutoff so that one side of a tube can be viewed at a time (as shown on the talk webpage links [9]) really clarifies the structure.

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