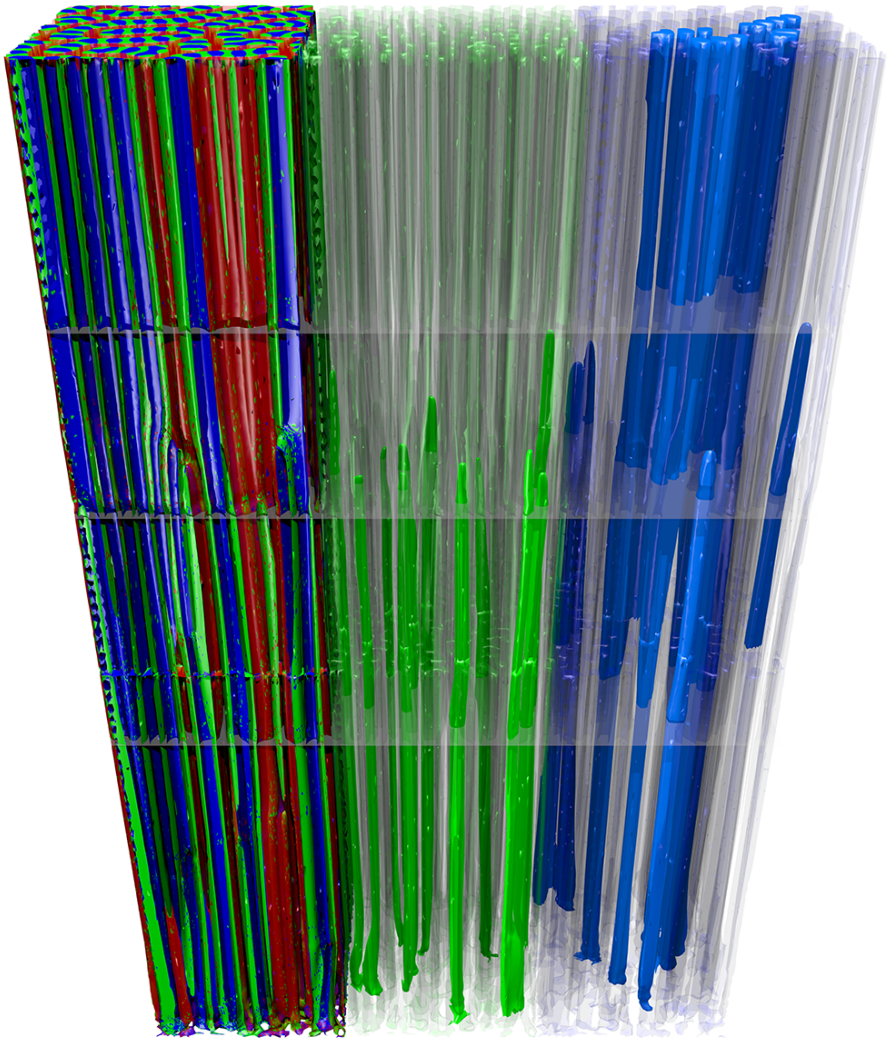
Research team uses computation and experiment to understand how novel material properties form

August 22 2017



A 3-D microstructure containing multiple solidification velocity changes. On the right, an exemption of intermetallic phases that shows the adjustments of the rods in the microstructure, such as the splitting, merging and overgrowing at different velocities. The gray planes indicate the height of the velocity change. Credit: High Performance Computing and Data Science Group, Karlsruhe Insitute of Technology and Karlsruhe University of Applied Sciences

Since the dawn of Enlightenment-era chemistry and physics, scientists have tried to document materials' properties different conditions. These investigations spawned the field of materials science and have helped humanity create aircraft and spacecraft, revolutionize healthcare, and build industrial processes to create products from adhesives and cosmetics to jet fuel and fertilizers.

However, as researchers attempt to create increasingly complex materials to address increasingly intricate industrial needs—such as improved material resiliency for high-temperature processes, or compression processes that effect materials for flight—the ability to uncover and understand materials' properties experimentally has gotten costly in terms of resources, energy, money and time.

A team of researchers led by Prof. Dr. Britta Nestler at the Karlsruhe Institute of Technology and the Karlsruhe University of Applied Sciences works on the frontline of advanced material design, using computation to model new material properties. The group primarily focuses on materials for which experiments are incapable of adequately characterizing and controlling the origin of their properties, or where such experimentation would be extremely time consuming to be done efficiently in a systematic manner.

Nestler, who was recently awarded the 2017 Gottfried Wilhelm Leibniz Prize by the German Research Foundation, and her team with the help of the High Performance Computing Center Stuttgart's (HLRS's) Cray XC40 Hazel Hen supercomputer—have scaled to new heights in their multiphysics and multiscale modeling and simulation efforts.

The Karlsruhe group develops the parallel simulation software Pace3D ((Parallel Algorithms of Crystal Evolution in 3D) and is a long-time user of HLRS resources, previously investigating material pattern formations such as multiphase directional solidification. One of the team's central goals is the computational analysis of the influence of varying melting conditions on material properties and microstructure quantities.

