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Material Challenges in Developing a Sustainable Metal Processing Infrastructure - Workshop Report

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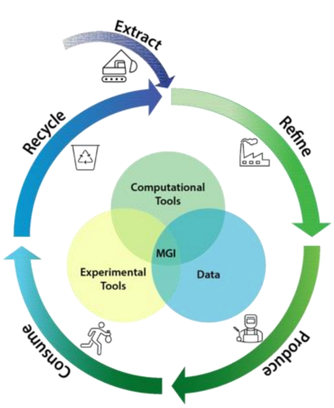

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Abstract

As metals and manufacturing industries continue to transition towards sustainable and circular principles, innovations are needed to address a variety of challenges. Multidisciplinary solutions are required across the materials lifecycle, from extraction, alloy design, manufacturing, reuse, and recycling. This special publication draws upon insights acquired from a NIST workshop held in July 2024 that convened experts from government, academia, and industry to identify challenges and opportunities for establishing a sustainable metals industry. The workshop emphasized the critical role of advanced extractive metallurgy, integrated computational materials engineering (ICME), and digital data infrastructures in accelerating the development of processing pathways and sustainable alloy design. Discussion about key materials systems included aluminum, steel, and critical materials. The workshop highlighted the need to redesign alloys to tolerate higher impurity contents, develop energy efficient extraction technologies, and optimize process-structure-property relationships to enhance material performance. Molten oxide electrolysis for steelmaking, recovery of valuable elements from metallurgical waste streams, and alloy design for high-recycled-content aluminum die castings are examples of specific areas for investment that were identified. The aluminum and steel sectors were examined as critical case studies, each facing unique challenges for developing a sustainable processing infrastructure, recycling integration, and maintaining performance amid rising impurity levels. The role of sustainable manufacturing was highlighted in the context of automotive applications, where life cycle assessment (LCA), high-volume closed-loop recycling, and new casting technologies are reshaping how metals are sourced and processed. Workforce development and educational revitalization emerged as essential enablers for ensuring that the U.S. maintains its capacity for innovation in extractive metallurgy and materials design. In summary, this document captures pathways toward a resilient and sustainable metals processing economy to meet future industry needs.

Keywords

Alloy Design, Circular Economy, Critical Materials, Extractive Metallurgy, Steel, Aluminum, Integrated Computational Materials Engineering, Life Cycle Assessment, Recycling, Sustainable Manufacturing.

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1. Introduction

As advanced manufacturing continues to evolve and infrastructure resilience becomes a priority, the demand for sustainable metals processing is growing. At the same time, the critical materials global supply chains are increasingly strained, raising concerns about their long-term resilience and sustainability. Addressing these challenges requires a fundamental shift in how to source, process, use, and recover metals, replacing linear production systems with more sustainable and circular approaches.

To identify key technology and metrology opportunities, the National Institute of Standards and Technology (NIST) hosted the workshop, "Material Challenges in Developing a Sustainable Metal Processing Infrastructure" on July 30th and 31st, 2024. The workshop brought leading experts from industry, government, and academia together to examine the pressing issues in critical materials supply, sustainable extractive metallurgy, alloy design, computational tools, manufacturing practices, and recycling technologies.

This document is a compilation of the seven topics covered at the workshop. Each section is a summary of the key technical considerations discussed for building a metal processing infrastructure that supports innovation, circularity, and national competitiveness. The topics covered included:

- **Critical Materials,** highlighting national initiatives for securing essential critical materials like lithium and cobalt through federal coordination, risk assessments, innovation hubs, and domestic investment.
- **Extractive Metallurgy,** for recovering critical materials from mining and industrial waste, including hydrometallurgical and electrochemical processes, emphasizing the need for revitalizing U.S. extractive metallurgy educational and workforce development programs.
- **Aluminum,** highlighting the importance of increasing recycled content in aluminum alloys while overcoming technical challenges related to impurities and legacy alloy regulations that limit the incorporation of scrap into smelted aluminum products.
- **Integrated Computational Materials Engineering and Data,** exploring the role of computational tools and materials modeling in alloy design, process optimization, and data integration to enable more efficient and sustainable production of materials.
- **Steel,** presenting emerging iron and steelmaking technologies, such as molten oxide electrolysis and hydrogen-based reduction, alongside strategies to manage scrap quality and alloy performance.
- **Sustainable Manufacturing,** highlighting the use of life cycle assessment to guide direct and indirect sustainability efforts, both of which are explored within the automotive and additive manufacturing sectors.
- **Recycling and Reuse,** outlining the economic and technical challenges in end-of-life material recovery, presenting promising strategies for improving separation and use of

recycled feedstocks, and highlighting the need for standards and certification frameworks to ensure performance of products made with recycled content.

