Autonomous synthesis of new ferromagnetic materials combines theory, informatics, and experiment

Data storage systems are coated with ferromagnetic materials. When the materials' performance is optimized, this provides superior performance and storage density. In a recent issue of *Science and Technology of Advanced Materials: Methods* (https://doi.org/10.1080/27660400.2022.2094698), researchers reported a robust procedure for the autonomous synthesis of novel ferromagnetic materials with large magnetocrystalline anisotropy (MCA) by combining theory, informatics, and experiments.

Large MCA is an essential parameter for ferromagnetic materials for energy savings and high density of memory devices. Masato Kotsugi, a professor from the Department of Materials Science and Technology at Tokyo University of Science, told *MRS Bulletin*, "MCA is related to the size of the memory device. In other words, the density of the memory is connected to the recording speed of the system. Consequently, higher MCA will accelerate the writing and reading of memory devices."

In this study, a function model was utilized to perform an initial calculation of the MCA energy. This model consists of a kernel function that predicts the surface smoothness and other properties related to the MCA energy. Kotsugi says, "Flatter surfaces increase MCA energies, so smooth surfaces are necessary. A useful material exploration cannot be achieved without selecting a suitable kernel function."

Subsequently, to perform a comprehensive materials exploration and determine the optimal candidates, a Bayesian optimization was applied as a sequential strategy for global optimization. Non-rare earth elements (Fe, Co, Ni, and Cu) were identified as the materials that are most suited for a fundamental strategy, where a four-layer periodic multilayer system was adopted. Pulsed laser deposition (PLD) was selected to fabricate the top three predicted multilayer magnetic materials.

"Alternative fabrication techniques such as molecular beam epitaxy (MBE) and sputtering were proposed, but due to morphology changes contributing to a large distribution of the MCA energies and the growth of large clusters greater than the atomic layer, respectively, PLD was suitably the preferred option," Kotsugi says.

Reflection high-energy electron diffraction (RHEED) and other characterization techniques were used to evaluate the properties and confirm the epitaxial growth of the simulated magnetic materials. RHEED patterns with sharp streaks indicate a smooth surface condition; however, sharp RHEED patterns were not seen for the novel materials fabricated. Kotsugi says, "This suggests that the surface and interface structure are not perfect and may be attributed to the growth process, either the flow rate or temperature of the PLD fabrication, which are important processing parameters to optimize."

The study revealed that $[Fe/Co/Fe/Ni]_{13}$ and $[Fe/Cu/Co/Cu]_{13}$ are novel ferromagnetic materials whose magnetic anisotropy exceeds that of previously known comparable ferromagnetic alloys. The innovation of novel magnetic materials for memory devices continues to serve as a main pillar for improving data storage density and accelerating data retrieval with reduced energy consumption. In the future, Kotsugi and his research group aim to optimize their autonomous synthesis procedure. This will include increasing the number of elements and layers of their predicted models to increase MCA energies.

Kotsugi says, "New materials are becoming more efficient through the introduction of data science."

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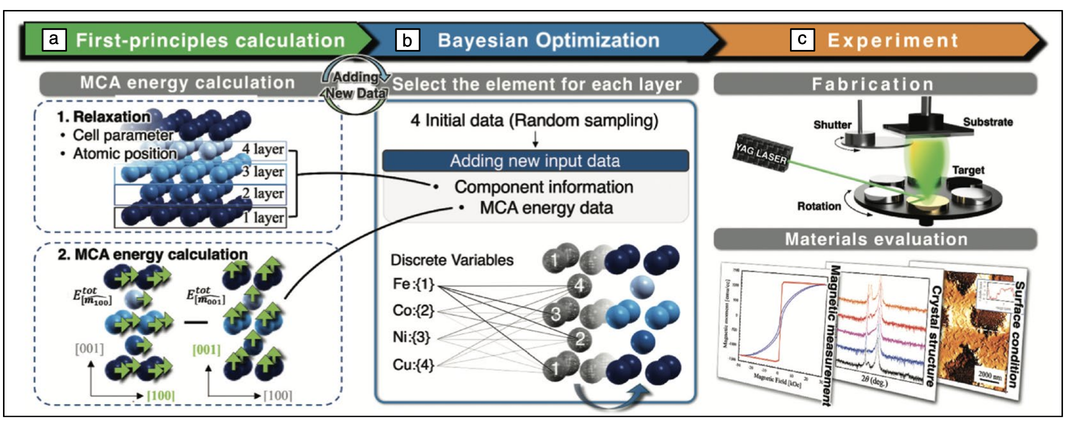

A detailed schematic outlining (a) first-principles calculations used to estimate the magnetocrystalline anisotropy (MCA) energy, followed by (b) Bayesian optimization used to select the element of each layer. To fabricate the predicted material, pulsed laser deposition was employed. Credit: *Science and Technology of Advanced Materials: Methods.*