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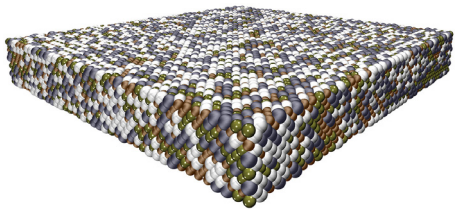
Framework drawing on paired distribution functions and atomic properties propels material generation 1,000 times faster than conventional methods.



Combining four or more elements in near-equiatomic compositions, high-entropy alloys (HEAs) has garnered attention in recent years for their superior functional and structural properties. Predicting new HEAs, however, requires more computer modeling resources than conventional alloys composed of fewer elements. One machine learning approach looks to streamline the process of finding new HEAs via computation.

Tetsassi Feugmo et al. propose a method combining artificial neural networks and evolutionary algorithms to generate HEA structures. An inverse design approach based on pair distribution functions and atomic properties provides researchers with a way to train a model on smaller unit cells to generate larger cells.

Previous attempts to simulate alloys involved approaches relying on special quasirandom structures (SQS) combining cluster expansions with Monte Carlo algorithms. Such approaches have been computationally intensive and suboptimal for simulating larger structures.

“Prior to our work, if you wanted to study an HEA material, you were limited in the system size you could consider,” said author Conrard Giresse Tetsassi Feugmo. “This meant that certain types of predictions, which occur on a larger length scale, were either not possible to predict or required very large computational resources.”

With the framework, the team generated structures larger than 40,000 atoms in a matter of hours -- roughly 1,000 times faster than SQS-driven approaches. Their method provides more efficient design exploration by allowing the same model to be used to generate multiple structures with same fractional composition.

The group hope the approach paves the way for simulating myriad properties of high-entropy alloys. They look to use it to optimize materials for automotive and aerospace applications.

Source: “Neural evolution structure generation: High entropy alloys,” by Conrard Giresse Tetsassi Feugmo, Kevin Ryczko, Abu Anand, Chandra Veer Singh, and Isaac Tamblyn, *Journal of Chemical Physics* (2021). The article can be accessed at https://doi.org/10.1063/5.0049000.

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