2. Critical Materials

Critical materials (including critical minerals) are essential to the U.S. economy, having unique properties that enable technologies such as microelectronics, batteries, magnets, electrical steels[1] used in electric vehicles, and renewable energy. Critical materials such as lithium, cobalt, nickel, and rare earth elements are in particularly high demand, yet their supply chains are often heavily concentrated in a small number of countries, thereby creating significant geopolitical and economic risks. The cost and timeline for the development of new production capabilities for these materials are frequently underestimated, creating additional risks in the supply chain. While some materials could become less critical over time due to the emergence of leapfrog technologies (e.g., the transition from compact fluorescent lighting to light-emitting diodes), the overall urgency remains to establish secure, resilient, and sustainable material supply chains. This section captures the key themes in critical materials that were presented and discussed during the workshop.

2.1. Federal Strategy and Definition of Critical Minerals

Recognizing the strategic importance of these materials, Congress codified the definition of "critical minerals" into federal law through the Energy Act of 2020 [1], which defines a critical mineral as a non-fuel mineral or mineral material essential to the economic or national security of the United States that has a supply chain vulnerable to disruption. Within this Act, both the U.S. Geological Survey (USGS) and the U.S. Department of Energy (DOE) were assigned distinct yet complementary responsibilities. The USGS is tasked with identifying and assessing critical mineral resources, while the DOE is tasked with advancing research, development, and commercialization strategies to diversify supply, develop substitutes, and enable circular material use. At the workshop, both the USGS and DOE provided presentations that highlighted their complementary roles within the critical materials space.

2.2. The U.S. Critical Minerals List - USGS

The USGS discussed the U.S. Critical Mineral List (CML) [2], which is updated every three years in coordination with other federal agencies. This list is key for identifying and managing the mineral supply chain vulnerabilities that are essential to the U.S. economy. The methodology used to determine the list of mineral commodities is based on the importance of the minerals to the U.S. economy and national security, and the potential impact of supply chain disruptions. The current list, updated in 2022, contains 50 mineral commodities. The CML is a key tool for federal agencies to guide research priorities and policy decisions. It also informs the decisions of U.S. industries related to material diversification, substitution, and recycling.

[1] An electrical steel is an alloy engineered specifically for optimal magnetic performance. These steels are widely used in the cores of transformers, motors, and generators to enhance energy efficiency and reduce heat generation.

2.3. Critical Materials Assessment - DOE

DOE presented a summary of their Critical Materials Assessment, which evaluates critical materials that are important to the energy sector. The 2023 assessment [3] evaluates the supply risks and importance of critical materials used in clean energy technologies. This assessment is based on U.S. national priorities, technology progression, and technology implementation directions. It builds upon prior DOE studies by incorporating updated market trends, geopolitical conditions, and technology deployment scenarios projected through 2035.

Unlike broader geological assessments, the DOE's analysis is application-driven, focusing on how material availability affects specific technologies such as electric vehicles, wind turbines, hydrogen electrolyzers, and power electronics. The report uses a structured methodology that evaluates materials based on their importance to energy technologies, supply risk, and the impact of supply disruptions, resulting in a tiered classification of materials into short-term and medium-term criticality categories.

The 2023 assessment highlights a growing set of materials as high-risk and high-importance, particularly those involved in batteries (e.g., lithium, cobalt, nickel, graphite), permanent magnets (e.g., neodymium, dysprosium, terbium), and energy production (e.g., solar cells: silicon, tellurium, and indium/gallium). It also identifies emerging vulnerabilities in materials not historically considered critical, such as aluminum, copper, and electrical steel, due to their increasing use in electrification and energy infrastructure. Beyond identification, the DOE outlines strategies to address risks, including substitution, efficiency improvements, recycling, and supply chain diversification. The report serves as a foundation for DOE's investment priorities in research and development (R&D) and informs cross-agency efforts to enhance critical material security for the U.S. energy sector.

