Physics informs machine learning for crack-free printing of metals

Machine learning (ML) is making significant inroads into materials research and discovery. ML trains computers to solve problems on their own, but methods are data-intensive. With limited data available, can we still train computers to make decisions to solve critical research problems?

In a recent study published in *Acta Materialia* (https://doi.org/10.1016/j.actamat.2021.117612), a research team led by Tarasankar DebRoy, a professor in the Department of Materials Science and Engineering at The Pennsylvania State University, demonstrated that machine learning can be used to solve important industrial problems even when limited experimental data are available. "Conducting machine learning using brute force will require a ton of experimental data due to the large number of variables involved in many important problems," says DebRoy, "but what if we could reduce the number of variables describing a phenomenon and use less data as a result?" DebRoy together with Barnali Mondal and Tuhin Mukherjee did just that to develop an index for predicting cracks in 3D-printed parts using ML.

It is known that 12 process variables and alloy properties affect crack formation in 3D-printed components. Using all of these variables in a machine learning model would require about 4,096 experimental data sets to forecast cracking based on the variables. To resolve this issue, the researchers computed eight mechanistic variables representing the physics of crack formation. Knowing that several of the variables were interdependent, the team conducted a Pearson's correlation analysis, (a measure of the strength of the linear relationship between quantitative variables), to isolate four independent variables. These were then used in a machine learning model to generate a Crack Susceptibility Index (CSI). The values of the CSI were calculated for 102 data sets (down from 4,096) from the literature.

"There is already an understanding that certain alloy compositions are more susceptible to cracks during additive manufacturing. What remains a mystery is how the various process variables influence the development of these cracks and hence, this study," says Mondal, a postdoctoral researcher in the Department of Materials Science and Engineering at The Pennsylvania State University, who played a key role in this research.

The results showed that unless used in concert, none of the individual mechanistic variables could successfully predict cracking in all the data sets. A CSI value greater than 0.65 indicated the presence of cracks. The solidification stress and cooling rate had the most and least influence on cracking respectively for all process variables studied. Process maps were also generated using the CSI to inform how different process parameters such as preheat temperature and printing speed can alter the mechanistic variables and cause cracks.

"These results also demonstrate that employing a physical understanding of processing in additive manufacturing and other fields can help bring out the best of both machine learning and physics-based mechanistic models to advance technology today," DebRoy says.

"This is an interesting study that utilized a physics-informed machine learning model to predict crack formation with high accuracy. Such models that can probe the effects of variables on the physics of cracking will have a great impact on the field of additive manufacturing," says Grace Gu, a professor in the Mechanical Engineering Department at the University of California, Berkeley, who was not involved in this study.

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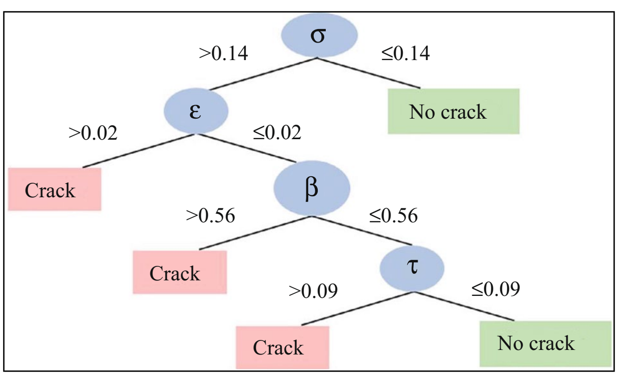

A decision tree constructed using four mechanistic variables—σ, ε, β, and τ—to predict crack formation in aluminum alloy printed parts. The decision-making criteria are based on the normalized values of the four variables. Credit: *Acta Materiala*.