The essential role of visualization for modeling nanotubes and nanodiamond

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Abstract

Visualization techniques to help understand the structure of carbon and its allotropes have been developed and applied to atomistic simulation projects which model different carbon systems on the nanoscale. Examples from ion implantation in diamond, the diffusion of hydrocarbons in nanotubes and the creation of nanodiamond from amorphous carbon under pressure are given.

Key words: visualization, carbon

1. Introduction

Carbon takes many different forms. It has a fantastic range of properties which result from different electronic configurations which give different geometical structures. Deducing the geometry of a sample that has been simulated is a crucial step towards understanding its properties. Visualization is essential for understanding sample geometries.

In a series of studies of diamond, graphite, amorphous diamond and nanotube structures we have developed techniques to visualize the sample geometries, especially in regions of defects and during transformations between different allotropes. Some of these such as animation, rotation, and slicing are useful in general, while others such as highlighting different atomic coordinations and bond lengths, are specific to carbon. Our AViz code [1,2] provides an easy way to actualize these for samples including as many as tens of thousands of atoms. Tracking of specific atoms under dynamic motion, and interactive three-dimensional visualization often provide the key to elucidation of the structure and properties. All projects were undertaken in close contact with experimental groups and visualizations provided a common language for discussions.

2. Background

A carbon atom has 6 electrons, and a nucleus with 6 protons and some neutrons, each of which has a wave nature. To visualize a carbon 12 atom showing this detail would require a very small nucleus with overlapping wave packets for the 6 protons and 6 neutrons and then 6 wavepackets for the electrons extending over a much larger range. Even if we simplify each atom to a point nucleus and just show the electronic density of the electrons, this remains a graphical challenge. In fact a 3 dimensional visualization of the electronic density of even the single electron of a single hydrogen atom is quite tricky [3]. This is generally done with techniques such as smoke rendering [4] and we have developed an adaption of AViz which uses color to help indicate density for such cases.

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Once carbon atoms form e.g. a graphite or diamond lattice, the electronic orbitals hybridize and it would be very hard to draw electronic densities in any way that the underlaying lattice structure could be understood for tens of atoms in a solid sample However the nature of the “bonds” between atoms is such that carbon atoms have 3 in-plane nearest neighbours in sheets of graphite bonded by sp2 orbitals and 4 neighbours in an sp3 bonded diamond lattice. Thus if we visualize the lattice structure in a way which indicates the number of neighbours in the colors of the atoms and “bonds” we will also have a good feeling for the nature of the bonds.

Atoms are not solid spheres and interatomic bonds are certainly not the cylinders one sees in ball and stick models or representations of molecules and solids! But, in a physical model physical objects signifying the atomic locations are needed as are connections to hold them in place. If we want to show a sample of atoms in a computer visualization with 3 dimensional perspective, then symbols marking the atomic sites are often required, and lines connecting neighbouring atoms provide an enormous aid to the eye. It is convenient to make these symbols balls or dots and to use the connecting lines to indicate the interatomic distances.

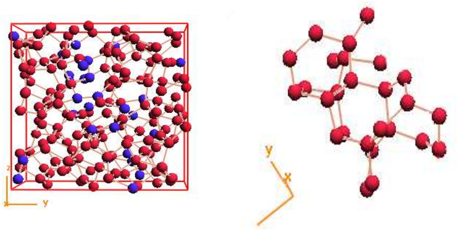

Fig. 1. Diamond nanocrystal in amorphous network, red (blue) atoms are sp^3(sp^2) bonded.

3. Searching for diamonds in haystacks and graphite in diamonds

Tiny nanodiamonds grow in samples of amorphous carbon when these are subjected to high pressures and temperatures[5]. Depending on the pressure we found 30 or more atoms in a diamond nanocrystal within a 216 atom amorphous carbon sample (with periodic boundary conditions). Our success statistics in growing nanodiamond exceed some others and we suspect this is due to our enhanced vision rather than chance.

Rotation is extremely useful here to aid visualization of the lattice structure. Selecting specific colors for atoms (and bonds between atoms) with specific coordination numbers enables us to glance at a sample of carbon and find the nanodiamond crystal in its amorphous matrix or the graphitic region in diamond damaged by ion implantation [2].

4. Nanotubes

Visualizations have also greatly aided two nanotube projects. The study of hydrocarbon diffusion in nanotubes used visualization intensively for debugging and also for understanding the nature (single file or normal) of the diffusion. Here the nanotube was drawn without bonds to make it semitransparent [2] and specific diffusing atoms were sometimes colored in order to trace specific particles. In another project, where we observed bending of nanotubes due to external forces, we chose to draw atoms as dots, and in different images drew interatomic distances of specific length ranges in order to show where bonds contracted and where they stretched [2].

More examples as well as technical details have been given in the manuscripts referenced below describing specific projects, Color and animated images for the different cases can be found on a website developed specifically for this project [6].

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