2.4. Critical Materials Innovation Hub

The DOE's Critical Materials Innovation (CMI) Hub [4], established in 2013 at Ames National Laboratory, is a research consortium focused on reducing U.S. dependence on high-risk critical materials. Initially, the organization targeted rare earth elements used in magnets and lighting, such as dysprosium, terbium, europium, neodymium, and yttrium. More recently, the organization has expanded its scope to include materials essential for batteries and semiconductors, including lithium, cobalt, manganese, graphite, indium, and gallium. The CMI supports DOE's strategic objectives by advancing research that enables the substitution of critical materials with more abundant alternatives, improves material recovery through next-generation recycling technologies, and strengthens supply chain resilience through diversification and domestic sourcing strategies.

CMI's work is organized into four core research areas: diversification of supply, development of substitutes, unlocking secondary sources, and crosscutting research. Enhancing and diversifying supply is achieved through expanding sources, developing transformative processes, and finding new uses for co-products. Developing substitutes focuses on designing products with less critical materials, but still meeting performance needs, such as magnets with less rare-earth content. Unlocking secondary sources focuses on improving manufacturing efficiency, expanding recycling, and optimizing co-production to support technologies like energy storage systems and electric machines. Crosscutting research advances new tools to forecast future critical material needs, supports enabling science, and drives environmental sustainability, supply chain security, and economic analysis.

2.5. Case Studies in Critical Material Supply Chain Vulnerability: Lithium and Cobalt

Lithium was highlighted in the workshop as an example of a critical material used within several key industrial sectors. While lithium is mined globally, the majority of lithium refinement capacity is currently located within China [5]. In 2015, the growth in clean energy technology began driving changes in the lithium global supply chains. By 2018, the increased demand for electric vehicle batteries and increased Australian lithium production resulted in a complete restructuring of the global market [6]. This three-year period highlights how sustained demand coupled with geopolitical dynamics may rapidly alter the critical material supply and reshape the broader global market.

Cobalt is another critical material that was highlighted, with increasing demand and significant importance across a wide range of industries. This demand is reflected in global mine production, which increased by approximately 375 % from 2000 to 2020 [7]. Much of this growth has been driven by the expansion of battery technologies. In 2000, approximately 50 % of global cobalt end-use was metallurgical grade, used in superalloys and cobalt carbides. By 2020, the market had shifted dramatically, where battery applications now account for the majority of global cobalt end-use [8].

The mining and refining of cobalt are highly concentrated in two countries, creating a supply chain vulnerability. The Democratic Republic of Congo accounts for nearly 76 % of cobalt global mine production [9]. Following extraction, much of this ore concentrate is then shipped to China for refinement, who controls more than 70 % of the global cobalt refinement capacity. The concentration of mining and refining capabilities of cobalt triggered discussions about the resilience and security of cobalt supply chains, particularly for clean energy, defense, and the tech sectors.

While not discussed at the workshop but relevant to this topic, the United States has leveraged the Defense Production Act to initiate strategic investments aimed at increasing North American cobalt mining and refining capacity [10], specifically supporting Electra Battery Materials in the construction of North America's first cobalt sulfate refinery in Temiskaming Shores, Ontario. Once operational, the facility will produce 6,500 tons of battery-grade cobalt sulfate annually, enough to support the production of over one million electric vehicles. The refinery is expected to process cobalt feedstock from emerging mining operations in the western U.S., providing an integrated supply chain within North America for critical battery materials.

3. Sustainable Extractive Metallurgy

As the global demand for metals continues to rise, novel sustainable extractive metallurgy processes have recently emerged to overcome some of the issues with traditional extractive methods. Sustainable extractive metallurgy focuses on minimizing waste, reducing environmental impact, improving circularity, and recovering materials from both primary and secondary sources. This section summarizes key insights from the workshop that include ongoing research into recovering critical minerals from metallurgical waste streams and emerging technologies such as hydrometallurgical and molten oxide electrolysis processes. In addition to technical advancements, the session also emphasized the pressing need to revitalize U.S. educational programs and workforce development in extractive metallurgy to ensure future innovation and industrial competitiveness.

