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Envisioning Structure-Property Relationships at the Nano and Macro Scales: Graphics for Presentation and Insight

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Introduction

The advent of high performance computers (HPC) has allowed materials researchers to simulate mechanical response of large complex three-dimensional (3D) nano-structures and predict their associated macro-properties. Envisioning complex structure-property relationships, embedded in massive HPC simulation data sets, is now possible with recent advances in computer graphic hardware and software. However designing insightful graphical tools is best accomplished within the context of the physics as understood by the researcher who also models the physics embedded in the HPC simulation. The same can be said when creating the mathematical models used in the HPC simulation. Insight occurs when both graphical and mathematical models are created within the context of the physics unique to each problem. At best commercial graphical tools are designed to present HPC simulation results generically that will benefit a broad range of problems. Hence a tradeoff exists between creating customized graphical models for insight or generic graphical models for presentation. Because researchers typically lack the programming skills required to create their own customized graphical models, insight is limited within the use of commercially available graphical tools. A solution to this dilemma is to create synergistic teams of computer scientists who are skillful graphical programmers and who work with discipline experts who provide the insight for designing a customized graphical interface. This a popular solution at national labs, but at academic institutions an opportunity exists to educate the next generation of researchers to be as skillful at graphical modeling as they are at mathematical modeling. This requires changing the curriculum to include graphical modeling as an insightful problem solving skill. Because academic institutions are notoriously slow to change the curriculum, creating synergistic teams has become more popular as a short-term solution. At Virginia Tech both approaches have been implemented with limited success when solving problems using HPC and scientific data visualization resources in the engineering sciences. Although many multidisciplinary examples can be cited the remainder of the paper focuses on material research problems that span the length scales from nano to macro.

Envisioning Structure-Property Relationships at the Nano-scale

Desktop computer graphics tools are commonly used by materials researchers to interpret and analyze properties associated with large 3D nano-structures. Many

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3D nano-structures that can be visually interpreted and analyzed at desktop computers, can also be analyzed and interpreted in immersive virtual environments (VEs) such as a CAVE™. In some cases immersive VEs can be more insightful from the researcher's viewpoint. The CAVE is a multi-person, room-sized, high-resolution, 3D video and audio environment [1]. In the current configuration, graphics are rear projected in stereo onto three walls and the floor of a 10x10x9 foot room and viewed with stereo glasses, Fig. 1.

Because it is more convenient for researchers to work at their desktop computers, there was a need to extend visual data analysis from the desktop to more insightful immersive VEs, such as a CAVE, when researchers see an advantage to do so. In collaboration with the National Center for Supercomputing Applications (NCSA) at the University of Illinois, the University Visualization and Animation Group at Virginia Tech created the VE application called Atomview using the CAVE Library, application programming interface (API), developed at the Electronic Visualization Laboratory, 1997. To promote future collaborations a new Linux-based open-source (GNU-GPL) VE API called DIVERSE was developed at Virginia Tech (1999) that emphasized extensibility using dynamic shared objects (DSOs) [2]. Using DIVERSE DSOs D_Atomview, developed at Virginia Tech (2001), could run on desktop computers, head mounted displays, and immersive desks, walls, or CAVEs [3]. D_Atomview was used to interpret and analyze result of a 3D Nickel nano-structures predicted by high performance computer molecular dynamic models [4], Fig. 1.

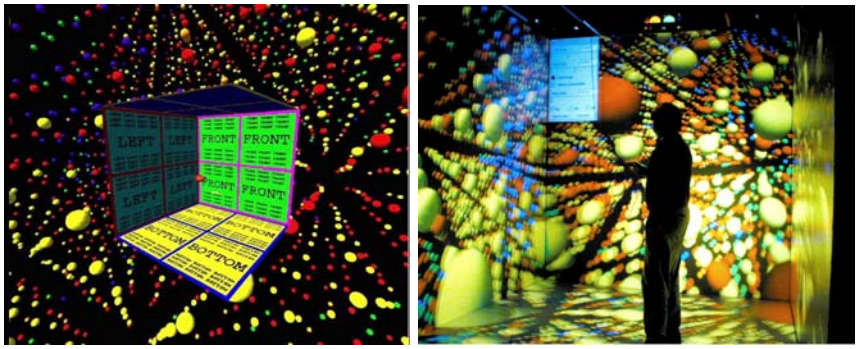

Figure 1: D_Atomview: a) right image, desktop CAVE VE-simulator embedded in a simple Nickel, Ni, nano-structure of 30,000 atoms, b) left image, actual snapshot of same structure projected onto the walls of a CAVE^{TM}, but VE immersion can only be experienced with head tracked stereo glasses while standing in the CAVE.

