Researchers use high-performance computing to drive alloy design

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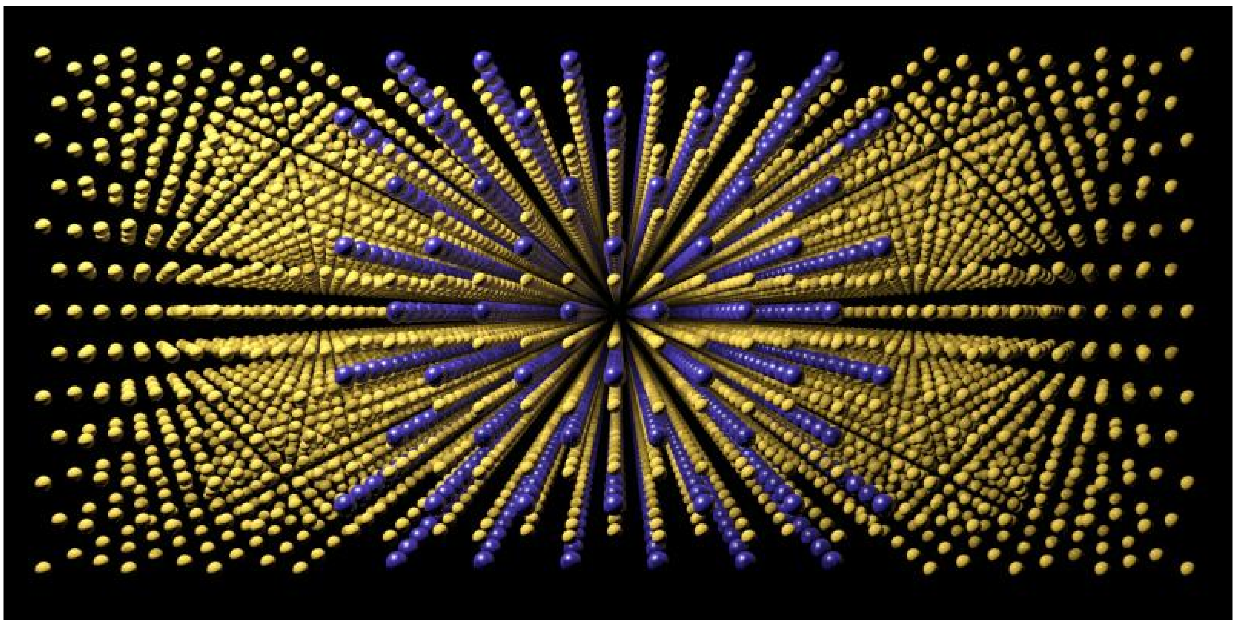


Using high-performance computing, ORNL researchers are modelling the atomic structure of new alloys to select the best candidates for physical experimentation.

The Department of Energy's Oak Ridge National Laboratory, FCA US LLC, and the foundry giant, Nemak of Mexico, are combining their strengths to create lightweight powertrain materials that will help the auto industry speed past the technological roadblocks to its target of 54.5 miles per gallon by 2025.

Automakers need powertrain materials that are not only lighter but also low cost and able to withstand the elevated temperatures and pressures in high-efficiency turbocharged engines. With the typical materials development cycle taking 10 to 20 years, there is little time to waste.

The ORNL-led project is part of a new initiative from DOE's Vehicle Technologies Office to develop new high-performance alloys. Ford, General Motors and FCA US are collaborating with national laboratories, universities and the casting industry to develop an affordable, 300 degrees Celsius-capable high-strength cast aluminum alloy.

