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Review

Artificial Intelligence—Engineering Magnetic Materials: Current Status and a Brief Perspective

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Abstract: The implementation of artificial intelligence into the research and development of (currently) the most economically relevant classes of engineering hard and soft magnetic materials is addressed. Machine learning is nowadays the key approach utilized in the discovery of new compounds, physical–chemical properties prediction, microstructural/magnetic characterization, and applicability of permanent magnets and crystalline/amorphous soft magnetic alloys. Future opportunities are envisioned on at least two fronts: (a) ultra-low losses materials, as well as processes that enable their manufacturing, unlocking the next step for higher efficiency electrification, power conversion, and distribution; (b) additively manufactured magnetic materials by predicting and developing novel powdered materials properties, generative design concepts, and optimal processing conditions.

Keywords: artificial intelligence; amorphous alloys; hard magnetic materials; soft magnetic materials; machine learning

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1. Introduction

Artificial intelligence (AI) has become a common keyword used across disciplines. The popularization of connected consumer components (e.g., smartphones and home appliances) and availability of smart (manufacturing) industrial components such as machinery sensors [1] have unlocked data quantity and quality previously unreachable that, associated with existing computing capabilities, has supported current AI significance growth. The use of AI in the area of materials science and engineering (MSE—exemplified by [2,3]) is gaining momentum, similar to other (very distinct) fields such as healthcare [4], smart cities/buildings [5,6], and transportation [7]. As a subset of the MSE universe with applicability in power conversion/distribution/transmission, data storage/transmission, and medicine, engineering hard and soft magnetic materials (HSMMs) are also facing the influence of AI. This movement is an expected step since HSMMs are directly involved in tackling growing challenges on more efficient electrification and mitigation of carbon footprint.

Due to the multidisciplinary character associated with HSMM research, it becomes relevant to address AI–HSMM status to understand current developments and to pave the way to enhance the associated research ecosystem further. This document will focus on addressing why AI has been implemented with engineering HSMMs—detailed in Section 2—and which multidisciplinary opportunities are envisaged, as summarized in Section 3; specifics on AI algorithms are discussed in [8–10].

2. AI—Hard/Soft Magnetic Materials: Why?

The driving forces for research combining AI–HSMM rely on at least three interrelated pillars: discovery of materials and/or prediction of their (physical) properties, materials characterization, and applications. Each one of them is discussed in further detail in the next subsections.

2.1. Discovery of Materials and/or Prediction of Properties

The first of the AI–HSMM pillars is the discovery of new compounds and/or prediction of their physical properties. Advances in HSMMs, similar to almost all other materials classes, have mainly occurred by trial-and-error cycles, impacting the time required to achieve milestones and increasing investments to accomplish them. Therefore, AI is expected to strengthen faster developments of novel and/or optimized HSMMs.

In the scope of hard magnetic materials, permanent magnets (PMs) have been a focus of AI utilization due to their unique role in enabling compactness and higher efficiency of systems constituted by them. Efforts resulting in enhanced performance and exploring the reduction of elemental criticality of some materials' families are strong value propositions to pursue. The combination of both features—performance and strategic use of critical elements—has currently resulted in limited applications of AI into Alnico, barium/strontium ferrites, and hybrid (bonded) magnets; conversely, for rare earth (RE)-Fe-B-based materials, AI efforts have intensified.

The first example within such space has utilized AI to train machine learning (ML) models, using a combinatorial high-throughput screening based on density functional theory calculations, to predict properties of RE(Fe, X)$_{12}$Y-type compounds, where X corresponds to a nonferrous alloying element [11]. Both intrinsic (e.g., uniaxial anisotropy energy) and extrinsic (e.g., maximum energy product $(BH)_{max}$) quantities have been scrutinized, indicating the possibility of bridging the gap of $(BH)_{max}$ existent among currently available compounds, typically observed between ferrites and Nd-Fe-B. In addition, it has enabled the creation of a respective RE-based hard magnetic phases database also allowing the estimation of thermodynamic stability and raw materials cost via a user-friendly interface [12]; in fact, it is worth noting that the number of databases that compile distinct materials classes and/or properties is continuously increasing [13]. In addition, potentially formable crystal structures of Nd-Fe-B-based alloys have also been assessed evaluating the elemental substitution of lanthanides, transition metals, and light elements. From a universe of 5967 samples, 20 of them were found to be potentially stable via high-throughput first-principle calculations. Based on (un)supervised learning, the average atomic coordination number and coordination number of iron sites have a major influence on the phase stability for novel Nd-Fe-B-based crystal structures [14].

