

Figure 1. Comparative visualization at 800 picoseconds of nanobowls at five temperatures (from left to right: 1000K, 1200K, 1300K, 1350K, 1500K). Rows show the full charge density field, registered bowl window, and segmented bowl (void space only).

Vis and Analysis for Computational Energy Materials Research

Innovation in renewable energy technologies demands advanced catalysis for use in battery, combustion and biomass conversion, and drives ongoing research initiatives at the US Department of Energy. Optimizing catalysis with atomic-scale nanostructures is central to these efforts. Complementing experimental synthesis, computational chemistry provides insight into the atomic-scale behavior of materials. Understanding and validating these simulations requires domain-specific analysis and visualization techniques. For geometry with thousands of atoms, volume rendering can mimic the appearance of electron microscopy methods, and represent uncertainties in exact surface location. In analysis, one goal is to compute measurements that correspond to real-world experimental data. These measurements need not be exact, as full density functional theory (DFT) would be impractical. However, accounting for bond length can have significant impact at this scale. Analyzing charge density volumes is well suited for this.

Analyzing Atomistic Simulations: Nanobowls

Data from atomistic simulations of nanostructured materials pose challenges to conventional scientific visualization and analysis pipelines. At the nanoscale, definition of surfaces is only approximate, with multiscale physical models and high uncertainty. Visualization and analysis of raw geometry (ball-and-stick models) are provide limited understanding, particularly for larger models (over 10k atoms). Computing approximate charge density volumes allows for more intuitive visualization, and often more realistic analysis of material interfaces. We propose a framework for generating, analyzing and visualizing charge density fields of atomistic simulations.

Using amorphous aluminum oxide nanostructures as catalyst supports has been proposed to engineer multipurpose catalysts that can mimic natural catalysis [1]. The stability of synthesized nanostructures under reaction conditions (Fig. 1) is key to their application. One underlying factor affecting stability of these structures is the atomic diffusion of aluminum and oxygen in the bulk and on the surface, which are temperature-dependent. The rate of volume decrease of the nanobowl as a function of temperature can be used as a qualitative indicator of the structural stability. We model the diffusion process in models consisting of 10k - 20k atoms (depending on nanobowl diameter), a molecular dynamics (MD) code. The goal is to determine which bowl structures are stable, for varying temperature and radius parameters. To determine this, we principally measure the bowl volume, and how it changes over a simulation run.

To construct the charge density volume, we plot charge density as a function of distance (radius) from Al and O nuclei (Fig. 2). We use these as radial basis functions in a kernel density model [6], discretized on a structured grid with 4 voxels per Angstrom. Since exact boundaries are not well defined, we use the charge density of the O-O bond as an upper threshold, and a colormap to represent the uncertainty region around the interface (Fig. 3). We then use the void and O-O thresholds to conduct statistical analysis of the surface. We compute a heightfield distribution to register each nanobowl, and compute the volume of the void space. These results correlate strongly with analysis of the raw geometry (Fig. 4). Other statistics (surface area, curvature of the bowl) are also computed in this framework.

Large-scale ball-and-stick raycasting

Volume rendering of charge density fields is useful for large-scale atomistic and electronic models. Nonetheless, domain scientists often prefer visualizations of the raw geometry, particularly ball-and-stick representations. Simple ball-and-stick rendering of even moderate-size models (over 1,000 atoms) appears cluttered and is difficult to interpret. Our GPU raycasting technique uses a grid acceleration structure [3] allowing for interactive rendering of large scale ball-and-stick models in conjunction with volume rendering, with correct depth sorting at every composited sample. This modality is useful for larger models (Figure 5) and can deliver both higher performance and better visual quality than rasterization approaches [2].

Interactive Autostereo Visualization and Modeling

Ball-and-stick rendering and comparative visualization of void space both benefit greatly from the improved depth perception of 3D stereo display. We have integrated our software with Dynallax [5], a tracker-based stereoscopic display. Stereo workstations could prove useful in a variety of materials visualization and modeling tasks, for example modeling *ab initio* geometry prior to simulation of bond formation in density functional theory computation.



Figure 5. Autostereo workstation.

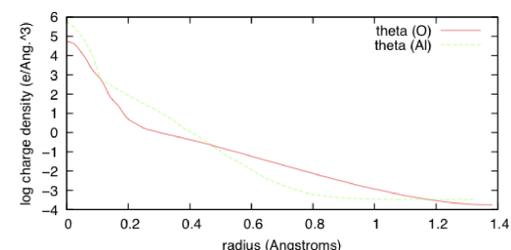


Figure 2. Charge density plots of Al-Al and O-O bonds obtained from a bulk compound DFT computation. These plots serve as radial basis functions in the kernel density model of our charge density field.