The team that created D_Atomview exemplifies the synergistic model of collaboration where researchers, D. Farkas in the Department of Materials Science

and Engineering and R. D. Kriz in Engineering Science and Mechanics, worked with computer programmers, J.T. Kelso and A.A. Ray in the Department of Computer Science. Because of time and resource constraints D_Atomview is not as full featured as the more popular commercial AMIRA VE software [5]. AMIRA like D_Atomview runs both on desktop computers and on immersive VE CAVE computers. Although AMIRA is not licensed open-source the desktop version of AMIRA is affordable, however the extensible CAVE version is not. Consequently researchers preferred to use AMIRA for day-to-day research on their desktop computers and only occasionally used D_Atomview in the CAVE. Extensibility from the desktop to the CAVE remains an important but unresolved issue. The solution will require that either new synergistic academic teams create new customized graphical models using open-source models like D_Atomview or the extensible version of commercial code becomes affordable.

A long term solution is to educate the next generation of researchers to become skillful at developing graphical models of their physics based simulation models. This requires changing the curriculum. With funding from the National Science Foundation Combined Research and Curriculum Development program, faculty at Virginia Tech created two courses where students analyzed complex nano-structures using desktop and immversive VEs [6]. This effort continues where the Department of Engineering Science and Mechanics offers a course each year on Scientific Visual Data Analysis and Multimedia (ESM4714). In this course students learn how to create customized graphical models both for presentation and insight [7]. Class projects encourage students to create their own customized graphical models based on projects associated with their senior projects, masters thesis, and Ph.D. dissertations.

Three examples follow that demonstrate how faculty and their students are using current HPC and scientific data visualization resources at Virginia Tech: 1) plastic deformation of gold nano-pyramids, 2) modeling nano-indentation of thin films, and 3) wave propagation in anisotropic media.

1) Plastic deformation of gold nano-pyramids: System-X and D_Atomview

Crushing deformations of gold nano-pyramids at the pyramid apex are simulated on Virginia Tech's tera-scale System-X computer using the LAMMPS open-source molecular dynamics code from Sandia National Labs [8]. Results are visually analyzed and interpreted in the CAVE using D_Atomview, Fig. 2, which highlights atoms associated with plastic deformations, e.g. dislocation glide. Planes of red atoms reveal slip planes and dislocations as the apex is being plastically deformed downward. Simulations reveal sequential formation of parallel slip planes that appear as inverted pyramids. Using immersion with head tracking nanostructures viewed in the CAVE reveals evenly space slip plane with curvatures not pre-

viously seen, Fig 2.

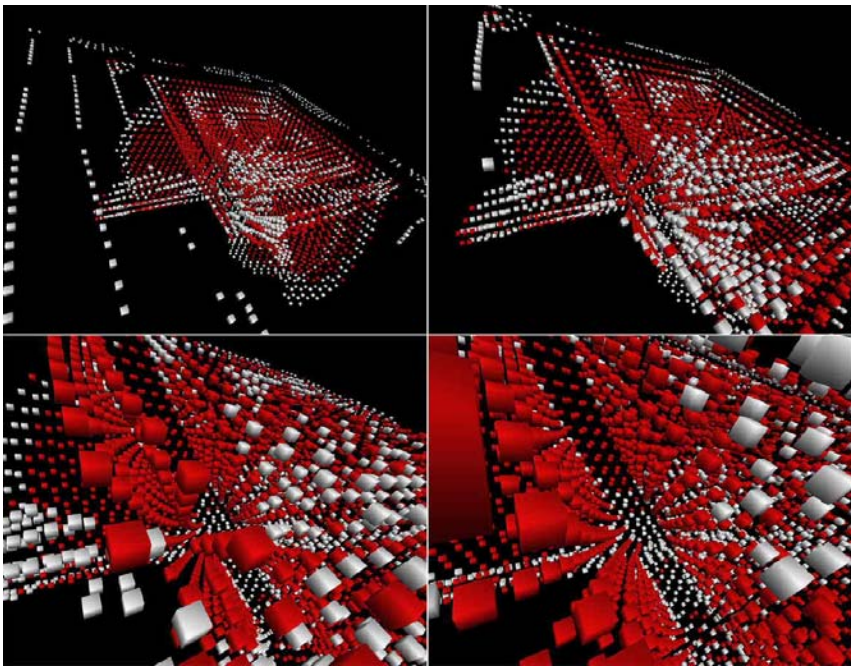

Figure 2: D_Atomview time sequence showing head tracked CAVE view while flying into the outermost slip plane shown in the lower right figure.