Addressing the mitigation in the use of (heavy) RE elements, a growing challenge faced in such PM class for at least a decade, diffraction data have been used in high-throughput experimentation assessing a combination of structural evolution and chemical composition variations [15]; as a result, a novel magnetic phase has been reported based on Fe-Co-Mo synthesized as a thin film whose magnetic results are illustrated in Figure 1. In a complementary way, along the same high-throughput line, the search of RE-free PMs has also been executed based on the combination of the Inorganic Crystal Structure Database with data mining/filtering. Applying boundary conditions considering, but not limited to, 3D and 5D elements, the magnetic moment per unit cell >0.5 μ_B/f.u., and compounds with hexagonal and tetragonal crystalline structures, Pt_2FeNi, Pt_2FeCu, and W_2FeB_2 have been proposed, as illustrated in Figure 2, as suitable phases to be further explored experimentally [16].

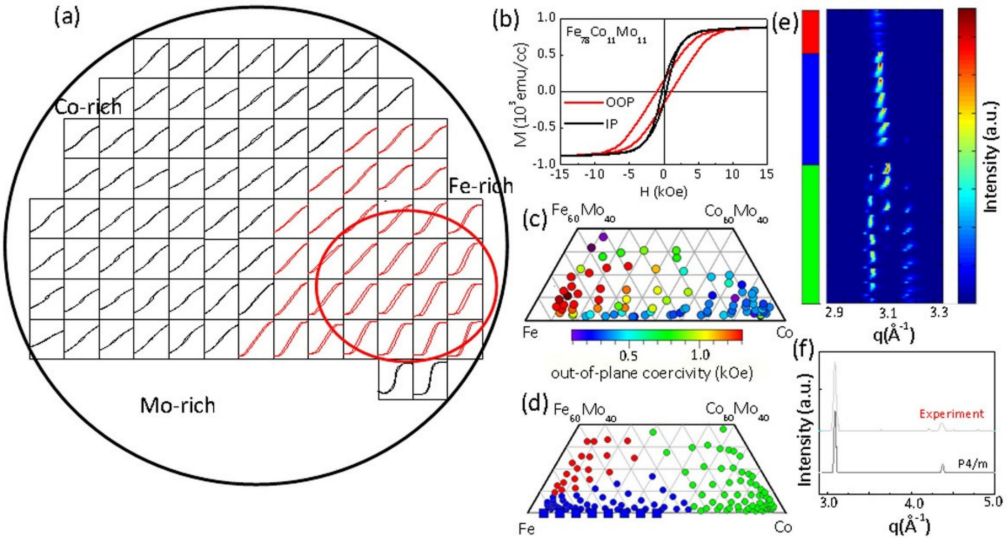

Figure 1. Maps (structural and magnetic) of Fe-Co-Mo: (**a**) hysteresis loops; (**b**) typical out-of-plane (red) and in-plane (black) hysteresis loop of $Fe_{78.4}Co_{10.8}Mo_{10.8}$; (**c**) out-of-plane H_c map of Fe-Co-Mo alloys; (**d**) diffraction data of Fe-Co-Mo; (**e**) intensity plot of X-ray diffraction patterns grouped by cluster result; (**f**) synchrotron X-ray results of $Fe_{78}Co_{11}Mo_{11}$ and calculated diffraction pattern. Further information available in [15]. The work is licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License (https://creativecommons.org/licenses/by-nc-sa/4.0/ accessed on 12 March 2021).

