Adventures in carbon visualization with AViz

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Abstract

We introduce and resolve several visualization challenges resulting from the Technion’s Computational Physics Group’s recent simulations of carbon allotrope systems such as CVD diamond, ion implantation for diamond membrane surfaces and nanotubes. These projects required larger and more intricate atomic samples than our previous studies, and therefore they required more flexibility in the selection of visualization parameters. The visualization solutions are provided within the framework of a new edition of our AViz code. AViz 6.0 enables variation of the fovy angle (field of view in the y direction) and of bond width, as a function of bond length, to aid three-dimensional perception, and includes options for sequential polymer bonding and easy compilation for different LINUX flavours in a single package.

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1. Introduction

The ability of carbon atoms to take different hybridizations and form diverse allotropes presents computational challenges. Carbon simulations fit into David Landau’s triangle of theory, experiment and simulation (see Figure 1 for a novel triangle interpretation) with a rather heavy weighting towards experiment and simulation for the amorphous phases. Simulation approaches to carbon allotropes range from ab initio, via tight binding molecular dynamics and classical potential studies to the approximate potentials in use for biological molecules. At the Technion, we have implemented several diverse simulation approaches to carbon since 1997 \cite{1} and we refer the interested reader to a recent review \cite{2} of our studies. In that review, we made a long overdue comparison between visualizations with the “ball and stick” approach of our AViz code, where bond hybridizations were identified by geometrical considerations, and electronic density DFT visualizations from VASP/VESTA. We were relieved to find consistency.

In the present paper we turn our focus towards optimizing the “ball and stick” visualization approach for large samples. One of the nicest aspects of research in Computational Physics is that while one’s computer is never powerful enough, over the years much larger samples have become possible. From 256 atoms in our first carbon study \cite{1} (and even less visualized within the central region of interest) we can now study tens of thousands with classical potentials for special cases, and routinely make studies of dynamic developments for tens of samples of 5120 and more atoms. However for such sample sizes, three dimensional visualization becomes far more challenging as we must pass thru

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many sample layers to access interesting regions. In the next section we will review our previous visualization efforts with the original AViz and then describe some dilemmas for visualization of the larger samples. We will then introduce AViz 6.0 with emphasis on the new features, videlicet variation of perspective and bond widths.

The revolution in computer power due to the introduction of “Beowulf” clusters of commodity processors is now being paralleled by a revolution in three dimensional visualization with the introduction of commodity stereo imaging. There are scientific implementations with diverse specifications as to types of screens/glasses. A stereo version of AViz has been prepared by H. Zilken [3] which last year required non-movable equipment costing a minimum 50,000 Euros for 5 or so people to view at once but can now run with a commodity projector, laptop and simple passive glasses. The stereo AViz has not yet been reproduced outside his laboratory, but probably will by the time this manuscript appears. More details will be given in a future report. Unfortunately while hardware costs have plummeted, mastery of software for algorithms and visualizations has remained elusive and still requires sophisticated expert support. This (as is also the case for High Performance Computing consultation support) is a point sometimes missed by university administrators.

2. Issues in 3D visualization of carbon

The two main macroscopic equilibrium allotropes of solid carbon, diamond and graphite have deep differences. The former is a hard insulator, the latter a soft conductor. There are sp² hybridized orbitals for the 3 in-plane nearest neighbours in sheets of graphite, and the 4 nearest neighbours of the diamond lattice are sp³ bonded. In [2] we discussed the calculation and visualization of the electronic density of carbon systems and confirmed that assigning atoms to have sp² or sp³ hybridized orbitals on the basis of the coordination number and bond lengths is valid. If we visualize the lattice structure with “atoms” drawn as balls, we may use different colors to indicate the atomic hybridization. Using “bonds” drawn as sticks between atomic centers to separate the atoms and assist in the realization of perspective we can obtain insight into structures of hundreds or thousands of atoms, [4]. In the simplest implementations we use different colors for the different hybridizations of the carbon atoms. In more complex implementations we may extend this by choosing different colors for 4 fold coordinated atoms that are neighbours of 3 fold coordinated ones, or even different colored bonds connecting atoms of different coordinations as shown in Figure 1. The configuration shown there, and in some of the subsequent figures, are split-interstitial defects where one additional atom is present in the sample. In this defect, instead of the additional atom taking a location between the existing lattice sites, it pairs up with one atom previously situated on a lattice site and instead of one on-lattice atom and one interstitial one they split the lattice site between them. It was long known that this is the most stable defect for diamond; in [1] we were able to show the route to its formation.