3.1. Extracting Value from Primary Metal Production Waste Streams

The extraction and refinement of ores and minerals for primary metal production generates substantial quantities of mine tailings and other material byproducts, which can accumulate over years. For instance, producing 1 ton of aluminum generates 2 tons to 2.5 tons of bauxite residue [11], contributing to a global accumulation exceeding 3 billion tons. However, workshop speakers challenged participants to think differently about these metallurgical waste streams. Often, they contain minerals in dilute concentrations that could be further extracted to produce valuable materials. Historically, the low concentrations and high energy costs of recovery made disposal the more economical option. However, the drive toward more sustainable and circular supply chains is motivating a reexamination of these waste streams, encouraging new research into sustainable extractive metallurgy.

Bauxite residue was discussed at length in the workshop. A byproduct of primary aluminum production, bauxite residue has significant management challenges due to its high causticity, fine particle size, complex mineralogy, and diverse elemental composition. Despite these challenges, bauxite residue is a potential resource for valuable minerals, with an average chemical composition (% mass fraction) of 5 % to 60 % Fe_2O_3, 5 % to 30 % Al_2O_3, 5 % to 50 % SiO_2, 0.3 % to 15 % TiO_2, 1 % to 10 % Na_2O, and 2 % to 14 % CaO [12]. Researchers from Worcester Polytechnic Institute (WPI) highlighted their recent hydrometallurgical studies that demonstrated the feasibility of a scalable, low-energy extraction process that yields high-purity metal oxides with high recovery rates, unlocking new opportunities for more effective resource utilization [13,14].

Beyond aluminum, other primary metal byproducts present opportunities for resource recovery. Boston Metal highlighted their molten oxide electrolysis technology, which has shown that valuable metals, including niobium, tantalum, and iron, can be effectively extracted from slag byproducts generated from primary tin production. This extractive metallurgy process is set to be commercially deployed by Boston Metal at a pilot demonstration facility in Brazil [15]. Additionally, the USGS is exploring the potential of sustainable extractive metallurgy to recover critical minerals from mined waste. Recent work by USGS has demonstrated that germanium can be characterized in mined waste using non-destructive analytical methods, advancing our understanding of its distribution and informing recovery potential [16].

3.2. U.S. Extractive Metallurgy Educational and Workforce Development

The U.S. extractive metallurgy education and workforce were discussed in depth during a presentation by Colorado School of Mines. The decline in U.S. educational programs dedicated to extractive metallurgy and mineral processing was highlighted. As of spring 2023, only 14 U.S. programs remained, enrolling just 590 undergraduate students, down 60 % from 2015, and graduating an average of only 12 mining engineers per school in 2023 [17]. In contrast, China supports 45 programs with roughly 12,000 students and 3,000 annual graduates [17]. This showcases the widening gap in developing the future extractive metallurgy workforce and presents a significant challenge in maintaining global competitiveness in the field of extractive metallurgy. The limited number of specialized degrees has led to a shortage of skilled professionals. This problem is further exacerbated by the impending retirement of experienced engineers, which threatens to hinder innovation in sustainable extractive metallurgy technologies.

The workshop discussions emphasized that revitalizing educational programs in extractive metallurgy and mineral processing is crucial not only to support a U.S. industrial workforce, but also to bolster the U.S. capacity to lead in the development of advanced and sustainable metallurgical solutions. Collaborative efforts between academia, industry, and government were proposed as essential to establish new degree programs, research centers, and public-private partnerships focused on technology development. These initiatives could position the U.S. as a leader in sustainable metallurgy, enhancing global competitiveness while addressing the growing demand for environmentally responsible resource extraction.

The Center for Resource Recovery and Recycling [18] (CR^3) was highlighted as a leading example of a public-private partnership advancing sustainable metallurgy. CR^3 brings together academic researchers and industry stakeholders to develop innovative technologies that enable the recovery, reuse, and recycling of critical and strategic materials. With university partners including WPI, Colorado School of Mines, and Katholieke Universiteit Leuven, CR^3 focuses on recapturing materials at end-of-life and feeding them back into production, improving industrial waste utilization, and supporting a circular economy in metals. By aligning research objectives with industrial needs, CR^3 helps accelerate the transition toward more sustainable resource use while strengthening domestic materials resilience and workforce development.

