Physicists present new way to predict magnetic alloy properties with machine learning

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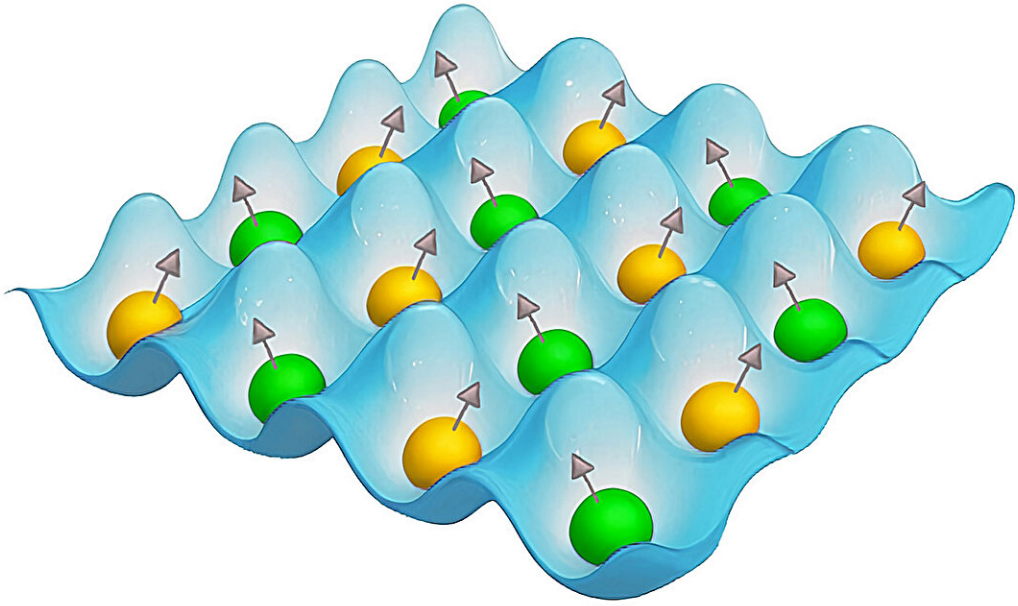

Magnetic structure of a material. The colored spheres represent atoms and the arrows stand for their magnetic moments. The curved surface illustrates how the atoms assume the most energetically favorable positions. The magnetic moments, likewise, adopt the most energetically favorable orientations. Credit: Pavel Odinev/Skoltech PR

Researchers from Skoltech and MIPT and their German, Austrian, and Norwegian colleagues have proposed and tested a new method for computer modeling of magnetic alloys. The method, which relies on machine learning, accurately predicted the energy, mechanical and magnetic characteristics of the alloy of iron and aluminum.

This has been made possible by accounting for the so-called magnetic moments of atoms that give rise to the effects of magnetism. The study is published in *Scientific Reports* and is a stepping stone toward modeling chromium nitride—an ultrahard and corrosion-resistant material used in metal forming, medical tools and implants.

Computer modeling of materials is often a balancing act between speed and accuracy. The gold standard for predicting material structure and properties with the least error is quantum mechanical calculations, such as solving the Schrodinger equation.

There are ways to accelerate these demanding computations, the most popular among them being density functional theory. The way DFT saves computation time is this: Rather than solve the equation with respect to the electron wave function, we find the so-called total electron density in the lowest energy state. However, even that only allows systems tens or hundreds of atoms large to be modeled on a supercomputer.

Larger systems require further simplification: Ignoring the electronic structure and considering so-called interatomic interaction potentials, which characterize the forces between atoms. Naturally, this sacrifices some accuracy in predicting a material's properties.

Recent years have seen the rise of a new solution that offers the best of both worlds. It retains the accuracy of quantum mechanical calculations and drastically increases computation speed even for systems numbering

thousands of atoms. One popular approach is to use machine learning to obtain interatomic potentials trained on quantum mechanical calculation results.