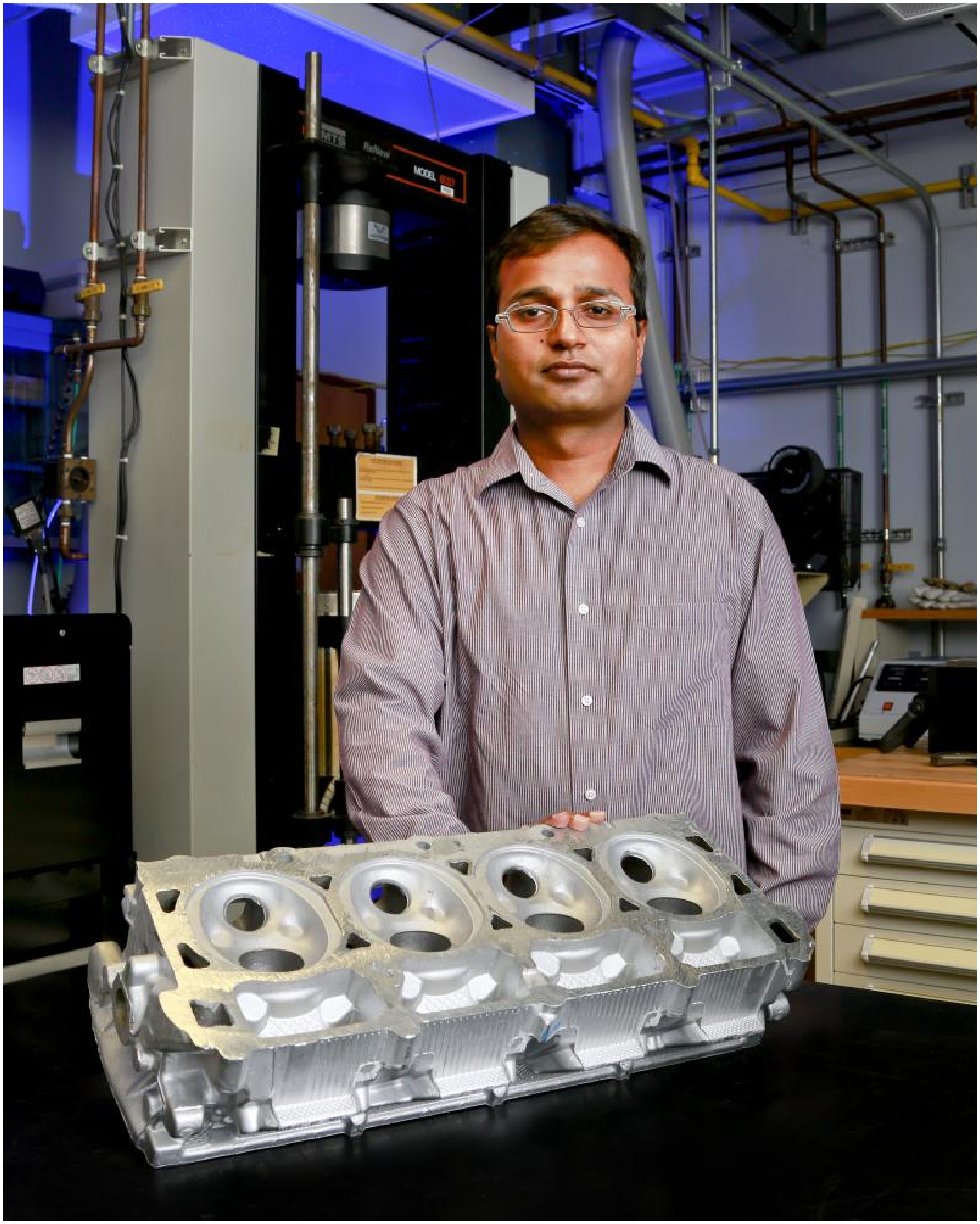
This target means engineering a material that is 25 percent stronger than current alloys and durable at temperatures 50 degrees Celsius higher, a necessity for next-generation engines. The real challenge is to accomplish this while keeping costs low for automotive manufacturers and consumers.

"The aggressive goals of these projects compress about half a century of typical materials development into a four-year project," said DOE program manager Jerry Gibbs.

A team of researchers from ORNL, FCA US and Nemak is using integrated computational materials engineering (ICME) to speed the development of new high-temperature aluminum alloys for automotive cylinder heads. ICME enables researchers to tailor new alloys at the atomic level to achieve desired properties such as strength and ease of manufacturability.

"Aluminum has been in mass scale production for more than a century, but current cast aluminum alloys cannot withstand the temperatures required by new advanced combustion regimes," said ORNL principal investigator Amit Shyam. "Our goal is to take high-temperature cast aluminum where it has never been."

ORNL is breaking new ground by scaling ICME to run on DOE's Titan supercomputer, the second fastest computer in the world. Using Titan's speed and parallel processing power, ORNL researchers can predictively model new alloys and select only the best candidates for further experimentation. This predictive capability dramatically reduces the time, energy, and resources devoted to casting trial alloys.



A team of researchers led by ORNL’s Amit Shyam is using high-performance computing to speed the development of new high-temperature aluminum alloys for automotive cylinder heads.

"Using approximately 100,000 cores simultaneously on Titan, we can increase the speed and scale of our first-principles quantum mechanics calculations by at least an order of magnitude," said ORNL researcher Dongwon Shin.

Before the shift to Titan, Shin was using a Linux cluster with approximately 300 cores to create atomistic simulations of single elements diffusing to intermetallic precipitates within the alloy. Now researchers can achieve larger scale simulations on Titan that are much closer to real world scenarios.

The team is also verifying the computational models through atomic scale imaging and analytical chemistry measurements. ORNL's scanning transmission electron microscopy and atom probe tomography allow researchers to identify and examine the location and chemistry of each atom in the alloy matrix, precipitates, and the interfaces between them.

ORNL and collaborators are creating a database that captures their aluminum alloy materials discoveries. This materials genome approach will help guide efforts to improve ICME capabilities and accelerate the development of new high-performance materials.

The Oak Ridge Leadership Computing Facility, a DOE Office of Science User Facility, approved six million hours on Titan for the ORNL alloy development project. The research uses microscopy resources at ORNL's Center for Nanophase Materials Science, a DOE Office of Science User Facility. The alloy development research is funded by the Propulsion Materials Program in the Vehicle Technologies Office of DOE's Office of Energy Efficiency and Renewable Energy.

Provided by Oak Ridge National Laboratory