In addition to traditional university degree programs, investing in workforce development through targeted short courses and certification programs was presented as a potential solution. Short courses and certification programs can rapidly equip professionals with the skills needed to support industry demands. As discussed at the workshop, through cultivating a pipeline of talent, the U.S. can ensure its ability to innovate and compete globally, fostering economic growth, and secure its position as a leader in sustainable extractive metallurgy.

4. Aluminum

The aluminum industry plays a crucial role in sustainable manufacturing in the U.S. as the demand for aluminum in products continues to grow. However, significant metallurgical challenges exist in the recycling and design of aluminum alloys derived from scrap. The session began with a comprehensive outlook on current and future aluminum production and the vision to produce cleaner, more sustainable aluminum in the upcoming decades. To meet increases in demand, future manufacturing will rely on recycled aluminum to replace primary aluminum production. However, utilization of recycled aluminum presents metallurgical and alloy design challenges that must be addressed for advancing a sustainable aluminum industry.

4.1. Vision of the Aluminum Industry – The Aluminum Association

The Aluminum Association presented their North American Aluminum Decarbonization Roadmap. The roadmap highlighted aluminum production as a key element to the U.S. manufacturing economy, where aluminum products are used across many industrial sectors such as automotive, aerospace, transportation, and construction. Approximately 164,000 workers are currently employed in the aluminum industry, which generates nearly $230 billion annually in economic output in the U.S. [19]. Demand for aluminum and its products continues to grow, resulting in investments totaling over $10 billion in the past decade to facilitate next generation growth. The total demand for aluminum in the U.S. is projected to grow by 80 % by the year 2050 [19].

Speakers highlighted that aluminum production emits approximately 1.1 billion tons of carbon dioxide annually [20], which accounts for about 3 % of global emissions [21]. To reduce environmental impacts, an aluminum trade group has set an ambitious goal to reduce domestic emissions by 92 % by the year 2050 [20]. Domestic production of aluminum will account for 73 % of the projected demand, while the remaining 27 % will be met by net imports [20]. Although North American aluminum production is roughly half as carbon intensive as the rest of the world, the need for importing aluminum to meet demand offsets much of these decarbonization efforts [19].

The increased use of recycled aluminum, as well as innovative technologies that produce clean power, will be required to meet industry goals. The use of scrap materials for aluminum production requires approximately 5 % of the energy used for processing bauxite ore used to make primary aluminum. Therefore, using more recycled material for aluminum parts will significantly decrease energy demands, and a goal has been set to use approximately 71 % of recycled aluminum in new productions by 2050. At the same time, renewable sources of energy are being explored and implemented for processing of aluminum. Some of these new technologies include the use of inert anodes in place of carbon anodes, phasing down the use of natural gas through the electrification of furnaces, and switching fuel from coal or natural gas to hydrogen [20].

4.2. Challenges for Recycled Aluminum Products

Several presentations highlighted the benefits and metallurgical challenges of smelting recycled aluminum over producing primary aluminum. The production of primary aluminum consists of mining, refining, smelting, and fabrication. Bauxite ore is mined from the earth and consists of different oxides including Al_2O_3, Fe_2O_3, and SiO_2. The ores are then refined to produce Al_2O_3, followed by smelting of the Al_2O_3 to produce aluminum and CO_2. The final aluminum is then fabricated into different product forms through wrought or cast processing. Each of these production steps requires significant amounts of energy. On the other hand, production of recycled aluminum requires only smelting, leading to a 95 % reduction of energy.

However there are challenges in using recycled aluminum, the final product quality can vary widely depending on how the material is recycled. The two types of recycling include open-loop recycling, where material is collected but the different alloys are not separated, and closed-loop recycling, where material is collected and separated by the type of aluminum alloy. Closed-loop recycling processes typically involve clean and well-sorted scrap, such as aluminum beverage cans, which can be used to make the original product. In contrast, mixed scrap found in open-loop recycling consists of inconsistent chemical compositions that make the production of new aluminum parts difficult.

