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FIELD GRAND CHALLENGE
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Grand Challenges in Metals and Alloys

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Editorial on the Research Topic

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INTRODUCTION

Metals and alloys have always been a staple of civilization, so much so that various epochs have been named after them: The Copper or Chalcolithic Age, the Bronze Age, and the Iron Age. Not only did people in the Ancient World develop the capability to melt these metals and alloys, they were also able to engineer them in quite sophisticated ways. For example, some bronze swords made in China during the Warring Sates period (475-221 B.C.) had a higher tin content on the blade's surface (17–21 at. %) compared to the center of the blade (10 at. %). This higher tin content provided both greater precipitation strengthening and solid solution strengthening, which gave the blade a harder edge that could better hold its sharpness. The higher tin content also made the sword's edge somewhat brittle, a deleterious effect that was mitigated by the softer, more ductile core (Baker, 2018).

One issue with bronze swords was that the components of bronze, tin and copper, are rarely found together geographically in the Earth's crust. Hence, supplies of the critical tin component were acquired from far-flung places. For example, tin from what would eventually become the counties of Devon and Cornwall in England is thought to be a source for some of the bronze produced in the Middle East as early as the second millennium B.C. The Phoenicians controlled the tin trade in the Mediterranean for much of the first millennium B.C., driving up the cost for the buyers.

Eventually bronze swords were supplanted by iron swords. This is not because iron swords were better—they weren't—but because iron was far more plentiful (copper, tin and iron are 0.0068, 0.00022, and 6.3% of the Earth's crust, respectively), easier to process (bronze has a lower melting point at 913°C compared to iron's 1538°C, but the innovation of including up to 4.3 wt.% carbon lowers the melting point to a more manageable 1147°C), and cheaper. This scenario was repeated millennia later in the Age of Sail. The mass-produced iron cannons that were manufactured in England starting in the early 18th century were not better than existing bronze cannons. In fact, bronze cannons could be made with thinner walls, were less likely to burst and had a lower coefficient of friction with iron cannonballs, meaning the cannonballs were less likely to stick in the cannon, but iron cannons were much cheaper to mass produce. This contributed to the dominance of the British Navy, as iron cannons were churned out in great quantities to provide 100–110 guns for a first-rate ship of the line (Baker, 2018).

As we look to make improved materials in modern times, there are lessons to be learned from the past. First, a material with an innovative advantage can completely supplant another material. Even though iron swords were worse than bronze swords, they won out on cost and availability, and were eventually developed—as steel swords—to be better than bronze. Thus, when developing new

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materials, better properties are good, but they are not necessarily the reason we select one material over another. A lower cost material that does the job adequately may be more desirable. Second, as tin could be considered as a strategic element before the development of iron, a different set of elements have now become strategic (Provis, 2015). Today we have strategic materials because of their origin or their rarity in the Earth's crust (Igogo et al., 2019). This raises the question as to whether new materials should be developed with such strategic elements even if they offer improved properties. Fortunately, opportunities exist to replace some strategic elements with the development of new alloys.

MATERIALS PROBLEMS

Practical challenges exist throughout society that could be solved or improved with better materials. With increasing global demand for sustainable energy and healthcare, two major areas of challenge in the 21st century are improved materials for energy applications and biomedical applications.

Energy Materials

In the energy sphere, almost every energy-related technology is limited by materials. Alloys that are resistant to creep, oxidation, and corrosion that can operate at higher temperatures than current alloys are needed so that the Carnot efficiency can be improved in steam turbine systems in power plants. For example, the martensitic/ferritic alloys that are currently used in power plants limit the operating temperatures to ≤600°C, limiting the efficiency to <40%. New materials, such as alumina-forming austenitic stainless steels, are needed to enable increases in operating temperatures to 750°C and improvements in efficiency to >50% (Viswanathan and Bakker, 2000). Affordable materials that can satisfy these requirements may also find use in supercritical CO_2 cycles and in tubing for concentrated thermal solar power. Another example is nickel-based superalloys, which were invented in the 1940's for use in gas turbine discs and blades and were subsequently developed as Nimonic alloys in the United Kingdom, Tinidur alloys in Germany, and Inconel alloys in the United States. The usable operating temperature of superalloys has steadily increased through both changes in composition and microstructural control (the change from equiaxed polycrystals to directionally-solidified elongated grains to single crystals). However, further significant increases in the operating temperature of Ni-based superalloys are unlikely since they are used very close to their melting point. To overcome this limit, many new metallic materials have been and are being explored, from intermetallics to refractory alloys, that can be used in gas turbines at higher operating temperatures.

