Agentic AI's Role in True Materials Discovery

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Abstract

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Materials discovery has driven invention throughout civilization [1]. Metal alloys allowed for complex tools and tall buildings, semiconductors allows for modern electronics, even the ability to widely produce aluminum allowed for modern aviation. However, this process of discovery has traditionally been quite slow. Even modern materials data sources such as MMPDS [2] have evolved modestly since their creation nearly a century ago [3].

Materials are folded into engineering design in two primary ways. The first is materials selection [4]. In this an engineer selects the best material for a part, component, or machine element. This selection is often sub optimal, in that to meet one critical specification often performance is sacrificed in areas with more margin of safety. For example, a system may need high strength and high thermal conductivity. To achieve high strength a steel or titanium is appropriate. To achieve high conductivity a copper or brass is better. If the margin of safety is negative for strength and positive for temperature, then a steel may be chosen at the lost of some temperature margin. It is a discrete choice of material. Often this choice is more subtile, for example an engineer choosing a 304 stainless steel versus a 304L stainless steel. The choice requires substantial product, design, manufacturing, and material knowledge.

The inverse of this approach is materials design [5]. Here the material is design to best meet all performance goals. Once the goals are determined and a specific material system is chosen (e.g., steel, aluminum, ceramic, polymer,Triply periodic minimal surface structures, etc), then a materials expert (usually with vast experience, also maybe a PhD) designs and develops that material using Integrated Computational Materials Engineering (ICME) [6]. This takes time and expertise, but allows for continuous variation in materials properties. However, it requires a scientist with expertise beyond the traditional design/manufacturing process and once the materials design in begun there is little possibility the jump to another material system.

Marquette's Computational Mechanics of Materials Laboratory and Shock Physics Laboratory had pioneered the use of statistical machine learning and data driven techniques to design and optimize Triply Periodic Minimal Surface (TPMS) structures [7] and other micro-architectured [8] and under-dense materials as well as other modern alloys (such as shape memory alloys [9] and ultraviolet sensitive resins [10]).

Specifically Marquette sees vast applications of TPMS structures. They are light weight while maintaining strength while moving above the diagonal line on an Ashby plot. They appear to have many energy applications. They look like radiators, they do not have the stress concentrations that would drive cracking in energy materials. They are 3D-printed to match an equation that is easy to modify. So they can be designed for specific heat transfer and energy goals. Since each system has an equation, they appear to be the best way to start jumping between material systems. They may act as a sandbox to play with materials design and discovery.

Machine learning tools can optimize within a material system. This, like materials design, is mostly a continuous problem. You can change the scale of pores continuously, you can change heat treatment times and temperatures continuously, you can change alloying concentrations continuously. The more difficult problem is when to jump to a new process (i.e., High-Purity VAR (HP-VAR) vs standard-grade VAR (SG-VAR) [1]) or when to jump to a new material system (i.e., go from copper to GRCOP).

To make this jump is discrete (harder to optimize with traditional optimization methods) and often more subjective. Ideally one could ask a materials expert when to jump to a new material or process. However, this can be difficult for a design engineering company (how many materials experts do they have?) and even the best materials experts may not have read the most recent article (e.g., that came out yesterday). What is needed is someone to ask " Do I jump to a new system" who can answer *yes/no* but also tell you how to move they data you have collected to the new system.

Agentic-AI may be the solution to *jumping* between material systems. It can reason and act in more subjective ways than supervised machine learning—all while incorporating all of your current data and the newest advances in literature. It will not replace the materials expert, but make the materials design process more agile and extensible. Again, while it will not replace the materials expert, it can open their blind spots, it can open new ideas, while ultimately lead to true materials discovery. Thus, Agentic AI-driven design of materials appears to be the best way to jump between materials systems.

References

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