

SCIENCE AND TECHNOLOGY

Expanding the boundaries of scientific knowledge and advancing the technological state of the art to solve problems of national and global importance

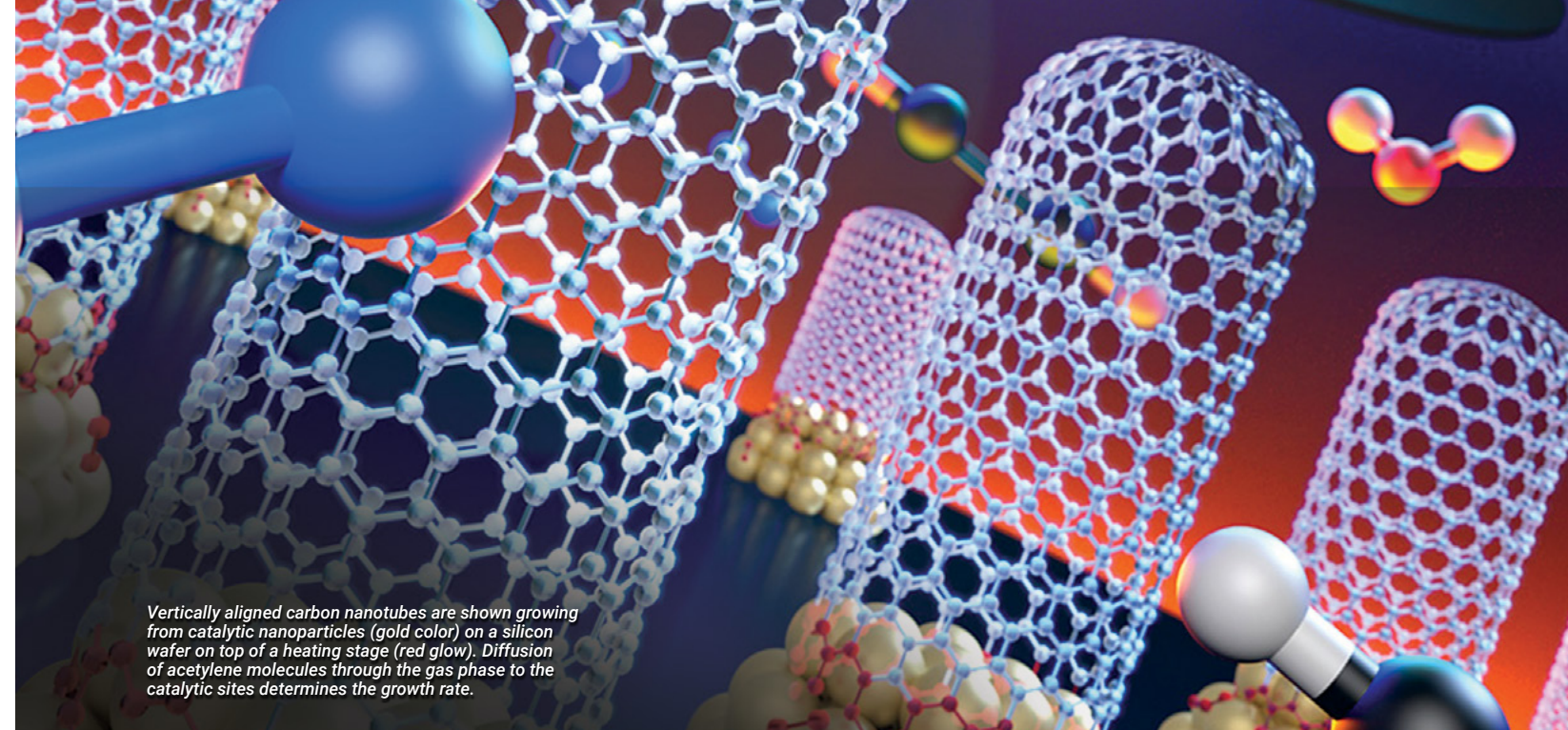
THROUGH its science and technology capabilities, the Laboratory makes fundamental discoveries about nature, develops innovative technologies that improve life and drive the economy, and carries out its mission to improve national security.

COGNITIVE SIMULATION AND MACHINE LEARNING

In May 2023, LLNL and SambaNova Systems announced the addition of SambaNova's spatial data flow accelerator to the Laboratory's high-performance computing (HPC) systems. The new hardware is part of an effort to upgrade LLNL's cognitive simulation program (CogSim), which combines artificial intelligence (AI) with HPC. Deep neural network hardware architectures are used to accelerate traditional physics-based simulations. Connecting the underlying physics to experimental data is an extremely difficult scientific challenge. CogSim AI techniques hold the key to teaching existing simulation models to better mirror experiments

and improve the feedback loop between experiments and models.