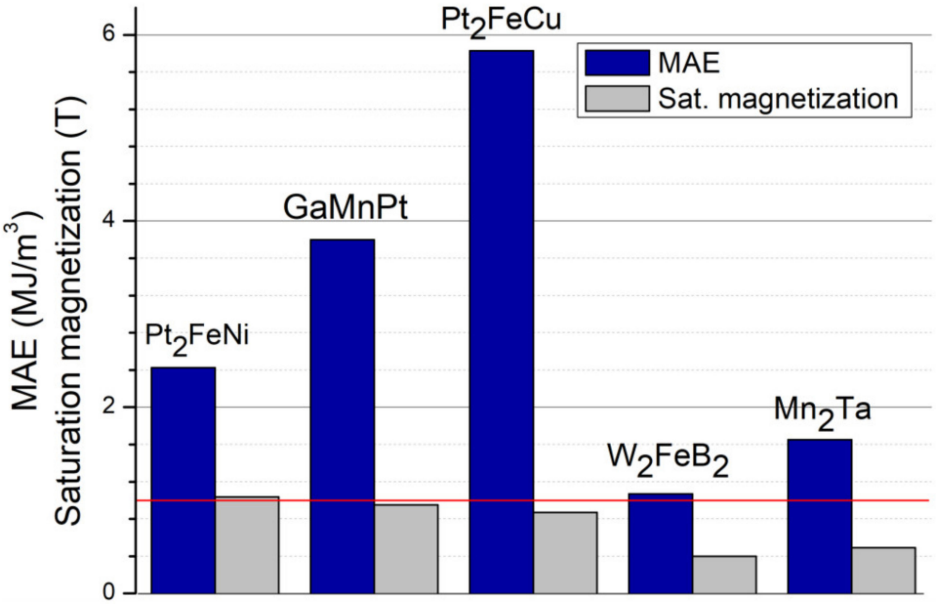

Figure 2. Magnetocrystalline anisotropy energy and saturation magnetization (polarization) of previously researched (Pt2FeNi) of potential candidates for PM. Red line indicates the threshold for a potentially successful PM. Further information available in [16]. This article or its components is available under the terms of the Creative Commons Attribution 4.0 International License (https://creativecommons.org/licenses/by-nc-sa/4.0/ accessed on 12 March 2021).

In the space of soft magnetic materials, where efforts are focused toward the minimization of magnetic losses [17], it is surprising that activities have been concentrated on amorphous and nanocrystalline alloys since, by volume, major market utilization occurs with Fe-Si (e.g., industrial motors, generators, transformers), Fe-Ni (e.g., shielding), and Fe-Co-V (e.g., aerospace) (macro)crystalline alloys. Such fact might be related to the technology maturity of the former, as evidenced by [18], compared to that of amorphous/nano-based counterparts. In this scenario, ML regression models have been trained to predict satu-

ration polarization J_s, intrinsic coercivity H_c, and magnetostriction λ of nanocrystalline Finemet (Fe-Si-B)-based alloys utilizing data mined from technical literature combined with experimental verification, as exemplified in Figure 3. Evaluations have considered chemical compositions and correlated them to processing conditions such as annealing temperature and time [19]. Discrepancies have also been noticed between predicted and experimental results [19], which have been attributed to the possibility of using inadequate data or limitations on the implemented (random forest) model(s).

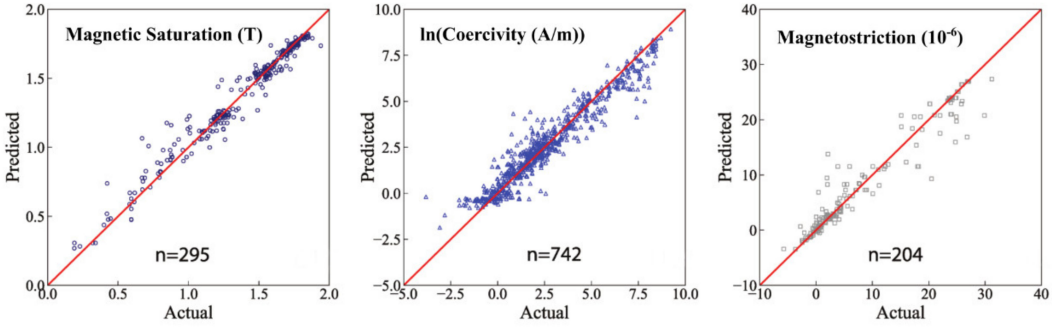

Figure 3. Experimental versus predicted (via machine learning) values of magnetic saturation (polarization), coercivity, and magnetostriction for Finemet-type soft magnetic alloys. Further information available in [19]. Reprinted with permission from Elsevier.

In addition, efforts utilizing ML have also been employed to develop Fe-based metallic glasses with an enhanced combination of Js and thermal stability (typically related to an onset crystallization temperature Tx) as illustrated in Figure 4 [20]. The proposed model, based on intrinsic elemental quantities such as atomic size and electronegativity, has predicted and been verified comparing with experimental data with accuracies above 93% for both Js and Tx, allowing the development of metallic glasses combining Js > 1.4 T and Tx > 800 K.

