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CAC and Paul Dawson and Matt Miller

Digital Materials: A Database for Developing and Testing the Properties of New Alloys

How do you decrease the time it takes to develop new engineering alloys?

Finding the Answer

Paul Dawson and Matt Miller from Cornell's Sibley School of Mechanical and Aerospace are focused on shortening the development time for new materials. High-performance computing clusters and database technologies at CAC are playing an essential role in this process by enabling more realistic simulations and the digital replication of traditional lab processes.

Digital Materials

New automotive vehicles are manufactured every year. The body might have a slightly different shape, the engine is probably more powerful, and a new color of paint might be topping the color chart.


But for all the modifications impacting the look, the construction of the auto remains the same. Changes in the materials used to build the vehicle often are needed to substantially alter design, but these changes occur much less frequently.

To change the material used for the structure, mechanical designers need reliable data illustrating critical properties, such as the strength and stiffness of the proposed structural material, at the beginning of the design process. The traditional laboratory-based process used to obtain property data take substantially longer than the time allowed to prepare a new product for market, and current methods make it impossible to obtain the needed data once the mechanical design process has begun.

Designers have chosen to use the same structural material year after year rather than face the risks of new materials.

Improved Research

Research Metrics

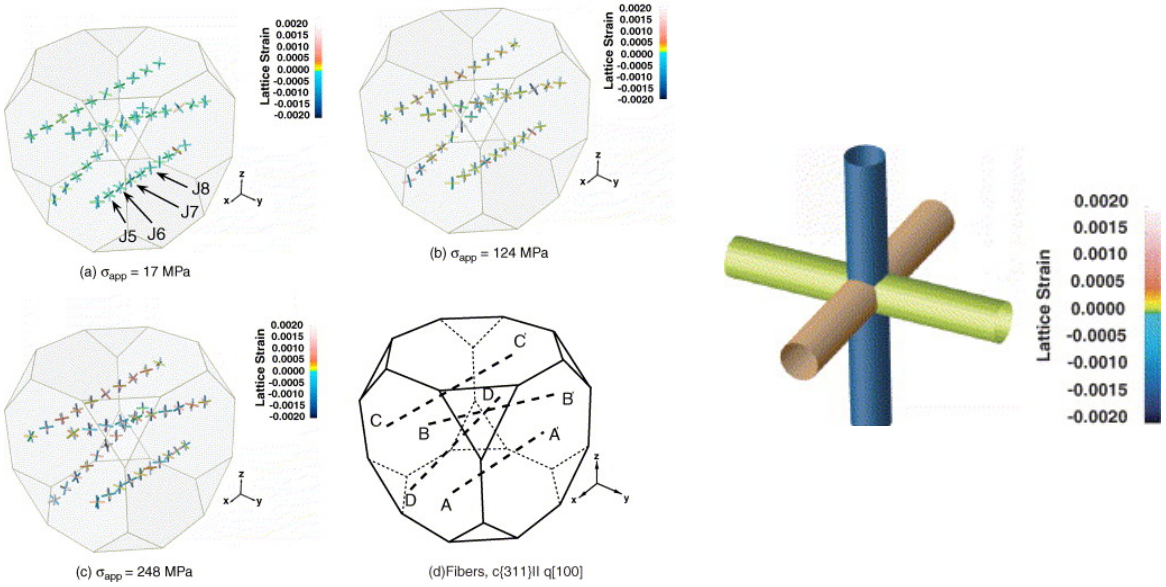
- Realistic simulations: Use CAC high-performance computing systems in order to provide required microstructural detail
- Easy access to digital materials in order to test properties: Work with CAC database consultants to design and deploy a alloy database that is scalable and easy-to-use

Research Challenge

The objective is to develop a simulation environment that mimics both in form and function the traditional laboratory-based methods for materials development. "We are creating an environment that intertwines traditional and digital methods," said Dawson. "Experiments and simulations must be used in complementary ways that collectively provide the needed properties. It's a 'no holds barred' approach."

Solution

Dawson and Miller created a digital representation of engineering alloys that is based on microstructural features visible under an electron diffraction microscope, as well as tools to operate on this material.



The information contained in the digital material is organized using an innovative database. Using the database, engineers can request a digital sample of a material, impose loading typical of its intended use, and use digital instruments to probe the reaction of the sample to these situations. The database contains structural information on material such a cooper/iron and aluminum/beryllium. The database was created by a team at CAC who worked hand-in-hand with the project team to understand the needs and directions of the project.

"We built the database to accommodate growth, in terms of new alloys, new properties, and new tests," said Linda Woodard, CAC consultant. "The database allows researchers to replicate in a digital environment the traditional processes done in labs to develop and test properties of new materials."

“Our work is resulting in a core – and dynamic – set of information that is accessible to a number of researchers who can draw data from it and add information to it,” added Dawson.

In addition to creating a database, CAC also provides HPC compute cycles to the research team.

The Clients

Paul Dawson

- Professor, Sibley School of Mechanical and Aerospace Engineering, Cornell University
- Research focus on the computational design and control of materials processes, including deformation and solidification/crystal growth processes
- Director, Deformation Processes Laboratory

Matthew Miller

- Associate Professor, Sibley School of Mechanical and Aerospace Engineering
- Research focus on the processing and properties of metals and alloys including steels, cooper, and aluminum, titanium, and nickel based superalloys

The Collaborative Relationship

HPC systems and database expertise at CAC have helped Dawson and Miller create more realistic simulations of materials at the levels of fidelity required.

“Often there are several features of the microstructure that influence the physical properties that designers need. Digital samples that include the needed features, in large enough numbers to be statistically meaningful, are large and complex. Simulating the responses under mechanical loading is challenging and impossible to accomplish on workstations. HPC is a must for success. Simulating virtual specimens with adequate microstructural detail cannot be done on workstations. The promise of parallel architecture is in replicating the behavior of realistic materials and, in doing so, opening the door for more easily introducing new materials in design.”

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