Steam turbines and gas turbines applications are obvious uses for improved high temperature materials, but affordable higher temperature alloys would also be useful in internal combustion engines. And, of course, for transportation applications, lighter high-strength alloys can improve fuel efficiency by lowering vehicle weights. Recently, this has occurred through the incorporation of both magnesium and more particularly aluminum alloys into electric vehicles. Even the best-selling vehicle in the United States, the Ford F150, is made mostly of 6,000 series aluminum alloys. However, steels continue to be used in vehicles because of their lower cost and in some case higher yield strength-to-weight ratio than aluminum alloys (Author Anonymous, 2021).

New alloys are not only needed for structural applications (Provis, 2015) but for functional energy applications as well. Demand for high-performance permanent magnets for motors is increasing rapidly in areas such as wind turbine generators and motors in both electric and hybrid cars. The rare Earth-based magnets, Sm-Co and Nd-Fe-B, are currently used for such challenging applications. For example, a typical wind turbine generator uses 250 kg of Nd while each Toyota Prius uses 1 kg of Nd. While these rare Earth magnets have the highest energy product, $(BH)_{max}$, of any material they are not without problems. For example, sintered $Nd_2Fe_{14}B$ is vulnerable to grain boundary corrosion, while Sm-Co magnets are quite brittle, prone to chipping and can fracture from thermal shock. Further issues with these materials are that over 95% of the strategic rare Earth metals are produced in a single country, and their price has been extremely volatile in recent years. For example, the price of dysprosium, which may be up to 6 at. % in some Nd-Fe-B magnets, hovered at less than $100/kg during the early 2000's, began a steady rise to around $150/kg until 2010, and jumped to nearly $3,500/kg in 2011 before falling thereafter. Mining of rare Earth metals is associated with severe environmental degradation and large energy usage for their extraction and processing due to the low concentrations of the elements in the ores. New permanent magnets that are significantly less expensive could prove useful even if they have a slightly lower $(BH)_{max}$. For example, ordered tetragonal NiFe has a comparable estimated energy product to Nd-Fe-B and Sm-Co magnets (40–64 MGOe for NiFe vs. 45 MGOe for $Nd_2Fe_{14}B$ and 30 MGOe for Sm-Co), and is much cheaper. The issue is that NiFe only transforms from the high-temperature f.c.c. phase at temperatures below about 320°C and, thus, orders too slowly for commercial use. New processing techniques or judicious alloying may produce usable NiFe permanent magnets.

Application of modern power electronics has the potential to reduce world energy consumption by 20%. However, neither the current high-performance amorphous, e.g., $Fe_{80}B_{20}$, nor nanocrystalline, e.g., HITPERM, NANOPERM, and FINEMET, soft magnets have the magnetic properties at higher temperatures to enable the full potential of wide bandgap semiconductors to be realized (McHenry et al., 1999; Silveyra et al., 2018). These semiconductors are needed for the next generation of power electronics and various electrical machines, including electric aircraft. Amorphous soft magnets were developed over 50 years ago and the development of nanocrystalline soft magnets started in 1988. New soft magnets based on high entropy alloys are showing promise to surpass the amorphous and nanocrystalline soft magnets, but further development is needed.

Thermoelectric alloys for energy harvesting are another area ripe for development, as these materials can be used for energy harvesting from waste heat as well as for refrigeration. Intermetallic compounds such as Bi_2Te_3 and PbTe are among the best metallic thermoelectric materials. However, their use is limited by the scarcity of tellurium and the toxicity of both tellurium and lead. This is a common problem with many thermoelectrics: they require the use of expensive or toxic elements. Half-Heusler alloys, such as NbCoSn, and alloys based on intermetallics such as the Heusler phase Fe_2AlV could offer the advantage of low cost and lack of toxicity but need further development.

Biomedical Materials

Moving on from energy into the biomedical realm, metallic alloys are used in three broad applications in the body: orthopedic implants, trauma fixation hardware, and stents. Various metals and alloys are also used in medical instruments, primarily stainless steel (often 316) but also titanium, tantalum, platinum, palladium, zirconium and gold (Tapscott and Wottowa, 2021).