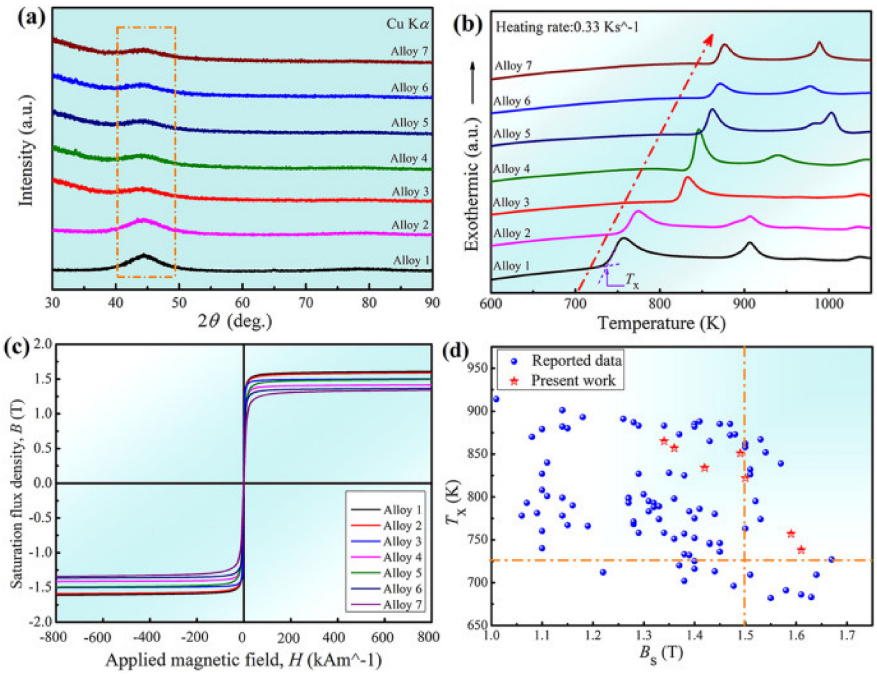

Figure 4. (**a**) X-ray diffraction patterns, (**b**) differential scanning calorimetry curves, (**c**) hysteresis loops, and (**d**) saturation polarization and Tx of designed (modeled via ML) and experimental Fe-based metallic glasses. Further information available in [20]. This article is licensed under a Creative Commons Attribution 4.0 International License (https://creativecommons.org/licenses/by-nc-sa/4.0/ accessed on 12 March 2021).

2.2. Characterization

A second research front addresses the characterization of engineering HSMMs. Traditionally, a physical/chemical approach implementing diffraction/image/elemental, magnetic, thermal, and other techniques gathers information for the system under consideration, and the combination of these results provides a path to tackle posted problems. In the scope of AI–HSMM, the research method still makes use of such an approach, reusing data for training purposes and adding to it AI-related contributions.

In the space of PMs, magnetic stability against temperature and/or demagnetizing fields is always a major concern. The knowledge of switching fields and where they occur provide valuable information on strategies to enhance H_c. Thus, the relevance of microstructural characteristics affecting the magnetization reversal process has been studied focusing on $Nd_2Fe_{14}B$ magnets [21]. Grains on the body edges have been recognized to represent the "weakest links" of the bulk, as illustrated in Figure 5, with a minor influence of other features including, but not limited to, the number of neighbors and sphericity. Consequently, the recognition of these sites allows determining specifically where H_c should be enhanced via, for instance, diffusion processes (already industrially implemented). In a similar scope, AI has also enabled the assessment of the local magnetic nucleation fields, now implementing electron backscatter diffraction data responsible for training supervised learning algorithms, to generate hysteresis curves of Mn-Al-C magnets, as illustrated in Figure 6 [22]. By using micromagnetic simulation of quasi-3D systems based on 2D images, the influence of microstructural features such as crystallographic orientation and size of grains have been assessed to identify "weak" regions of the magnet and identify partial dependences on the relations of such features to predict magnetic results.

