Breaking the trial-and-error loop in Material Design through Machine Learning

Machine learning predicts elastic behavior of multi-component alloys using information from simple two-component alloys

Humans have created alloys and composite materials to get the desired properties such as thermal conductivity, ductility or strength. They would choose contributing materials on a case-by-case basis, solely on chemical intuition. They would make the composite material, test the properties, change the composition and test again. Automating the task can be more efficient, but it still requires a prior understanding of the possible options for the choice of contributing materials and the physical properties of materials involved.

An alternate and more efficient approach would be using mathematical methods to design any material. The technique would use a verified recipe of constructing very few known materials so that it can also successfully predict the associated unknown physical characteristics. Otherwise termed as ‘Machine learning’ (ML), such methods can ‘learn’ and make logical decisions on their own based on limited data. Thus, they have the potential to significantly reduce the time and resources required to develop new materials for a given application.

Prof Alankar, who heads the ICME and Materials Genome Lab in the Department of Mechanical Engineering at IIT Bombay, and his team, revisit the elastic behaviour of materials to demonstrate the power of machine learning in Material Design. They use information about simple alloys to train machine learning algorithms to predict the elastic properties of more complex alloys. They showed that ML could find a set of directly measurable quantities that can be used to design alloys that have more than two elements and the desired elasticity. The work, partly funded by

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The elasticity of a material refers to a material's ability to recover from deformation, which can be inferred by measuring elastic constants. We can quantify the elasticity of materials using quantities such as Young's modulus, which tells us how easily a material can stretch and deform. Elastic constants can be determined using a mathematical modelling method called density functional theory (DFT). However, DFT-based models accurately describe the physics of materials only at 0K or 'absolute zero' temperature (-273 ℃). Since the physical properties described by DFT models are not accurate at temperatures that the alloys would be used at, designing simple alloys using DFT often faces a considerable roadblock. Prof Alankar's work uniquely addresses this by developing an ML model based on the mathematical approach but that can be applied on easily available experimental data, and which can further be extended for any temperatures and operating conditions.

The researchers first 'trained' the ML models to learn elastic properties of all plausible combinations of 2 element alloys obtained through DFT models. Through this procedure, the ML algorithm learns to automatically predict important properties of materials. It comes up with a numerical representation of the binary alloys using a set of physical descriptors or 'features'. The researchers then tested the ML models on the same dataset to shortlist a few easily measurable features of materials, such as melting temperature, atomic radius, thermal conductivity, which could predict elastic properties of all possible combinations of alloys. Talking about this feature selection, Prof Alankar elaborates - "We were expecting a few of the known features in the shortlist. However, we were not certain about their importance. e.g. atomic radius turned out to be the most critical." ML thus provides a platform to identify and explore the unknown properties and how they are related to the material structure, which otherwise is complicated to be derived mathematically.

The crucial achievement of this work, however, was established when the researchers were able to successfully validate these trained ML models on the real experimental data of elastic constants of a five-component alloy comprising of the elements, Nickel (Ni), Chromium (Cr), Iron (Fe), Molybdenum (Mo) and Tungsten (W). Prof. Alankar expresses, "To start with, we have used data of binary alloys and have been able to predict elastic constants of multi-component alloys. Other than being able to correlate with experimental data, this is the outcome that we celebrated."

Prof Alankar's innovative work lays the path for discovering and characterising novel 'perovskites', a class of calcium titanium oxide-based minerals that can be engineered to make new materials, and other extraordinary multi-component alloys. Prof. Alankar and his team are already investigating this in their upcoming works by enforcing underlying physical laws in the ML- models, also known as 'Physics-informed machine learning'.

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