Two common experimental systems of mixed hybridizations are diamond - graphite conversions with intermediate amorphous phases at high temperatures and pressures and mixed diamond - graphite - amorphous phases from CVD growth at low pressures. Most of these are either entirely nanoscale or nanoscale in regions of interest. Identification of these structures provides a REAL VISUALIZATION challenge when analyzing results of simulations. We need to be able to visualize the nature of interfaces either between diamond and graphite, or between nanodiamonds with different crystal orientations.

2.1. Diamond-graphite conversion

Several projects of this type were carried out [5, 6] and [7] with A. Sorkin and R. Kalish exploring nanodiamond growth, amongst other issues. Because the primary concern was evaluating band gaps from the density of states, and therefore a tight binding code was needed, sample sizes were small enough that a simple two color scheme was sufficient. More recently we have begun to model the production of diamond membranes, wherein which photonic crystals can be created. This is an elusive, but potentially important goal for guiding single photons in micro-sized structures to yield promising optical devices. The experimental side is described in [8] and the complementary information desired from simulations is mainly geometric. Larger samples are needed for accurate characterization, and hence we use classical potentials.

The simulation modelling approach in this project is to mimic the laboratory experiments and develop a heavily damaged (rich in broken bonds) buried layer in diamond by ion-implantation. If the damage is light, the damaged region returns to a diamond structure on subsequent annealing [1]. But if it is severe the diamond converts to graphite.
The layer which was converted to graphite would be etched away, leaving a sharp interface. Unfortunately, the optical quality of the resultant diamond-vacuum interface has been insufficient to enable the utilization of such membranes as high quality wave guides. In [9] we carried out a molecular dynamics study of this system with a Brenner potential, Langevin thermostat and 5120 atoms in each sample. In summary, 20 carbon atoms were sequentially inserted at a random place between layers 11 and 12 and shot at an angle of 7 degrees with KE of 350eV. We found that damage extended for about 20 (out of 40) layers. We created 10 sets of random locations, each implanted and simulated with 3 different annealing/quenching schedules, with a range of temperatures. With two methods to analyze sp2 content and many different schedules/temperature all multiplied by 10 sets of initial random coordinates, a large number of samples were investigated. All the results of this study (where we concluded that high (but not too high) annealing temperatures give the sharpest interface) can be found in [9] and we will only address the visualization questions in the present paper.

At the left of Figure 2 the final state of one sample is shown. Blue (dark) bonds connect sp3 hybridized atoms and yellow (light) ones connect sp2 ones. We developed the blue(dark)/yellow(light) color scheme for carbon hybridization visualization in [10] in the days before the color online possibility and it is helpful as long as only two colors are needed. It is also the best way for color-blind researchers to understand visualizations. It is clear there is a degraded region in the sample center, but it is difficult to view details. Since the aim here is to etch out the graphitic material, we also prepared an image where this is missing. When observing in two dimensions this does not make a large difference, but on rotation of the sample it assists; such images can be viewed on [11]. We do, of course, realize that in real samples the unsupported atoms, that remain sp3 hybridized and hence are shown in the image, would also be etched away. An algorithm of the bootstrap percolation [12] type is appropriate here, and such a study is in progress now.

2.2. CVD grown samples

It is not economically feasible to use the same single crystal diamonds, valued for engagement rings, for industrial purposes. Diamond is transparent, hard and stable at high temperatures, desirable attributes for esoteric applications such as windows in satellites, [13]. Industrial diamond films grown by CVD (Chemical Vapour Deposition), consist of either micron sized diamond crystals or of nanodiamonds surrounded by amorphous regions, and are severely affected by impurities like hydrogen. Our earlier tight binding calculations of diamond and amorphous regions in CVD
Figure 2: On the left we reproduce an image using dark (blue) bonds to connect sp\textsuperscript{3} hybridized atoms and light (yellow) bonds to connect sp\textsuperscript{2} hybridized ones. On the right the same data is shown with the sp\textsuperscript{2} atoms and their connecting bonds removed for clarity.

Figure 3: Image at the left of a nanodiamond surrounded by amorphous carbon is similar to that selected for the volume cover of [15]. Image at right is of a split interstitial with the bond width adjusted for the length.
diamond films emphasised comparison between LDOS and NEXAFS spectra [14]. Hydrogen plays an important rôle in these interfaces and we made a classical (Stillinger-Weber) potential combined with a PLATO tight binding study of hydrogen location in mixed crystals, [16]. An image of a sample with a nanodiamond surrounded by amorphous carbon is shown on the left in Figure 3. More recent simulations in this project involve several differently oriented nanocrystallites and their interfaces, complicating visualization requirement even further.