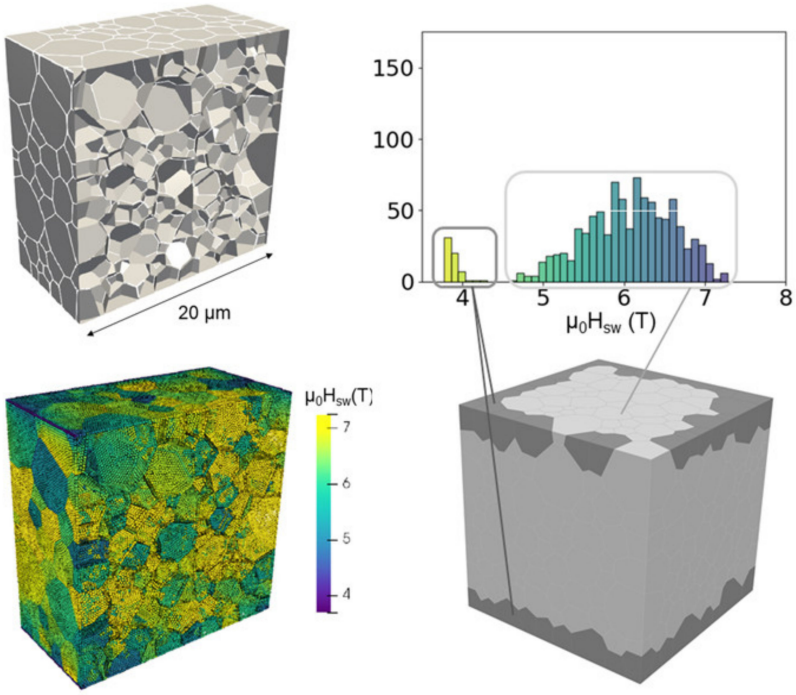

Figure 5. Representation of structure with identification of grain with lower switching fields (positioned on the edges) [21]. This article is licensed under a Creative Commons Attribution 3.0 License (https://creativecommons.org/licenses/by/3.0/ accessed on 12 March 2021).

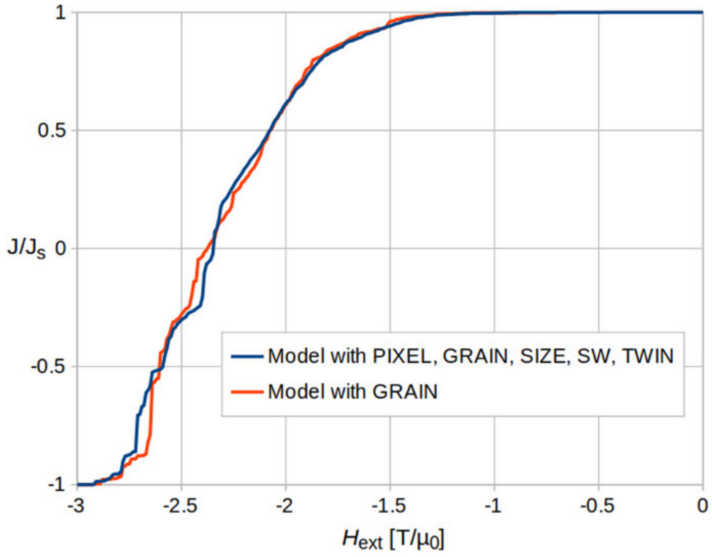

Figure 6. Examples of magnetization curves of Mn-Al-C PM implementing distinct models [22]. This article is licensed under a Creative Commons Attribution 4.0 International License (https://creativecommons.org/licenses/by/4.0/ accessed on 12 March 2021).

In the universe of soft magnetic materials, Finemet-based alloys have also received attention in characterization-related efforts. From the structure-processing standpoint, ML and the calculation of phase diagrams (CALPHAD) approach were combined to scrutinize relationships between processing (e.g., composition, temperature, and annealing time) and structural (mean radius and volume fraction of Fe_3Si phase) parameters [23]. Models implementing the k-nearest neighbor algorithm indicated that specific combinations of temperatures and chemical compositions lead to nanocrystals of pre-determined mean radius applying short annealing times (0.5 h), as exemplified in Figure 7, whereas volume fractions above 70% can be obtained for a broader temperature window and annealing times (>0.5 h), although it narrows the potential selection of chemical compositions.