2) Modeling nano-indentation of thin films: System-X and AMIRA

Nano-indentation based technology is an important way of addressing the mechanical properties of thin films, such as hardness. When addressing properties at the nano-scale new phenomena appear in Fig. 3 and nano-structures appear that are different from the well known macroscopic counterparts. To completely understand mechanical behavior at the nano-scale, EAM molecular dynamics computer simulations were used to model material behavior on Virginia Tech's tetra-scale System-X computer. These simulations can now attain the spatial scales typical of nano-indentation and can provide great detail about the mechanisms underlying materials response. The simulations also provide information on the mechanisms responsible for the size effects and the particular response of films of varing thicknesses. Visualization of simulation results, using AMIRA, Fig. 3, have provided great insight into the actual process of emission of the first dislocations responsible for incipient plasticity as the films are indented. Simulations of thinner films reveal that contact stress required for the emission of the first dislocation is not significantly dependent on the film thickness.

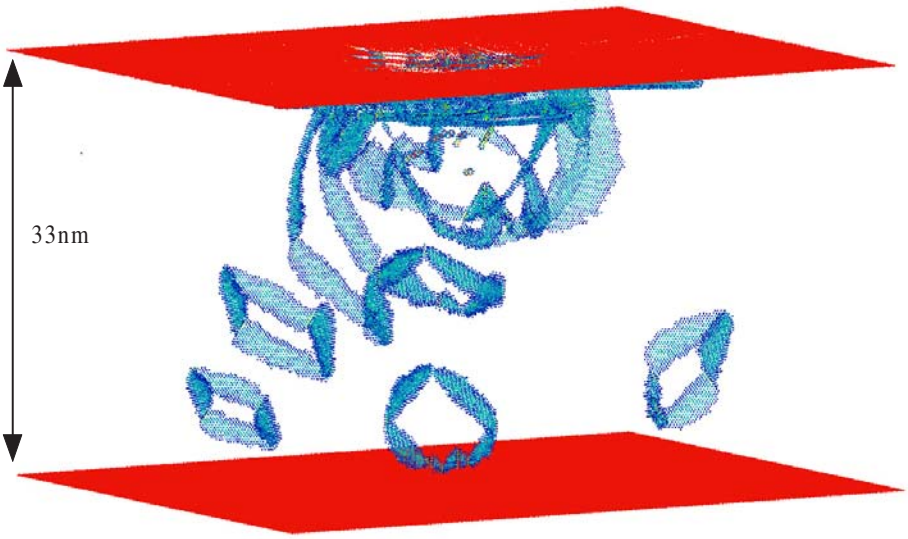

Figure 3: Dislocation loops in a thin film of a Ni crystal, whose red plane normal is oriented in the [111] direction, simulated by indentation on the top surface with a radius of 15nm.

3) Wave propagation in anisotropic media: PV-Wave, VRML and DIVERSE

There are many macro-properties that can be associated with any given nano-structure. Here a crystal of Calcium Formate, $Ca[HCOO]_2$ is studied because of it's unusual orthorhombic anisotropy. Orthorhombic symmetry reduces the fourth order elastic stiffness tensor, Cijkl, to nine independent components. Components of the fourth order tensor are macro-properties associated with the alignment and orientation of polar covalent bonds between atoms. For long wavelengths propagating along principal material axes, x_i, waves "see" the material as a continuum and the corresponding wave speeds (macro-properties) are related to individual terms of the fourth order tensor. Using Voigt contracted notation waves propagating along the $x_i$axes include only the diagonal terms of the contracted 6x6 stiffness matrix $C_{\alpha\beta}$, where $\alpha\beta$ = 1,2,3,4,5,6, which define the geometry of wave speeds along those axes. Wave velocities off-axis form 3D wave-velocity sheets require the collection of all terms of the fourth order stiffness tensor, defined by Christoffel's equations of motion [9],

$$[C_{ijkl}v_iv_l - \rho v^2\delta_{ik}]\alpha_i = 0, \tag{1}$$

where v_i is the "pointing" or plane wave propagation direction, ρ the density, v is the wave velocity (eigen-values), and α_i is the wave displacement vibration direction (eigen-vectors).