3. **AViz 6.0**

3.1. *Earlier AViz codes*

AViz is designed for atomistic visualization of large ordered or amorphous condensed matter systems. It can be used interactively during simulation or in post-production mode, and runs on LINUX systems using Qt and Mesa.

3.2. *Motivations for the upgrade*

AViz was written some 10 years ago by Geri Wagner and Adham Hashibon, based on older OpenGL codes in use by group members. Once they left for more senior positions the Technion group muddled along with minor updates. There are several motivations for our recent preparation of a substantially new, coherent, version of the AViz code, including:

- AViz collected various useful improvements (mainly from Technion undergraduate projects) such as the option for sequential bonds in polymers prepared by Yuval Shyuv, which never made it into the main distribution.
- LINUX versions changed and a series of patches and notes to AViz instructions failed to keep up. The preferred flavour of LINUX within the atomistic simulation community also changed, with a high demand for Debian/Ubuntu which has some differences from the Red Hat/Fedora/Centos systems popular in many computers at the Technion.
- Several of the current Computational Physics Group members developed a wish list of new features, partly motivated by our ability to simulate much larger systems which required adptions to the visualization techniques.

Thus it became desirable to incorporate some modifications and prepare a Debian/Ubuntu release. (We note that the stereo version of AViz developed by Herwig Zilken is based on SUSE Linux.)
Figure 5: A screen shot of an example of linear width variation as a function of bond length.

Figure 6: A screen shot of the implementation of the quadratic variation for the split interstitial.
3.3. Variable perspective

In order to obtain good 3D insight a realistic perspective is desirable. However, if one’s aim is to determine lattice structure, sometimes a direct view is desirable. This has been achieved in AViz 6.0 by enabling adjustment of the fovy (field of view in the y direction) parameter of the underlying OpenGL. An example with the same fovy value as that shown in Figure 2 is given on the left of Figure 4 and one with a much lower value (so it appears “straight-on”) is given on the right.

3.4. Variable bond width

The bonds in AViz have usually been considered as an aid to depth perception or connectivity rather than important in their own right. The exception has been several attempts to show bonds of very specific lengths when simulating nanotubes, in order to highlight regions of bond compression and stretching [17]. However, when trying to elucidate details of grain boundaries, variable bond width could help understand the nature of the connectivity. Two options are provided, linear and quadratic width variation as functions of bond length. In Figure 3 on the right, a split interstitial is shown with the quadratic variation option. One may observe that two of the bonds connecting the split interstitials are shorter and two are longer. In Figure 5 thickness as a function of width for linear variation is shown. In Figure 6 a screen shot including the panel for bond width selection is shown.

4. AViz howto

There are two guides [4, 18] in the archival literature to introduce users to the implementation of AViz, but the former, more detailed guide, is not accessible to many potential users, and so a brief account is now presented.

4.1. Initialization and the basic boxes

AViz requires a data set in the .xyz format; an example for the split interstitial defect shown in Figures 8, 1 and 6, is given below. The first lines states how many atoms, the second is a comment line to identify the file and third and subsequent lines contain a symbol to identify the atom, followed by its x, y and z coordinates (as real numbers). Take care that the number of rows matches to number in the first line. AViz also allows further columns for additional parameters. These could be velocity, or other atomic attributes depending on the physics issues involved. In this case they give information that is redundant with the initial symbol and provides information on the local geometry of the atom’s surroundings.

The basic idea is that one initializes AViz with the command aviz then interacts with its interface to first select the dataset and then optional viewing parameter files. In the sample data file (called split.xyz) there are 42 atoms and the letters were used as explained in [4] to provide different colors for atoms with different coordination numbers, see Figure 1 for the colored implementation of part of this datafile.

This is quite a complicated procedure, and not terribly helpful for large samples. Similar information is provided by the varied bondwidths as we described above. One may simply replace all the letters by C if using the variable bondwidth choice, or one can combine the two approaches for optimal characterization. The file (which is linked on the website [19]) is:

