Using AI to predict new materials with desired properties

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Aluminum alloys are lightweight, energy-saving materials which are used for various purposes, from welding materials for buildings to bicycle frames. Credit: Jozef Polc via123rf

Scientists in Japan have developed a machine learning approach that can

predict the elements and manufacturing processes needed to obtain an aluminum alloy with specific, desired mechanical properties. The approach, published in the journal *Science and Technology of Advanced Materials*, could facilitate the discovery of new materials.

Aluminum alloys are lightweight, energy-saving materials made predominantly from aluminum, but also contain other elements, such as magnesium, manganese, silicon, zinc and copper. The combination of elements and manufacturing process determines how resilient the alloys are to various stresses. For example, 5000 series aluminum alloys contain magnesium and several other elements and are used as a welding material in buildings, cars, and pressurized vessels. 7000 series aluminum alloys contain zinc, and usually magnesium and copper, and are most commonly used in bicycle frames.

Experimenting with various combinations of elements and manufacturing processes to fabricate aluminum alloys is time-consuming and expensive. To overcome this, Ryo Tamura and colleagues at Japan's National Institute for Materials Science and Toyota Motor Corporation developed a materials informatics technique that feeds known data from aluminum alloy databases into a machine learning model. This trains the model to understand relationships between alloys' mechanical properties and the different elements they are made of, as well as the type of heat treatment applied during manufacturing. Once the model is provided enough data, it can then predict what is required to manufacture a new alloy with specific mechanical properties. All this without the need for input or supervision from a human.

The model found, for example, 5000 series aluminum alloys that are highly resistant to stress and deformation can be made by increasing the manganese and magnesium content and reducing the aluminum content.

"This sort of information could be useful for developing new materials,

including alloys, that meet the needs of industry," says Tamura.

The model employs a statistical method, called Markov chain Monte Carlo, which uses algorithms to obtain information and then represent the results in graphs that facilitate the visualization of how the different variables relate. The machine learning approach can be made more reliable by inputting a larger dataset during the training process.

More information: Ryo Tamura et al. Materials informatics approach to understand aluminum alloys, *Science and Technology of Advanced Materials* (2020). DOI: 10.1080/14686996.2020.1791676

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