In a recent paper published in *Acta Materialia*, the researchers detail fully 3D simulations of an aluminum-silver-copper (Al-Ag-Cu) alloy as it solidifies and compare microstructure characteristics with experimental photographs. For the first time, researchers have used a combination of theory and experiment to induce tailored velocity changes in order to design the microstructure and, in turn, material properties. The team chose Al-Ag-Cu due to the wealth of experimental data with which to compare their simulation results. The method sets the stage for larger simulations of more complex materials.

"With the knowledge we've gained from our recent computing runs, we have a framework to go to technically relevant systems that often have experimental difficulties," said group leader Johannes Hötzer. "We decided to investigate the Al-Cu-Ag microstructure pattern to show the validity of the model and the possibilities to compare it with a wide range of experimental data."

Solidification speed changes

Materials scientists are often seeking to understand the limits of

materials—the hottest temperature a mixture can operate at, the highest pressure it can withstand, among others. One topic of interest is understanding properties of eutectic materials consisting of two (binary eutectic) or three (ternary eutectic) distinct solid phases in a microstructure arrangement that results in the lowest melting temperature. The Nestler team has recently focused on ternary eutectics with three alloy components.

Using Hazel Hen, the team simulates how certain process conditions—such as solidification velocity or processing temperature—effect a eutectic material's microstructure. To deduce correlations, the team needs large-scale 3D computations to simulate a representative sample of microstructural patterns. Before its recent simulations, for example, the team hypothesized that when an Al-Ag-Cu transforms from liquid to solid, the speed of the solidification transition plays an important role in how a microstructure's pattern splits and merges, and how the length and width of the fibers that subsequently form influence the material's strength at higher temperatures.

However, researchers only had 2D experimental data available, preventing them from unequivocally proving or disproving their hypothesis. Experimentalists and computational scientists needed to see this process unfold in 3D, and they could do that with the help of a supercomputer.

The team created multiphysics software package Pace3D for incorporating a wide variety of material models and implemented a highly optimized version in a collaboration with the Fredrich Alexander University Erlangen-Nuremberg, using the university's computational framework waLBerla (widely applicable Lattice Boltzmann from Erlangen).

This code breaks down massive 3D simulations into roughly 10,000

computerized cubes, then solves a variety of physics equations within each cell for millions of time steps—each step is in the range of 0.1 to 1.0 microseconds. To observe velocity variations, the team ran sets of simulations with variations in solidification velocity. Each simulation needs roughly one day on approximately 10,000 of Hazel Hen's CPU cores.

Experimentalists were surprised with the outcome. Based on their 2D experiments, they assumed that the eutectic microstructures grew quickly in a straight, largely uniform manner. However, simulation revealed many rearrangement processes during solidification, and illustrated that microstructure patterns change more slowly but on longer length scales than assumed. These results were later confirmed by synchrotron tomography, an imaging technique that allows researchers to study material properties on a fundamental level.

Tailored Microstructures

The team's accurate simulation results represent a proof of concept for its ability to simulate microstructure formation in more complex, and more industrially relevant, materials under a wide variety of material and physical conditions.

As experiments continually get more complicated—the Karlsruhe experts in computational materials modelling have collaborated intensively with experimentalists doing zero-gravity material design research on the International Space Station—computations will continue to play a larger role. Nestler indicated that experiments such as those on the ISS were extremely important, but also expensive and time consuming to prepare; supercomputing methods help researchers to make large strides toward charting tailored materials with specific properties for particular applications while also bringing down the cost.

Computing also allows researchers to run many permutations of the same simulations with very subtle differences—differences that would otherwise require dozens of individual experiments. "In our simulations, we can vary physical and processing conditions, such as the solidification velocity, which have an influence on microstructure. By controlling this parameters, we end up getting a well-designed, tailored microstructure," said Nestler.

By understanding how to subtly change speed and temperature profiles during the production of complex materials, Nestler points out that large-scale parallel computations support materials scientists in designing an extremely well-suited material for a specific task. These materials can be used for air and aerospace technologies, as well as in industrial processes where materials are exposed to extremely high temperatures or pressures.

For example, conducting simulations of a nickel, aluminum and chromium-34 alloy, the team could show how the microstructure's alignment improves by establishing controlled process conditions, resulting in a higher creep resistance, meaning that the material will not deform when exposed to mechanical or temperature-based stress.

"Our main goal is to design particular microstructures for multi-component alloys, for cellular or particle based systems that are based on its application," Nestler said. "The application defines what new materials should look like or should be able to sustain, and we can now design, in a controlled manner, the particular microstructure that is needed."

These simulations were carried out using Gauss Centre for Supercomputing resources based at the High-Performance Computing Center Stuttgart.

More information: Johannes Hötzer et al, Influence of growth velocity variations on the pattern formation during the directional solidification of ternary eutectic Al-Ag-Cu, *Acta Materialia* (2017). DOI: 10.1016/j.actamat.2017.07.007

Provided by Gauss Centre for Supercomputing