Three-dimensional wave surface topologies reveal complex structure-property relationships not previously understood. The collection of velocities corresponding to directions vg in the x_1-x_2, x_1-x_3, and x_2-$x_3$planes shown as 2D wave-velocity surfaces shown in Fig. 4a. The outer-most wave-velocity surface corresponds to the fastest quasi-longitudinal (ql) wave and the inner two wave surfaces are quasi-transverse (qt) and pure transverse (t). Calcium formate exhibits an unusual wave 3D wave-velocity surface topology, where all three wave-velocity surfaces combine into a single connected surface, Fig 4a. This unusual topology is uniquely defined by the inequality $C_{11} > C_{33} > C_{66} > C_{22} > C_{55} > C_{44}$, written in contracted notation [9]. Although the simple schematic in Fig. 4a shows connectivity, the entire 3D wave-velocity surface is not shown. In Fig. 4a connectivity occurs at wave-velocity intersection points a, b, c, and d, which are shown only in principal material planes. Perhaps similar points occur away from the principal material planes. The entire 3D wave-velocity surface is created by solving Christoffel's equation for velocities, v, in all possible propagation directions, v_k, away from the principal planes. Displacement vibration directions, α_k, are mapped as color onto these velocity surfaces [9]. Since velocities, v, and their vibration directions, α_k, are only functions of Cijkl, these 3D wave-velocity topologies uniquely represent the fourth order stiffness tensor, Cijkl, Fig 4b.

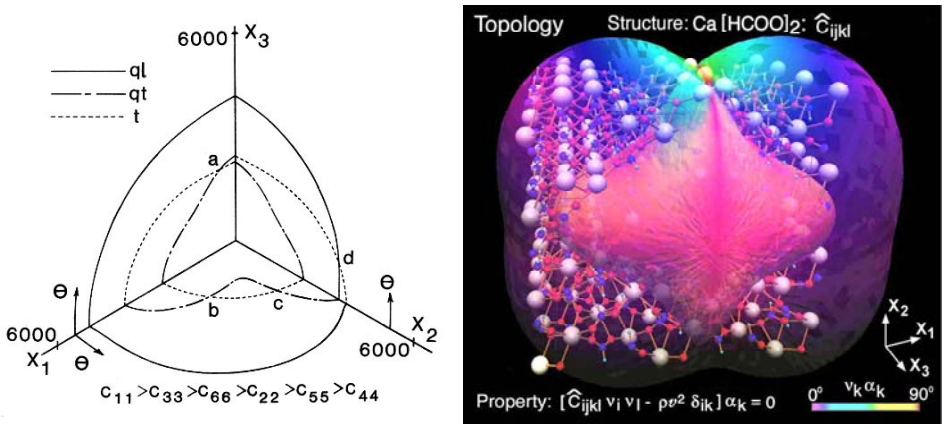

Figure 4: Calcium Formate 3D wave velocities (m/s): a) left image shows a simple schematic isometric view of velocities in three principal planes resulting in a connected wave-velocity surface, b) right image shows 2x3x3 unit cell nano-structures embedded in the complete out-of-plane 3D wave velocity surfaces. The outer two surfaces used PV-Wave software [10] to create VRML files with translucency. Final images are displayed using the DIVERSE API.

Closer observation of these 3D topologies in an immersive VE, not shown here, revealed that no new velocity intersection points occur outside principal planes.

These observations were only possible in an immersive VE. Hence, starting the analysis at the desktop VE-simulator, Fig. 4b, and then moving results into the CAVE proved to be an insightful experience. This demonstrates that immersive VEs such as a CAVE are not primarily used for presentation but for insight.

Discussion of Results and Future Opportunities

The advent of high performance computing (HPC) has created a data-rich but information-poor working environment for materials researchers interested in interpretation and analysis of HPC results of large-scale nano-structures. Graphical representation of complex nano-structures and their corresponding macro-properties is now possible at desktop computers because of high-speed graphics cards and new open-source and affordable commercial graphics software applications and their APIs. Many of these desktop graphics applications are now routinely used to assist in the interpretation and analysis of HPC results.

New graphical software such as AMIRA and DIVERSE allow researchers to work both at their desktop and in immersive VEs as necessary. This was demonstrated by creating simple VRML graphical models and using DIVERSE to study the nano-structure and macro-properties of waves propagating through a crystal of Calcium Formate embedded in 3D translucent wave-velocity surfaces that represent the fourth order stiffness tensor of the same material. Immersive VE environments were more useful when analyzing wave-velocity (macro-properties) topologies. Immersive VEs such as a CAVE also proved to be insightful when studying the formation of nano-structures associated with large plastic deformations.

Future opportunities in the area of visual analysis and interpretation of HPC results exist because of the growing trend of faster, cheaper, and easier-to-use desktop computers and affordable commercial software. Faster numerical calculations allow researchers to study larger problems. Faster graphics hardware transforms data-rich HPC results into meaningful information-rich 3D images and animations. With curriculum change future scientists will create computer graphical models, like mathematical models, which will become an integral part of how each scientist models, creates, and understands their physical world. Until then we must rely on creating synergistic teams of computer scientists and discipline experts to create customized graphical models for insight. Virginia Tech continues to do both.

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