AI and machine learning (ML) are widely used throughout the Laboratory to accelerate scientific discovery. For example, LLNL materials and computer scientists have developed a novel ML model that can predict 10 distinct polymer properties from known data sets more accurately than ever before. Discovering suitable polymer materials for use in applications ranging from packaging to solar cells depends on accurately predicting the properties of candidate materials. The model's success lies in a new polymer representation that compactly captures the polymer's structure combined with powerful graph-based ML techniques that autonomously learn how to best describe that structure. Previous ML approaches to predicting polymer properties could not capture the polymer's periodicity, leading to inaccurate predictions. The new ML model will enable new concepts in polymer chemistry to be rapidly tested and iterated upon for a large application space.



Vertically aligned carbon nanotubes are shown growing from catalytic nanoparticles (gold color) on a silicon wafer on top of a heating stage (red glow). Diffusion of acetylene molecules through the gas phase to the catalytic sites determines the growth rate.

NANO FORESTS, BIG POSSIBILITIES

Carbon nanotubes (CNTs)—hollow graphite cylinders measuring up to 5 nanometers in diameter and tens of micrometers long—are the focus of several Livermore research efforts. CNTs have unusual strength, stiffness, and thermal and electrical conductivity. They enable faster proton transport than that in biological channels. LLNL scientists have keen interest in scaling up the production of packed arrays of vertically aligned single-walled CNTs, often called forests. Order and alignment of CNTs strongly influence the material's macroscale performance. Use of forests rather than unorganized CNT structures could revolutionize a host of commercial applications, such as energy storage and water purification. The LLNL research team demonstrated growth of vertically aligned single-walled CNTs at wafer scale under a variety of synthesis conditions and derived a kinetics model to interpret the observed growth trends. The model indicates that appropriate choice of the growth recipe and fluid dynamic conditions can significantly increase the production throughput of CNT forests.

Other LLNL scientists have applied a neural network interatomic potential within advanced computational models to understand the hydrogen bonding of water confined in single-walled CNTs. This potential allowed an efficient, computationally accurate examination of confined water for a wide range of

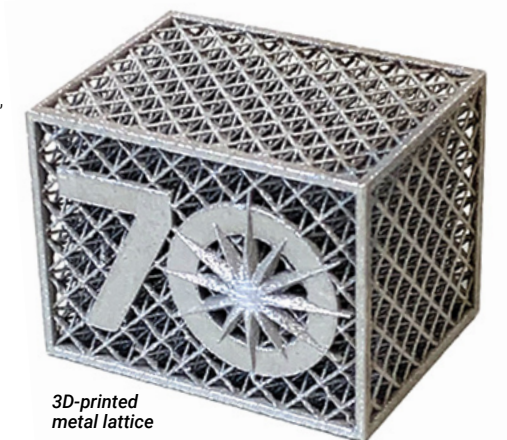
CNT diameters at time and length scales beyond the reach of conventional first-principles approaches. An improved understanding of hydrogen bonding in nanopores bridges knowledge gaps in the structure and dynamics of confined water and promises to advance various applications, including ion-selective membranes for water desalination.

ADVANCING COMPONENT DESIGN AND MANUFACTURING

Over the last decade, Laboratory breakthroughs in additive manufacturing—often called 3D printing—have enabled production of nanoscale precision components with previously unobtainable properties made from an ever-expanding variety of materials. An invention this year was a 3D-printed material capable of replicating characteristics of biological tissue. Engineers and chemists at LLNL and Meta produced a material that is stretchable to around 200 times its original properties, and as its gradient transitions from soft to stiffer material, its toughness increases by 10 times. It can be tailored for energy-absorbing materials, soft robotics, and wearable electronic devices, including those for enhancing human performance. Other researchers at the Laboratory developed a method for detecting and predicting strut defects in 3D-printed metal lattice structures during a print using a combination of monitoring, imaging techniques and multiphysics simulations. The ability to monitor build quality in situ to decide, on the fly, if the part will satisfy quality requirements

is important for manufacturing high-strength, low-density metallic lattices.

Laboratory engineers are also making major strides toward closing the gap between design and manufacturing. This year, they adapted the Livermore Design Optimization (LiDO) code to accelerate the development cycle for new parts. LiDO works in tandem with Serac—a high-order nonlinear thermomechanical simulation code—to automatically generate optimal designs based on performance metrics. Previously, designers had to write unique code to integrate Serac simulations into the LiDO framework, requiring every solver to use a separate subroutine or wrapper function. Now, designers can use a single wrapper for all Serac solvers, reducing the time, energy, and maintenance burden to facilitate changing design needs. LiDO is integral to a DOE HPC initiative that aims to create "digital twins" for expediting design and production of aerospace components.



3D-printed metal lattice



LLNL computer scientists stand by the new SambaNova artificial intelligence hardware that upgrades the Laboratory's cognitive simulation capabilities.