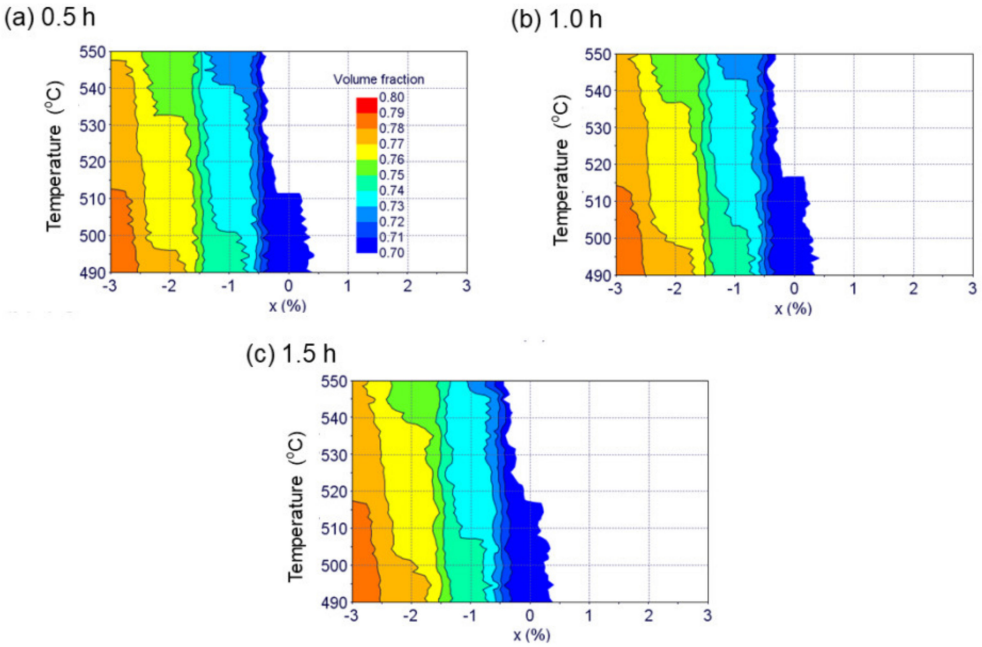

Figure 7. Example of volume fractions of nanocrystalline phase predicted after distinct periods of annealing time ((**a**): 0.5 h; (**b**): 1.0 h; (**c**): 1.5 h) as a function of different Fe and Si (x %) content [23]. Reprinted with permission from Elsevier.

Within the crystalline soft magnetic alloys space, ML has been explored with image processing (a typical utilization of AI). As illustrated in Figure 8, 1.26% Si non-grain-oriented steel photomicrographs have been classified considering crystallographic texture and hysteresis curves data to assist in the identification of higher efficiency materials [24]. Implementing the concept of transfer learning, together with the convolutional neural network used as feature extractors, it is shown that a specific architecture with k-nearest neighbors classifiers enables 100% accuracy in identifying lower losses materials within a fraction of a second. Results of comparable nature can also be found in the literature [25,26] with reported accuracy (constantly) superior to 88%. Furthermore, it is also worth noting that mechanical performance of stamped steels has been evaluated via nondestructive magnetic data collection processes [27]. Due to variations among batches of industrial coils (rolls), suppliers have a growing interest in real-time quality control. The use of a "micromagnetic characterization system" is claimed to identify mechanical properties using polynomial equations from magnetic properties, monitoring for instance yield strength variation of steel strips from a single coil (roll).