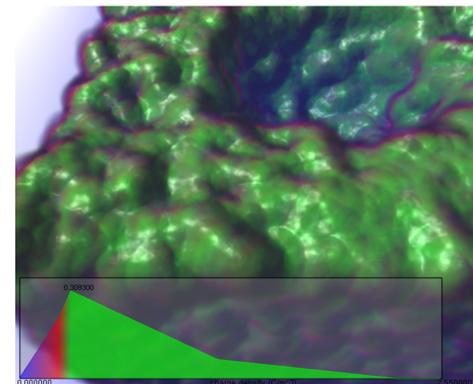


Figure 3. Uncertainty-driven classification of the nanobowl surface. Void space is color mapped to blue at a charge density of zero. The charge density cutoff for O-O bonds (green peak) serves as an upper bound. Using our charge density field, the surface is defined somewhere in between.

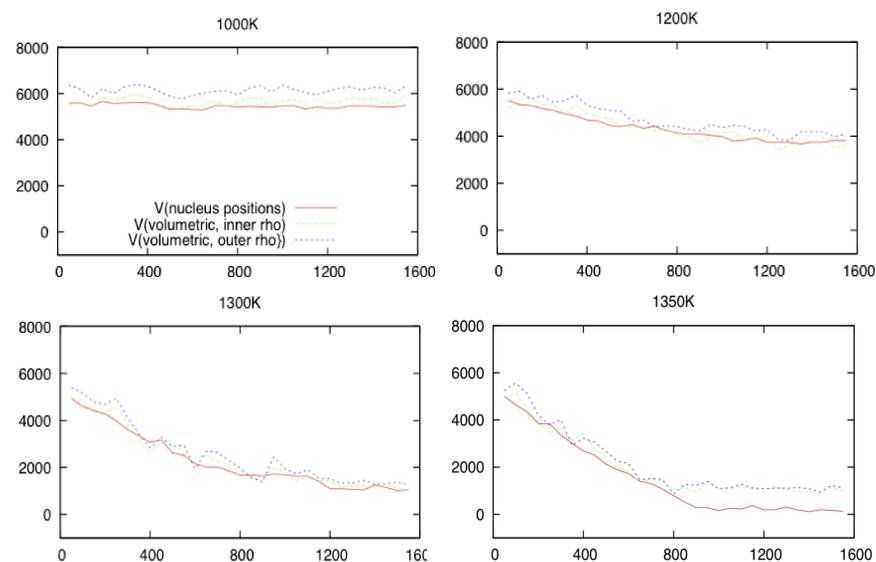


Figure 4. Analysis of bowl volume (cu. Angstroms), over simulation time (picoseconds), for the first 4 runs shown in Fig. 1. We compare our charge density classification approach to volume measurements of the raw geometry data, computed over a heightfield of interpolated nucleus positions. We tabulate lower and upper thresholds corresponding to our uncertainty classification (Fig 3).

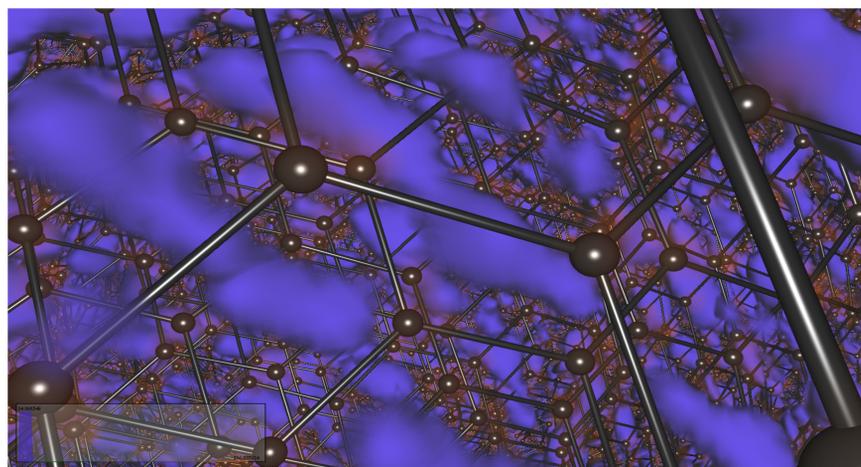


Figure 5. Volume and ball-and-stick rendering of a 740,000-atom graphite-diamond hybrid "supersoot" structure, used as a battery capacitor, showing void space in between carbon chains. Data courtesy of Kah Chun Lau and Larry Curtiss, Materials Science Division (ANL).

References

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