Engineering the World's Strongest Iron-based Bulk Superconducting Magnet using AI (Highlights)

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June 17, 2024. Iron-based high-temperature (high-T_c) superconductors have good potential to serve as materials in next-generation superstrength quasipermanent magnets owing to their distinctive topological and superconducting properties. However, their unconventional high-T_c superconductivity paradoxically associates with anisotropic pairing and short coherence lengths, causing challenges by inhibiting supercurrent transport at grain boundaries in polycrystalline materials.

In this study, reported in *NPG Asia Materials* [1], we employed machine learning to manipulate intricate polycrystalline microstructures through a process design that integrates researcher- and data-driven approaches via tailored BOXVIA software [2]. We focused on an optimization process for enhancing the critical current density of polycrystalline $(Ba,K)Fe_2As_2$. To achieve this, we integrated Bayesian optimization, a machine-learning approach, which empowers data-driven experiments even when operating with limited prior data. Our adopted methodology is based on a collaborative framework, initially designing a researcher-driven process that ensures the simultaneous accumulation of data to promote a data-driven process. This collaborative relationship, shown in Figure 1, is reliant on the continuous reference to the furnished dataset. Ultimately, these two processes yield an optimal parameter set that facilitates the fabrication of permanent magnet prototypes under various conditions.

Our approach resulted in a bulk $Ba_{0.6}K_{0.4}Fe_2As_2$ permanent magnet with a magnetic field that is 2.7 times stronger than that previously reported [3]. Additionally, we demonstrated magnetic field stability exceeding 0.1 ppm/h for a practical 1.5 T permanent magnet, which is a vital aspect of medical magnetic resonance imaging.

Nanostructural analysis revealed contrasting outcomes from the two (data- and researcher-driven) processes, opening the door to redefining what makes for a 'superior' superconducting material. The researcher-driven technique yielded a tightly packed grain boundary network structure, maintaining an approximate spacing of 25 nm. Conversely, the data-driven process led to a distinctive bimodal grain boundary arrangement, with spacing dimensions of approximately 25mm and a broad range of 50-200 nm. Furthermore, this approach introduced densely packed intragranular defects with spacings on the order of several nanometers.

Numerical simulations based on the finite element method showed excellent agreement with the experimental results, suggesting the existence of a uniform supercurrent distribution $J_c(B)$ within the bulk material. This attribute, which is characteristic of polycrystalline superconducting materials, represents a significant advantage.

The magnet structure consisted of a randomly oriented polycrystalline material, which is notably the most robust among unconventional high-T_c superconductors. The production of this superconductor could be efficiently scaled through conventional ceramic processes, aided by the straightforward predictability and optimization achievable using numerical models. Consequently, these iron-based superconductors hold substantial promise as pioneering, next-generation, and high-strength magnets suitable for practical applications. This potential extends to challenging environments, such as liquid hydrogen cooling (~20 K).

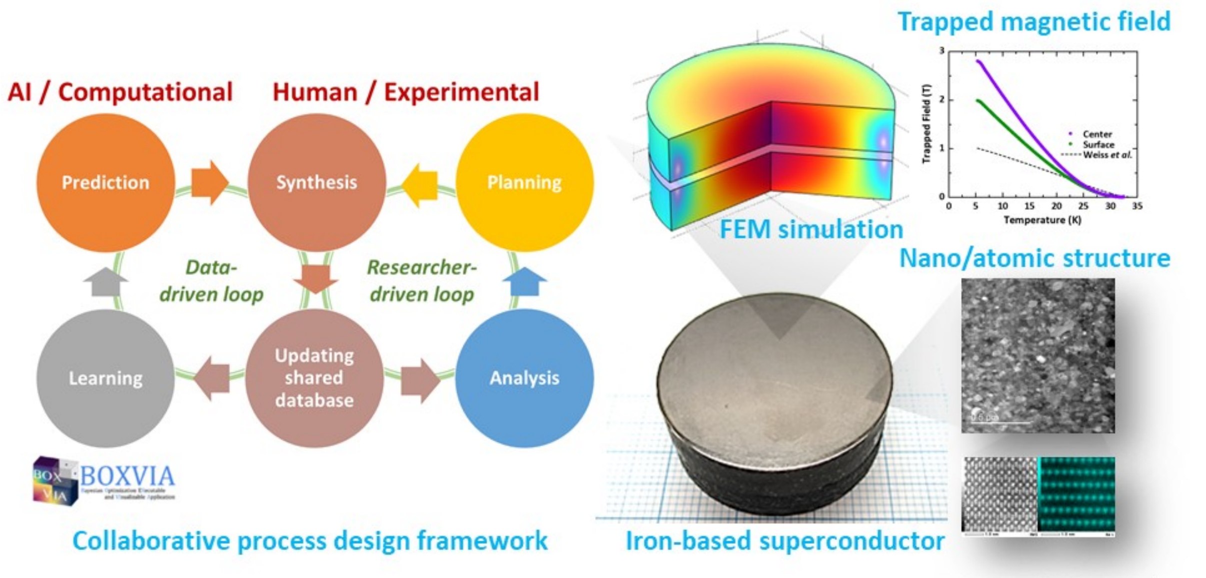

Fig. 1. The world's strongest iron-based bulk superconducting magnet has been manufactured [1]. Machine learning using Bayesian optimization was employed to improve the superconducting properties of potassium-doped barium iron arsenide $(Ba,K)Fe_2As_2$ via tailored BOXVIA software [2]. Two large disk-shaped samples were fabricated using common industrial processing techniques under the best conditions deduced from data- and researcher-driven methods. After magnetizing the samples, they could retain a magnetic field of 2.83 T as a quasi-permanent magnet, around 2.7 times the previous record [3], with decay rates less than -0.1 ppm/h, crucial for MRI scanners. The two approaches produced divergent microstructures, opening the door to redefining what makes for a superior superconducting material.

The paper, "Superstrength permanent magnets with iron-based superconductors by data- and researcher-driven process design," is available open access at *NPG Asia Materials*: https://www.nature.com/articles/s41427-024-00549-5.

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