An ally for alloys: AI helps design high-performance steels

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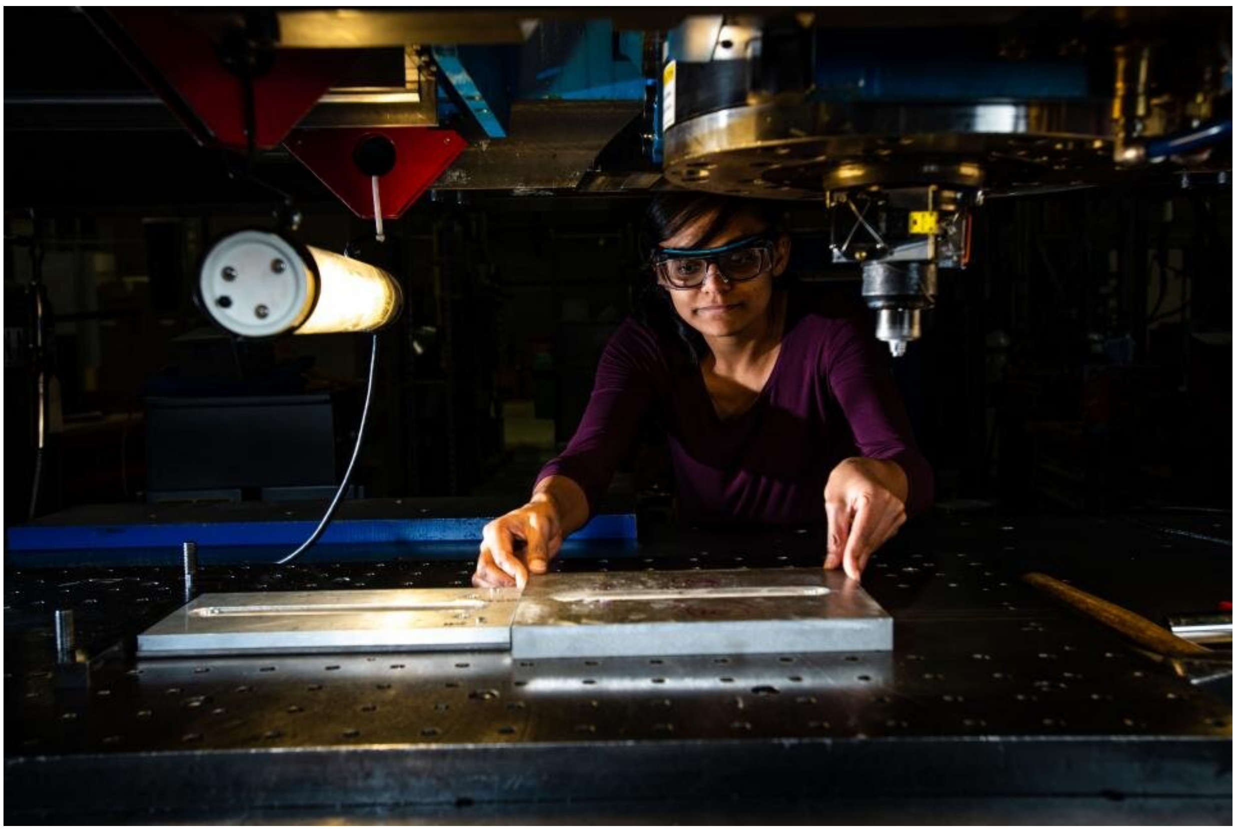

PNNL's distinctive capabilities in joining steel to aluminum alloys enable lightweight vehicle technologies for sustainable transportation. Credit: Andrea Starr | Pacific Northwest National Laboratory

Machine learning techniques have contributed to progress in science and technology fields ranging from health care to high-energy physics. Now, machine learning is poised to help accelerate the development of stronger alloys, particularly stainless steels, for America's thermal power generation fleet. Stronger materials are key to producing energy efficiently, resulting in economic and decarbonization benefits.

"The use of ultra-high-strength steels in power plants dates back to the 1950s and has benefited from gradual improvements in the materials over time," says Osman Mamun, a postdoctoral research associate at Pacific Northwest National Laboratory (PNNL). "If we can find ways to speed up improvements or create new materials, we could see enhanced efficiency in plants that also reduces the amount of carbon emitted into the atmosphere."