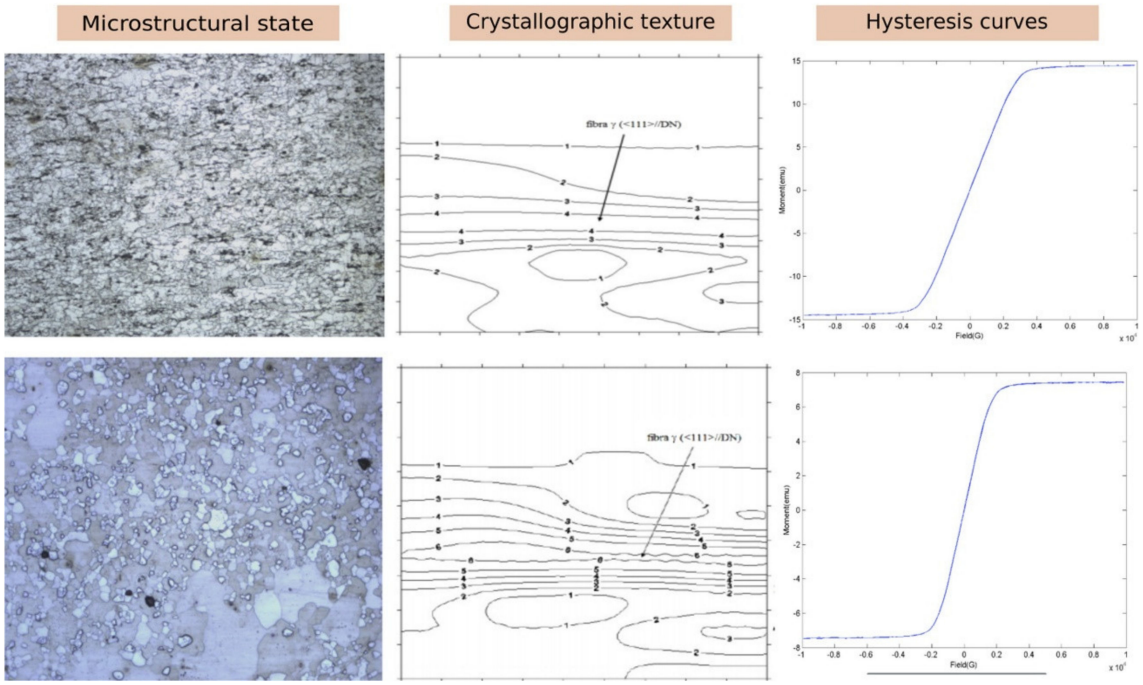

Figure 8. Conventional forms of characterization typically implemented in the manufacturing of electrical steels. Micrographs have been used to separate lower= and higher-efficiency materials [24]. This article is published under the terms of the Creative Commons Attribution-Non-Commercial-No Derivatives License (CC BY NC ND) (https://creativecommons.org/licenses/by-nc-nd/4.0/ accessed on 12 March 2021).

2.3. Applications

The third front that explores interactions AI–HSMM addresses the implementation of such materials. Different from the two previous pillars where data treatment/assessment considers mainly a magnetic compound and its respective physical/chemical features, this last front combines—directly or indirectly—material's properties to end-use conditions/performance. Despite specific results related to materials be apparently limited, it is still possible to capture AI potential in relevant cases.

Dealing with electromagnetic applications, a fundamental quantity always involved refers to a magnetic field. In this scope, the feasibility of predicting Maxwell's equations solutions for a coil, transformer, and interior permanent magnet motor has been investigated and is illustrated in Figure 9 [28]. Based on empirical evidence data generated from finite elements, a convolutional neural network was trained to map magnetic field distri-

butions. The developed model was capable to approximate field distributions positively, compared to finite element analysis results. In a similar way, AI is supporting the design of geometries aiming at the minimization of losses of individual soft magnetic components. In the example of inductors, it has been possible to verify several designs considering inductance value restrictions and geometric dimensions, finding "automatically" a set of optimal characteristics focusing on ferrite-based materials [29]. It is interesting to note that this has reduced the time to complete such development, but also investments required for prototyping (e.g., preparation and construction of molds for experimental trials).