Orthopedic implants have long been made of stainless steel, titanium, or cobalt-chromium alloys, but each has its own set of issues. First, stainless steels, such as 316L, contain nickel, which can elicit a cutaneous histamine reaction. Second, it is very difficult to polish titanium alloys to a surface finish comparable to other implant alloys. Third, debris particles from the wear of cobalt-chromium implants can produce an immunogenic, and possibly a carcinogenic response. One issue common to all metallic implants is that their high elastic modulus compared to that of bone leads to stress shielding and bone loss: the lower elastic modulus of titanium (110 GPa) compared to stainless steel and cobalt-chromium alloys (190 and 210 GPa, respectively) gives it an advantage in this regard. As populations age, the use of orthopedic implants and replacement implants is increasing, making the need for better alloys more urgent.

Trauma fixation hardware is also made from stainless steel and titanium, but there is growing interest in biodegradable alloys based on magnesium and zinc, particularly for screws and wires, and small bone fracture (Kim et al., 2020). Controlling the corrosion rate of the latter materials involves judicious alloying, particularly so that large quantities of hydrogen do not evolve in the case the corrosion of magnesium alloys, and so that the alloys retain sufficient strength as they corrode to prevent premature refracturing. Tantalum is also being considered for trauma fixation hardware.

Finally, most stents are made of vacuum-melted stainless steel (316 VLM) and nickel-titanium shape-memory alloys (which are self-expanding) both of which can have issues with the nickel allergy noted earlier (Mani et al., 2007). Other materials that have been used or considered for stents are platinum-iridium alloys, tantalum, and commercially-pure titanium. There is interest in biodegradable stents based on high-purity iron and magnesium alloys. Again, this is likely to be an area of growing usage and an opportunity for new materials to present an advantage over those currently in use.

MATERIALS SOLUTIONS

While in the above section we focused on energy applications and biomedical applications there are many other areas where there are materials challenges. For example, the wear, and corrosion that slowly break down materials cost the world economy hundreds of billions of dollars per year. Thus, there are challenges for developing new or improved alloys in all sectors of the economy with improved durability and corrosion resistance as well as reduced cost. Such developments will, no doubt involve the traditional approaches of experience and serendipity. The 2015 Report from the Basic Energy Sciences Advisory Committee (Hemminger et al., 2015) “Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science” points out several challenges to moving Materials Science forward, including “Mastering Hierarchical Architectures and Beyond-Equilibrium Matter”; “Understanding the Critical Roles of Heterogeneity, Interfaces, and Disorder”; “Revolutionary Advances in Models, Mathematics, Algorithms, Data, and Computing”; and “Imaging across Multiple Length Scales”.

Many recent advances are driving new alloy development. The use of *ab initio* calculations to find new materials and predict their properties, such as corrosion behavior and saturation magnetization, is proceeding rapidly. Machine learning is also of growing interest for developing and optimizing alloys (Butler et al., 2018), although a problem here is that researchers tend only to publish papers on good alloys and not on bad ones. Complete training of models using both good and bad alloys is necessary to teach artificial intelligence programs how to identify promising new alloys. Calculations based on thermodynamic data using a variety of commercial databases are also useful for developing new alloys, although their accuracy is limited for non-traditional alloys due to the lack of available data. A variety of additive manufacturing techniques is moving sustainable, low-waste processing forward and leading to the development of new alloys which are more amenable to additive manufacturing than some traditional alloys. Additive manufacturing will also be useful for producing gradient materials that could lead to advances in biomedical applications. Advanced microstructural characterization techniques, such as aberration-corrected transmission electron microscopy and atom probe tomography using a local electrode, have become commonplace and enhance our understanding of microstructural evolution. New ways of thinking about alloy development are also the basis of many new developments in alloy design, as embodied in the ideas of high entropy or multi-principal component alloys that are not based on one particular metal, but based on several metals (Cantor et al., 2004; Yeh et al., 2004; Baker et al., 2019). The Combinatorial Materials Science approach could accelerate the development of such alloys.

CONCLUSION: THE ROLE OF THIS JOURNAL

This brings us to the role of this new journal on metals and alloys. The journal will not only focus on fundamental Materials Science but also on commercial applications. It will help identify where new materials offer a key advantage over those currently in use. It will publish theoretical and modeling papers and also papers on experimental work, and will be especially interested in papers that combine the two. New processing techniques will be of interest along with advanced microstructural characterization methods, particularly techniques that involve dynamic characterization. The journal will cover both physical properties and mechanical properties of metals and alloys. Of particular interest will be materials of commercial importance that can be produced in environmentally-friendly ways that are sustainable. Finally, the journal will be open-access so that the published research is available to the widest possible audience.

AUTHOR CONTRIBUTIONS

IB developed the conceptual content and wrote the document.

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