AI behind deepfakes may power materials design innovations

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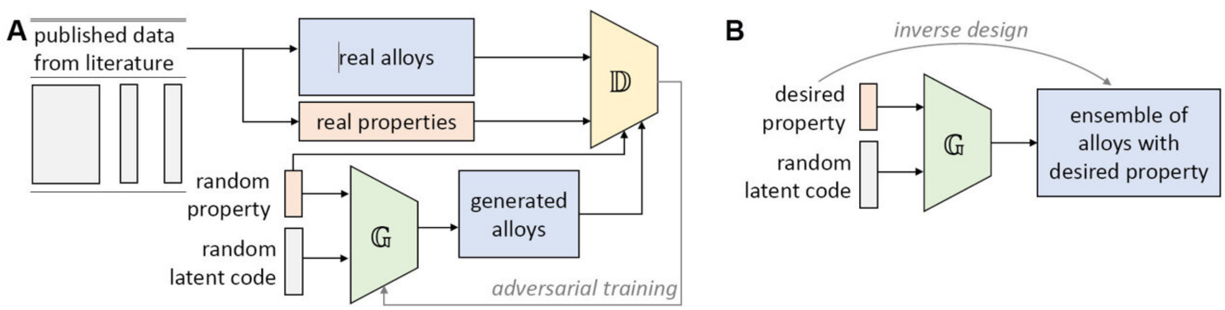

Figure 1. Schematic illustration of generative modeling for inverse design of materials using a conditional Generative Adversarial Network. (A) Adversarial training procedure in which the Generator and Discriminator compete for superior performance. (B) Inverse design using the trained Generator. Credit: DOI: 10.20517/jmi.2021.05

The person staring back from the computer screen may not actually exist, thanks to artificial intelligence (AI) capable of generating convincing but ultimately fake images of human faces. Now this same technology may power the next wave of innovations in materials design, according to Penn State scientists.

"We hear a lot about deepfakes in the news today—AI that can generate realistic images of human faces that don't correspond to real people," said Wesley Reinhart, assistant professor of materials science and engineering and Institute for Computational and Data Sciences faculty co-hire, at Penn State. "That's exactly the same technology we used in our research. We're basically just swapping out this example of images of human faces for elemental compositions of high-performance alloys."

The scientists trained a generative adversarial network (GAN) to create novel refractory high-entropy alloys, materials that can withstand ultra-high temperatures while maintaining their strength and that are used in technology from turbine blades to rockets.

"There are a lot of rules about what makes an image of a human face or what makes an alloy, and it would be really difficult for you to know what all those rules are or to write them down by hand," Reinhart said. "The whole principle of this GAN is you have two neural networks that basically compete in order to learn what those rules are, and then generate examples that follow the rules."

The team combed through hundreds of published examples of alloys to create a training dataset. The network features a generator that creates new compositions and a critic that tries to discern whether they look realistic compared to the training dataset. If the generator is successful, it is able to make alloys that the critic believes are real, and as this adversarial game continues over many iterations, the model improves, the scientists said.

After this training, the scientists asked the model to focus on creating alloy compositions with specific properties that would be ideal for use in turbine blades.

"Our preliminary results show that generative models can learn complex relationships in order to generate novelty on demand," said Zi-Kui Liu, Dorothy Pate Enright Professor of Materials Science and Engineering at Penn State. "This is phenomenal. It's really what we are missing in our computational community in materials science in general."

Traditional, or rational design has relied on human intuition to find patterns and improve materials, but that has become increasingly challenging as materials chemistry and processing grow more complex, the researchers said.

"When you are dealing with design problems you often have dozens or even hundreds of variables you can change," Reinhart said. "Your brain just isn't wired to think in 100-dimensional space; you can't even visualize it. So one thing that this technology does for us is to compress it down and show us patterns we can understand. We need tools like this to be able to even tackle the problem. We simply can't do it by brute force."

The scientists said their findings, recently published in the *Journal of Materials Informatics*, show progress toward the inverse design of alloys.

"With rational design, you have to go through each one of these steps one at a time; do simulations, check tables, consult other experts," Reinhart said. "Inverse design is basically handled by this statistical model. You can ask for a material with defined properties and get 100 or 1,000 compositions that might be suitable in milliseconds."

The model is not perfect, however, and its estimates still must be validated with high-fidelity simulations, but the scientists said it removes guesswork and offers a promising new tool to determine which materials to try.

More information: Arindam Debnath et al, Generative deep learning as a tool for inverse design of high entropy refractory alloys, *Journal of Materials Informatics* (2021). DOI: 10.20517/jmi.2021.05

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