A particularly difficult challenge in open-loop recycling is the contamination of the aluminum alloys with iron. Iron contamination in aluminum often leads to the formation of intermetallic phases during solidification since the maximum solubility of iron in aluminum is very low (< 0.04 % mass fraction). These intermetallic phases are generally undesirable and have a negative effect on the properties. When combined with other metallic elements such as manganese, such as in 5XXX series aluminum alloys, iron contamination can often lead to cracks during forming processes [22]. The reduction of iron in recycled aluminum is possible, but the removal of iron generally increases the cost of production, making the overall production process economically unfeasible in some cases. Many similar effects can be seen in aluminum scrap containing other elements, such as silicon and magnesium, where undesirable intermetallic phases precipitate and impact forming processes.

The production of high recycled content aluminum alloys requires an understanding of the impurity effects on the microstructures of the materials and the resulting properties required for forming operations. A general rule-of-thumb in recycled aluminum is that higher impurity contents generally increase strength at the expense of reduced ductility. Consequently, increasing chemical composition specifications to tolerate higher amounts of impurities is often not recommended. Practical approaches to managing recycled content include improving alloy separation processes during scrap sorting, using scrap aluminum for the production of alloys with composition ranges that can tolerate higher amounts of contaminants, and reconsidering or substituting alloys used for certain products that may not have aggressive service conditions.

Government and industry regulations may unintentionally create demand for primary aluminum production because of legacy specifications. One example of a legacy specification, developed decades ago when fewer aluminum alloys were available, is a mandate to use specific grades such as 3003 or 5052 for highway road signs. These alloys typically have strict composition limits and little tolerance for impurities. For example, aluminum alloy 3003 has a low limit for magnesium, meaning recycled 5XXX cannot be absorbed due to the high magnesium content~~s~~. Similarly, aluminum alloy 5052 can tolerate only small amounts of manganese and copper, restricting the use of recycled wrought 5XXX and 3XXX alloys that contain high contents of manganese and copper. Strict limits on impurities and scrap compatibility effectively prevent the use of recycled material, forcing most products with legacy alloy specifications to rely on energy-intensive primary aluminum. Workshop participants discussed whether products like road signs, which commonly specify these alloys, should continue to rely on primary aluminum, or whether regulations should be updated to accommodate greater use of recycled content.

4.3. Sustainable Aluminum Alloy Design

The potential for expanding sustainable aluminum alloy designs, with particular focus on castable aluminum alloys was highlighted. In contrast to wrought aluminum alloys, which are typically lean in solutes and have a low impurity tolerance, cast aluminum products can tolerate more impurities and tend to be rich in solutes. In the automotive industry, internal combustion engine blocks typically serve as a primary application for recycled aluminum due to these characteristics of cast aluminum alloys. The use of recycled aluminum in electric vehicles is currently being researched. A potential application for recycled aluminum involves structural high-pressure die casting (HPDC), although these alloys need to be carefully designed due to the structural requirements of the large castings. Many cast aluminum alloys do not meet the requirements for structural applications of HPDCs, and structural alloys often have a low tolerance for impurities, limiting the use of scrap aluminum. Research into HPDC can also be challenging due to the heterogeneously distributed microstructures and properties in the castings, the cost and time sinks when studying large melts, and the resulting limited ability to study much of the composition space due to the number of alloying elements involved. However, a careful, sustainable approach to the design of aluminum alloys for structural HPDCs can lead to many benefits, including the energy savings from using recycled material, light-weighting of electric vehicles, consolidation of many cast parts, and cost reduction per vehicle.

At Oak Ridge National Laboratory, small-scale experiments using a mixed scrap stream of 5XXX and 6XXX series aluminum alloys are being conducted. This scrap mix reflects the typical composition of aluminum parts from Ford F-150 vehicles that are now approaching end-of-life. The mixture of these aluminum alloy series can be simplified to the aluminum-magnesium-silicon-iron system [23], and the composition ranges can be matched to existing structural cast alloys with similar composition ranges, including alloys such as Magsimal 59, Magsimal Plus, C446F, and Castaduct 42. Of these, Castaduct 42 was first studied by varying the mass fraction of silicon over a range typically seen in an example scrap stream. Increasing the silicon content of these alloys promotes the formation of silicon-containing intermetallic phases, and higher mass fractions result in larger precipitate sizes. The strength did not change significantly, but a clear decrease in ductility was observed with an increase in silicon mass fraction. The loss in ductility is due to the increased phase fraction of the brittle, primary $Al_{13}Fe_4$ intermetallic [24].

