Resilient Energy Systems
Mission Campaign

DISCOVERY OF NEW HIGH-FREQUENCY MAGNETIC MATERIALS ENABLED BY ARTIFICAL INTELLIGENCE

This project will harness artificial intelligence (AI) to develop new high-frequency magnetic materials in support of the development of more resilient electrical grid components. Using AI in both the identification and synthesis of these new materials will dramatically shorten the time needed to develop these materials.

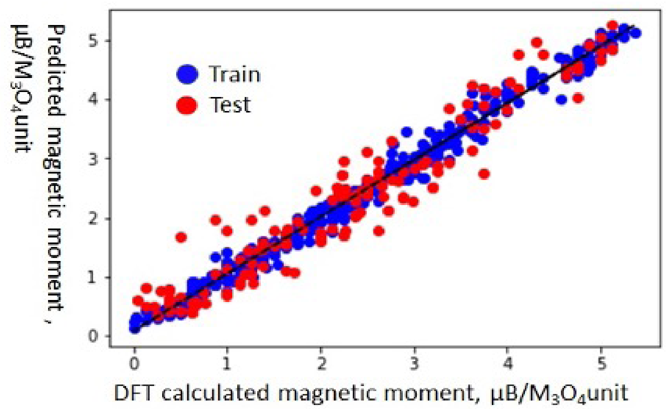
THE CHALLENGE

Solid-state transformers are a promising approach to making the electrical grid more resilient. Solid-state transformers can be more resistant to attack, and they can be more easily replaced than the massive, foreign-made, grid-scale transformers that are currently used. The optimum solid-state transformer would take advantage of the high switching speeds that are enabled by ultrawide bandgap switches, but unfortunately, current inductor materials have magnetic hysteresis losses that are too high at these frequencies. We need better high-frequency inductors to realize the potential of solid-state transformers.

The goal of this project is to use artificial intelligence to identify and synthesize new high-frequency ferrites to support new electrical architectures in power systems (such as solid-state transformers). This will dramatically shorten the time to develop new materials and allow us to test them in circuits within a three-year project period.

APPROACH

We are attacking this problem using articial intelligence (AI) in all stages of the work from initial identification of target materials to the synthesis and characterization of the materials. We will train AI to identify new materials that have improved high-frequency magnetic properties using density functional theory (DFT) calculations. DFT calculations are generally extremely accurate, but are too time-consuming to effectively search the massive number of unknown ferrite phases. So, a series of DFT calculations can be used to train AI to find candidate material more quickly and efficiently. The new materials identified by AI can then be subjected to full DFT calculations. If the AI is accurate, the materials will be synthesized.



AI being trained to determine the magnetic moment of unknown magnetic ferrites. Red dots represent the AI determinations; the closer they are to the black line, the more accurate the determination.

Synthesizing new materials can be as challenging as identifying materials that should be synthesized. Simply knowing the ultimate materials' components and structures doesn't mean they can be synthesized. We will use the DFT simulations to calculate the X-ray diffraction (XRD) pattern of each desired material. Then, when we attempt to synthesize the material we will collect XRD in real time and compare the patterns to the pattern of the desired product in real time using AI. The AI can adjust the reaction conditions and monitor the output of the reaction until the correct phase is synthesized. In time, the AI will become more efficient at synthesizing new, unknown phases as it learns the influence of the synthetic parameters such as time, concentrations, and temperature.

These reactions will be designed to produce nanoparticles, which leads to rapid reactions that produce materials that remain in solution, easing the collection of real-time XRD. Once we successfully produce the desired nanoparticles, the nanoparticles can undergo warm compaction to create toroidal inductors that can be wound with wire to test the inductors in the circuits of interest.

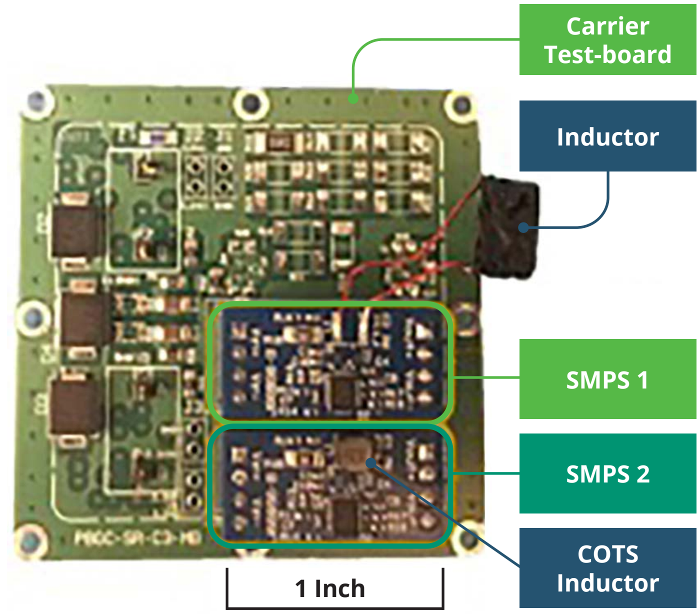
EXPECTED RESULTS

Developing new magnetic materials tends to follow a trial-and-error approach, and it typically takes decades of work to develop new materials with improved properties. We expect this research to yield new materials with improved high-frequency properties in less than three years. These materials will go from discovery to application in realistic circuits within the lifetime of this project.

In addition to the dramatic impact this can have in Sandia's development of new electrical architectures for the grid, this represents a new approach to materials development. It replaces the intuition and guesses of researchers that typically guide new materials development with a rigorous AI approach. This approach is general and can be applied to many systems that are in need of improved materials. This will have a wide range of impacts in areas of interest to Sandia including defense applications, fusion reactors, non-proliferation, and sensing.

EXPECTED IMPACT OF THIS RESEARCH

The project outcomes will include a new approach to materials discovery and synthesis that can be applied to a number of other systems. We anticipate leveraging these results to apply for further funding from agencies such as the Department of Energy's (DOE's) Basic Energy Sciences program, DOE's Office of Energy Efficiency and Renewable Energy, and the Advanced Research Projects Agency-Energy (ARPA-E). On the practical side, we will have developed new materials for high-frequency magentic material applications. This will move us to a Technology Readiness Level (TRL) of at least four, and we will be able to look to technology transfer to get the materials manufactured so we can apply them in systems of interest, such as solid-state transformers.



A test bed for comparing custom Sandia inductors to commercial off-the-shelf (COTS) inductors.

RESILIENT ENERGY SYSTEMS

Sandia's investment in this project is part of its Resilient Energy Systems portfolio of projects, coordinated R&D that addresses the resiliency of the nation's energy systems and other critical infrastructures to threats. This work supports the second thrust: *Materials, Device, and Cyber Innovation* in the area of new high-freqency magnetic materials. The materials developed here will enable new electrical architectures such as solid-state transformers that can support a more resilient national electrical grid .

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