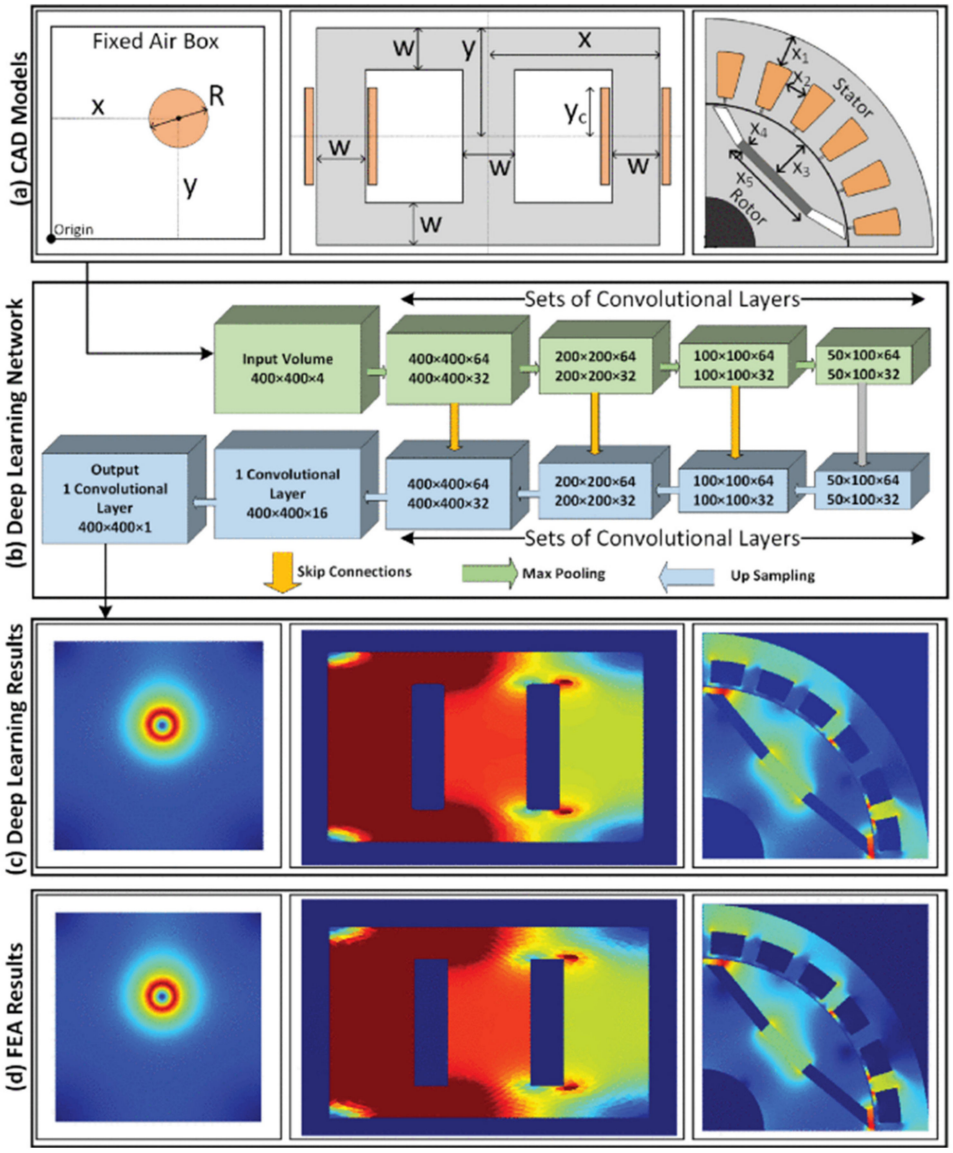

Figure 9. (**a**) Geometrical definitions, (**b**) learning network, (**c**) field predictions, (**d**) finite element results [28]. Reprinted with permission from IEEE.

3. AI—Engineering Hard and Soft Magnetic Materials: Summarizing the Present and Future Directions

The implementation of AI in the discovery and/or properties prediction, characterization, and applicability of engineering hard and soft magnetic materials has been addressed. Value propositions and/or features for each front have been identified and summarized by theoretical—often combined with experimental—results, illustrating AI–HSMM status.

In the discovery/properties prediction space, two paths have been pursued implementing (mainly) machine learning: (i) delineation of AI capabilities so that known results can serve as the base to provide guidance and validate novel developments (e.g., presence of weakest grains on the surface of hard magnets) and (ii) (full) anticipation of novel phases. Thermodynamic stability, combined with magnetic performance, also constitutes examples of typical information able to be acquired. The (material) characterization context currently brings interesting opportunities for enhancing quality control: training algorithms with microstructures representing materials with different features, as in the case of magnetic losses for electrical steels, but potentially applicable to others as intrinsic coercivity of permanent magnets (as exemplified in [30]) has the potential to support industry in further refinements of process control. Lastly, in the space of applications, there is apparently a limited implementation of AI linked to magnetic materials per se, although it is already possible to confirm its value in predicting results in both individual components, as inductors, and (sub)systems such as industrial motors.

The progress of AI–HSMM might be envisaged to be driven by exploring some specific fronts. The first one refers to the development of ultra-low coercivity materials, combined with saturation polarization above 1.8 T and processes that enable their mass manufacturing. This topic will continue to gain industrial relevance considering that requirements for higher energy efficiency have become more demanding from governmental agencies as well as from end users. Here, if AI can be used to explore combinations of cost-accessible materials, comparable to silicon steels, and manufacturing conditions monitoring power losses as main output (in a faster and more predictive in nature that commonly implemented with the (factorial) design of experiments), technoeconomic impacts will be unique. Within such scope, signs of progress could also be envisaged when additive manufacturing is considered: by now, the development of systems dedicated for the processing of soft magnetic materials (and especially products manufactured by them) are still very limited.

In the space of applications, convergence between finite element analysis and AI has the potential to be disruptive: results from the former constitute today the base of traditional designs of novel developments (e.g., industrial motors); however, if associated with AI rising capabilities, such combination might build a faster new normal in exploring electromagnetic phenomena and their engineering.

Lastly, it is worth noting that although the focus of this text is mainly on engineering hard and soft magnetic materials, AI has also been implemented in activities scrutinizing other relevant topics, such as chiral magnets [31], 2D magnets [32], and ferromagnetic compounds [33].

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