Alloy design requires the optimization of several conflicting property objectives, as well as balancing processing efficiency with higher costs. Changes to improve one property often have a negative impact on another, such as the strength-ductility tradeoff seen in many common engineering alloys. Reducing impurity contents may dramatically increase processing costs. As the models and data needed to represent all the processing-structure-property linkages are not always available, alloy development has often been empirical. CALPHAD (Calculation of Phase Diagrams)[2] based computational tools have been instrumental in accelerating alloy development [25].

The effectiveness of a CALPHAD-based alloy design relies heavily on the accuracy of the underlying databases. When investigating a new alloy space, one needs to ensure that the database selected includes all the needed composition space. It is particularly important when considering alloys with higher impurity contents whether a given database is appropriate or may require additional evaluations to accurately represent the higher impurity contents. (That is, a given database may have been evaluated for Al-rich alloys with much lower impurity concentrations, and one may need to modify the phase descriptions to better describe the thermodynamics for higher alloy concentrations.) An example of this was illustrated when evaluating higher Si and Fe contents in Al alloys. In efforts to optimize the processing of Al-Mg alloys with higher Si and Fe impurity contents, initial solidification phase fraction predictions for the $Al_{13}Fe_4$ using various commercial CALPHAD databases contradicted experimental results [24]. After optimizing the thermodynamic database, the Al-Mg-Si-Fe composition space could be used to limit the amount of primary $Al_{13}Fe_4$ that forms during solidification. Three alloys were chosen from the CALPHAD results for experimental validation, and each alloy showed no primary $Al_{13}Fe_4$ formation upon solidifying.

Alternative processing methods were also presented as an attractive means for utilization of sustainable solutions for recycled aluminum alloys. Primary $Al_{13}Fe_4$ is largely undesirable due to its large size and brittle morphology. Manipulation of the particle size and morphology can effectively mitigate the negative impacts of the intermetallic phase on mechanical properties. Additive manufacturing processes, such as laser powder bed fusion, are promising methods for achieving desirable microstructures and properties. The high solidification cooling rates and resulting small solidification structure in as-deposited samples has been shown to limit the size and morphology of primary $Al_{13}Fe_4$ that forms during solidification.

[2] CALPHAD is a phase-based approach to modeling the composition, temperature, and pressure dependence of material properties [25,26].

5. The Role of Integrated Computational Materials Engineering (ICME) and Data in Sustainable Metallurgy

This session highlighted the critical role of computational tools, modeling, and data in advancing sustainable metal processing. ICME integrates materials science, manufacturing processes, and product design, providing a comprehensive framework for developing more sustainable materials and processes. The ICME approaches discussed at the workshop rely on CALPHAD-based tools and databases to help integrate across time and length scales. This section summarizes presentations and discussions at the workshop that outline the key challenges and opportunities for ICME to promote sustainable materials design.

5.1. Applications of ICME

ICME and CALPHAD-based tools, such as Thermo-Calc Software or CompuTherm, can be used to optimize the sustainability of materials by considering their full lifecycle. New materials can be engineered to use less energy and be more recyclable through strategies such as optimizing heat treatments, increasing the use of scrap in primary production, designing for longer in-use lifespans (e.g., improved corrosion or wear resistance), and enhancing recyclability of materials and parts. The audience was challenged to consider how sustainability and recyclability might be more intentionally integrated into existing system design frameworks that link processing, structure, properties, and performance as seen in Figure 1. The question posed was whether sustainability should be considered a new element in this chain, as part of the performance metric, or as part of the processing. The separate "Processing" and "Performance" links indicate some of the additional elements that would be considered in the design process to incorporate sustainability. The "Sustainability" is added to the Processing-Structure-Property-Performance paradigm as a suggestion.