42
Split interstitial
J 5.3012 5.29852 7.09405 9
H 6.16665 6.12665 8.05686 7
J 5.25262 7.05947 5.22232 9
H 6.17108 8.1017 6.13538 7
J 5.2896 7.08316 8.92685 9
J 5.31561 8.92685 7.12608 9
H 6.18016 8.00222 9.86069 7
H 6.08953 9.89518 7.95577 7
J 5.31865 8.94514 10.72933 9
On the first call a visualization window and a dialog box open. The dialog box is the smaller box in the screen shot of Figure 6. The “File” pulldown button in this box enables file selection. Once this is completed, the next task is to invoke the “Mode”, “Style”, “Size” and “Quality” selection pulldown buttons, initially in that order, although further enhancement can be done later at will. “Mode” gives a choice of spheres for atoms and other objects such as rods, pores or cones for quadrupoles, spins etc. Examples of AViz visualization of spins (with cones) is given in [20] and of quadrupoles (with rods) in [21]. “Style” includes a dot option which is both helpful for very large systems while one is setting global parameters and requires a quick response and also for use in its own right in “smoke rendering” visualization, [2]. “Size” is atomic size and may be adjusted to suit for all options except dots. “Quality” relates to rendering and can be increased once a frame is ready to be recorded.

4.2. Tuning the images

The upper options open pull down menus or new dialog boxes, the one shown in Figure 6 is the “Set Bonds” box that opens either directly or from the “Elements” box. The “Set Bonds” box enables the following actions described left to right from top to bottom. First, there are two pulldown buttons to select between which atoms (as identified by the symbols in the first column of the dataset) bonds will be drawn. The default is absent and must be changed in order for a bond to be shown. Then color is selected, then type (thin, thick or the varying thickness with length introduced in the new 6.0 version). Bond emmission is related to the lights (set in the “View” dialog box). The length selection is crucial. One of the reasons AViz was created was our dissatisfaction with packages that preselect lengths of bonds
between different types of atoms. Freedom of choice is important but if the length is not selected carefully one will either see no bonds, or bonds between quite distant atoms, totally obscuring one’s vision. Finally “Apply” and “Done” are needed, or if all is lost “Cancel” and start again. We note that in Figure 1 some of the atoms in this data file are not drawn, this is done by simply not ticking the “Show Atoms” box in the “Atoms” dialog box, see Figure 7.

Once the first image from data or sets of data is prepared, further processing can be carried out to enhance it. A contour surrounding the data is the default, and is shown in all figures except at the left of Figure 2. Axis labels are given in the lower left corner. Contours and axes are controlled by the “Settings” button. Options for slicing and cutting the sample are provided via the “View” button. The annotation option is invoked via the “Elements” button. Within the main AViz window there are radio buttons to change the viewpoint and an “Auto” option at the lower right to spin the sample thru such rotations continuously.

4.3. Animation

Animation is easy with AViz. One simply records the xyz data thruout a simulation and then place all .xyz files in a “filelist” file and upload that instead of a .xyz file. If the data files are numbered e.g. split.0001.xyz etc, then a simple command ls split*.xyz > splitlist will create the filelist file called splitlist. Once a filelist is selected and uploaded, a dialog box (as shown in Figure 8) appears and one may select options such stepping thru the files, or cycling them. (Note that file names ending with .0001.png are not appreciated by pdflatex and one needs to change the name when using the resulting image in a publication.) It is recommended to tick the “Keep ViewScale” box in order to keep size scaling and the contour location fixed. The “Tracks” button enables one to follow the path of each atom, useful when tracking diffusion of, for example, hydrogen atoms out of nanodiamonds.
4.4. Recording the output

AViz outputs the images from the main window into .png files. The “Snap” button provides a single screen shot whose quality is improved when AViz is run in full screen mode. “Autosnap” gives successive png files, and in a given session the output files are named (e.g. for split.xyz) split.0001.xyz etc, no matter how they are created, be it with successive filelist files, a sample rotation or a zoom in or out. AViz does not provide tools to turn successive .png files into movies since there are so many ways to do this. The simplest is to use the linux convert command to make an animated .gif file. (The command convert split.*.png split.gif creates the animated gif file split.gif, which can be easily viewed in your web browser of choice.) To avoid jerkiness on a complete rotation, recall at which axis orientation you started and when you get back there remain at that point for a few frames before ceasing the autosnap, because this split.gif file will loop and the waiting gives a smoother join. This procedure is reasonable for up to 500 files and adequate for most presentations. Examples of these rotations can be found at [11] for the diamond membrane project. At the Technion we have also used a commercial codes that enable the preparation of .mpg files with the addition of music. (We remind readers that it is illegal to use music without permission, but there are libraries of music that can be used with acknowledgement and one can always create one’s own.)

5. Summary

We have produced a substantial upgrade to our AViz code, with several new features as well as a code that is hopefully easier to install. All details about the new AViz 6.0 as well as files for downloading can be found at [19].

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