Such potentials give better predictions of material properties than their experimentally sourced analogs. However, machine learning interatomic potentials do not necessarily account for the magnetic moments of atoms, and this can cause errors in modeling magnetic materials.

To model the properties of such materials, a group of physicists and mathematicians from MIPT and Skoltech updated its Moment Tensor Potentials method for obtaining machine learning interatomic potentials, generalizing it to version mMTP. This new "magnetic" MTP has already been used to predict the energy of iron in its para- and ferromagnetic states. The new study in *Scientific Reports* applies the method to the two-component alloy of iron and aluminum.

Ivan Novikov, a senior research scientist at Skoltech and an associate professor at the MIPT Department of Chemical Physics of Functional Materials, commented, "Our team is developing machine learning potentials that speed up the quantum mechanical calculations needed to describe the properties of materials by approximately five orders of magnitude.

"Over the past three years, machine learning potentials with magnetic moment have been emerging, and we created our own mMTP and validated it on the system of iron. In the new paper, we sought to validate the potential on a two-component system and demonstrate the algorithm for building a dataset for training the potential."

The researchers compiled the dataset on the basis of quantum mechanical calculations, and used it to train five mMTPs. The team then tested how well the potentials could predict the structure and the

magnetic properties of the iron-aluminum alloy depending on the proportion of aluminum.

The first stage of the study, which lasted the longest, involved creating the dataset for model training. Sixteen-atom systems were chosen for the quantum mechanical calculations. The systems differed in the number and relative positions of the iron and aluminum atoms. For every configuration, density functional theory allowed the team to find the positions of the atoms, lattice geometry, and magnetic moments that corresponded to that particular system's lowest energy state.

Next, the researchers introduced perturbations into the system by displacing atomic positions and extending or compressing the lattice vectors, which characterize lattice geometry. The final stage involved exciting the magnetic moments for the structures from both the first and the second stages using density functional theory and the constraints it imposes on magnetic moments. The resulting dataset contained more than 2,000 configurations, both excited and in an equilibrium state.

The scientists then proceeded to train an ensemble of five mMTPs on the newly formed dataset and test their predictions of a configuration's equilibrium magnetic moments and lattice vectors against quantum mechanical calculations. The new method proved highly accurate regardless of the proportion of aluminum in the alloy.

Magnetic MTP predictions agreed well with the experiment, too. The researchers considered how the ratio between the metals in the iron-aluminum alloy affects the lattice vectors. It turned out that the geometry of the lattice remained unchanged for the proportion of aluminum between 20% and 40%. A quantitative mismatch was observed, but it could be accounted for by the fact that modeling assumed the absolute zero of temperature, unlike the experiment.

The scientists went on to compare the magnetic moments of the alloys given by mMTP and by quantum mechanical calculations. The values agreed with each other and with theory: As the proportion of aluminum grew, the alloy's magnetic properties diminished. But while mMTP predicted a complete loss of ferromagnetism at 50% aluminum, quantum mechanical calculations didn't. This mismatch calls for further investigation.

The researchers are planning to supplement their method with active learning, so that the selection of configurations suitable for training the potential will happen automatically. This will enable multicomponent paramagnetic systems and materials at nonzero temperatures to be studied.

"Combining our knowledge and the 2022 research findings on iron with this new paper on the iron-aluminum alloy, we will add active learning and verify mMTP on another material—chromium nitride," Novikov said.

"Specifically, we will be able to predict the variation of specific heat capacity and examine paramagnetic states. I am in favor of the approach when you begin by thoroughly validating your method and only then do you turn to practical matters. And this is the path our research has been taking so far: First we validated MTP on benchmark systems, and we're now at a point where we can start predicting the phase diagrams of more complex materials."

More information: Alexey S. Kotykhov et al, Constrained DFT-based magnetic machine-learning potentials for magnetic alloys: a case study of Fe–Al, *Scientific Reports* (2023). DOI: 10.1038/s41598-023-46951-x

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