Mamun is the lead author on two recent, related journal articles that reveal new strategies for machine learning's application in the design of advanced alloys. The articles chronicle the research outcomes of a joint effort between PNNL and the National Energy Technology Laboratory (NETL). In addition to Mamun, the research team included PNNL's Arun Sathanur and Ram Devanathan and NETL's Madison Wenzlick and Jeff Hawk.

The work was funded under the U.S. Department of Energy's (DOE's) Office of Fossil Energy via the "XMAT"—eXtreme environment MATerials—consortium, which includes research contributions from seven DOE national laboratories. The consortium seeks to accelerate the development of improved heat-resistant alloys for various power plant components and to predict the alloys' long-term performance. The inside story of power plants

A thermal power plant's internal environment is unforgiving. Operating temperatures of more than 650 degrees Celsius and stresses exceeding 50 megapascals put a plant's steel components to the test.

"But also, that high temperature and pressure, along with reliable components, are critical in driving better thermodynamic efficiency that leads to reduced carbon emissions and increased cost-effectiveness," Mamun explains.

The PNNL–NETL collaboration focused on two material types. Austenitic stainless steel is widely used in plants because it offers strength and excellent corrosion resistance, but its service life at high temperatures is limited. Ferritic-martensitic steel that contains chromium in the 9 to 12 percent range also offers strength benefits but can be prone to oxidation and corrosion. Plant operators want materials that resist rupturing and last for decades.

Over time, "trial and error" experimental approaches have incrementally improved steel, but are inefficient, time-consuming, and costly. It is crucial to accelerate the development of novel materials with superior properties. Models for predicting rupture strength and life

Recent advances in computational modeling and machine learning, Mamun says, have become important new tools in the quest for achieving better materials more quickly.

Machine learning, a form of artificial intelligence, applies an algorithm to datasets to develop faster solutions for science problems. This capability is making a big difference in research worldwide, in some cases shaving considerable time off scientific discovery and technology developments.

The PNNL–NETL research team's application of machine learning was described in their first journal article, "A Machine Learning Aided Interpretable Model for Rupture Strength Prediction in Fe-based Martensitic and Austenitic Alloys," published March 9 in *Scientific Reports*.

The paper recounts the team's effort to enhance and analyze stainless steel datasets, contributed by NETL team members, with three different algorithms. The ultimate goal was to construct an accurate predictive model for the rupture strength of the two types of alloys. The team concluded that an algorithm known as the Gradient Boosted Decision Tree best met the needs for building machine learning models for accurate prediction of rupture strength.

Further, the researchers maintain that integrating the resulting models into existing alloy design strategies could speed the identification of promising stainless steels that possess superior properties for dealing with stress and strain.

"This research project not only took a step toward better approaches for extending the operating envelope of steel in power plants, but also demonstrated machine learning models grounded in physics to enable interpretation by domain scientists," says research team member Ram Devanathan, a PNNL computational materials scientist. Devanathan leads the XMAT consortium's data science thrust and serves on the organization's steering committee.

The project team's second article, "Machine Learning Augmented Predictive and Generative Model for Rupture Life in Ferritic and Austenitic Steels," was published in *npj Materials Degradation*'s April 16 edition.

The team concluded in the paper that a machine-learning-based predictive model can reliably estimate the rupture life of the two alloys. The researchers also described a methodology to generate synthetic alloys that could be used to augment existing sparse stainless steel datasets, and identified the limitations of such an approach. Using these "hypothetical alloys" in machine learning models makes it possible to assess the performance of candidate materials without first synthesizing them in a laboratory.

"The findings build on the earlier paper's conclusions and represent another step toward establishing interpretable models of alloy performance in extreme environments, while also providing insights into data set development," Devanathan says. "Both papers demonstrate XMAT's thought leadership in this rapidly growing field."

More information: Osman Mamun et al, Machine learning augmented predictive and generative model for rupture life in ferritic and austenitic steels, *npj Materials Degradation* (2021). DOI: 10.1038/s41529-021-00166-5

Osman Mamun et al, A machine learning aided interpretable model for rupture strength prediction in Fe-based martensitic and austenitic alloys, *Scientific Reports* (2021). DOI: 10.1038/s41598-021-83694-z

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