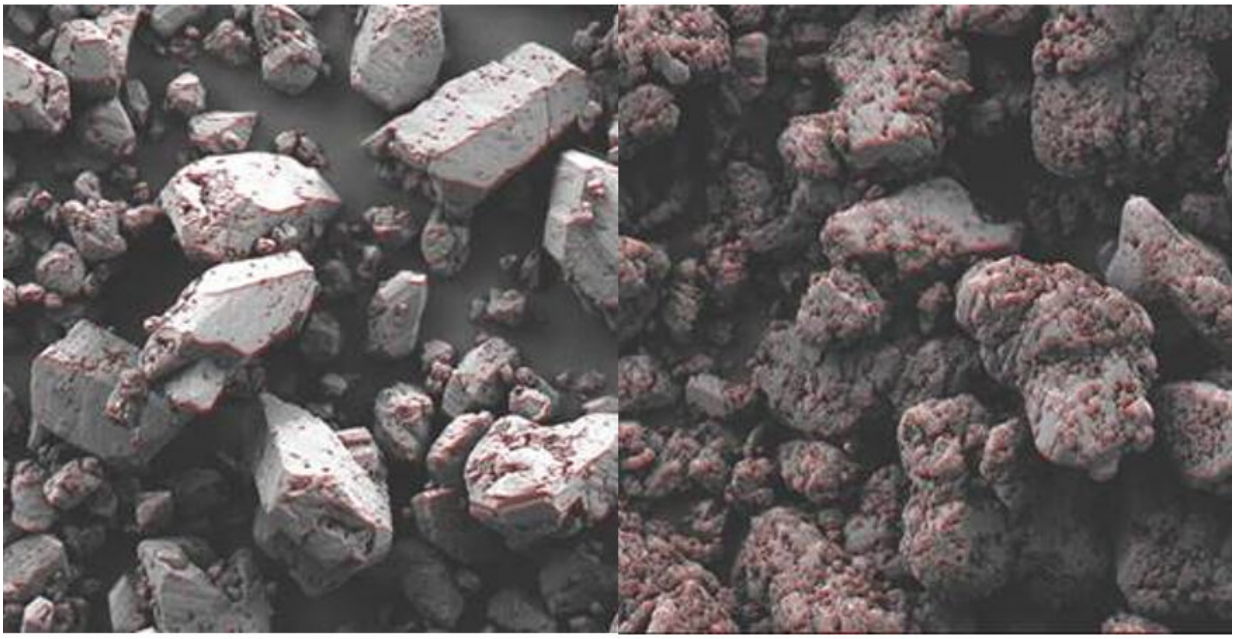
# Machine learning accelerates high-performance materials development and deployment

March 4 2020, by Rose Hansen



Examples of two different TATB crystal structures synthesized under different conditions, shown at identical magnifications. Credit: Lawrence Livermore National Laboratory

Lawrence Livermore National Laboratory (LLNL) and its partners rely on timely development and deployment of diverse materials to support a

variety of national security missions. However, materials development and deployment can take many years from initial discovery of a new material to deployment at scale.

An interdisciplinary team of LLNL researchers from the Physical and Life Sciences, Computing and Engineering directorates are developing machine-learning techniques to remove bottlenecks in the development cycle, and in turn dramatically decreasing time to deployment.

One such bottleneck is the amount of effort required to test and evaluate the performance of candidate materials such as TATB, an insensitive high explosive of interest to both the Department of Energy and the Department of Defense. TATB samples can exhibit different crystal characteristics (e.g., size and texture) and therefore dramatically differ in performance due to slight variations in the conditions under which the synthesis reaction occurred.

The LLNL team is looking at a novel approach to predict material properties. By applying computer vision and machine learning based on scanning electron microscopy (SEM) images of raw TATB powder, they have avoided the need for fabrication and physical testing of a part. The team has shown that it is possible to train models to predict material performance based on SEM alone, demonstrating a 24 percent error reduction over the current leading approach (i.e., domain-expert assessment and instrument data). In addition, the team showed that machine-learning models can discover and use informative crystal attributes, which domain experts had underutilized.

According to LLNL computer scientist Brian Gallagher, lead author of an article appearing in the journal Materials and Design: "Our goal is not only to accurately predict material performance, but to provide feedback to experimentalists on how to alter synthesis conditions to produce higher-performance materials. These results move us one step closer to

that goal."

LLNL materials scientist Yong Han, principal investigator and corresponding author of the paper, added: "Our work demonstrates the utility of applying novel machine-learning approaches to tackle difficult materials science problems. We plan to expand on this work to tackle data sparsity, explainability, uncertainty and domain-aware model development."

**More information:** Brian Gallagher et al. Predicting compressive strength of consolidated molecular solids using computer vision and deep learning, *Materials & Design* (2020). DOI: 10.1016/j.matdes.2020.108541

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