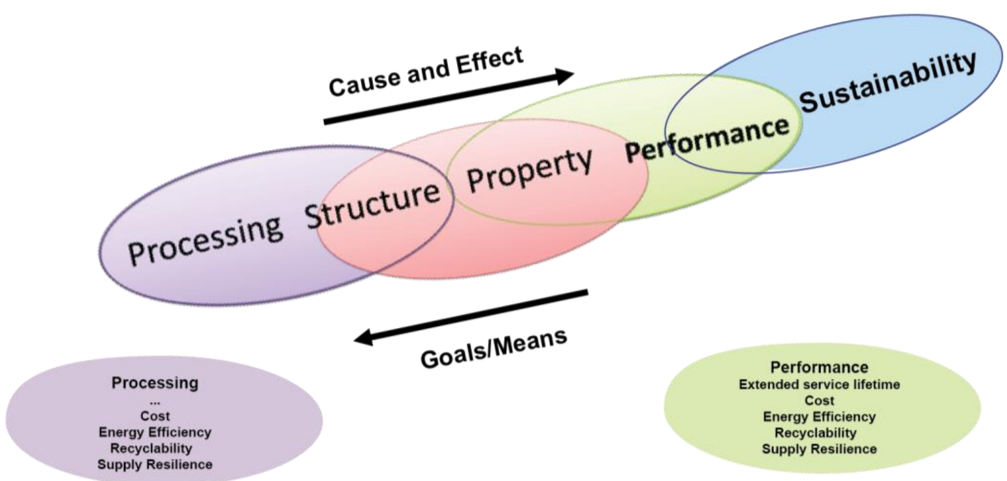

Figure 1. Processing-Structure-Property-Performance Linkages.

One of the biggest challenges in implementing an ICME approach that includes sustainability is having sufficient phase-based data to support the design. While there are several commercial and open source multicomponent thermodynamic and diffusion mobility databases for many of the technologically relevant alloy systems, there is a need to improve the descriptions of impurity elements in these different alloy systems. This need was exemplified in the previous section 4.3 in designing sustainable Al alloys. Further development of other phase-based thermophysical and thermomechanical property data is also required, including liquid viscosities, surface tension, thermal conductivity, electrical resistivity, molar volume, and elastic constants.

Examples illustrating how ICME has supported the development of more sustainable alloys and processing approaches, include designing new alloys to improve high temperature performance of turbine engines and reducing the need for certain critical materials [26]. Another effort to increase aerospace sustainability through alloy design is developing new lightweight TiAl alloys for aerospace applications to reduce emissions and increase part lifetimes as a part of the European Clean Sky 2 initiative [27]. Torralba et al. [28] demonstrated that new high entropy alloys (HEA) could be designed using electronic waste and alloy scrap sources. Navazani et al. [29] investigated using higher contents of Cu in the Al-Cr-Fe-Mn-Ni HEA system that enabled greater fractions of scrap steel, which typically have a high fraction of Cu impurities, to be used as a primary source material. Another example of efforts to develop sustainable Al alloys (section 4.3), is when the unwanted detrimental phases resulting from higher impurity contents are converted to less detrimental phases. This approach has been demonstrated for increased Fe impurities in aluminum alloys, where manganese is added to form a more desirable precipitate, converting $Al_9Fe_2Si_2$ to $Al_{15}Si_2M_4$, where M=Fe, Mn [30]. CALPHAD and other ICME tools can help identify alternative precipitates in complex alloy systems.

More efficient heat treatments can also substantially reduce energy and emission costs. Optimization of the heat treatment process allows novel processing cycles to be developed that use less energy for cast materials. A two-step heat treatment for Ni-base superalloys avoids incipient melting, saves energy, and produces more consistent creep properties [31]. This method has been expanded to also include 9 % to 12 % mass percent Cr ferritic-martensitic steels [32].

Several processing innovations driven by ICME methods were also presented. The first innovative process involved the toxic red mud that is a solid waste derived from bauxite refining processes. The red mud is rich in iron and other useful elements; however, it has an extreme alkalinity that can leach and contaminate groundwater. Making use of toxic red mud as a source for iron was highlighted as a pathway to recycle primary metal production products as investigated by Jovičević-Klug et al. [33]. This work demonstrated how thermodynamic calculations can be used to optimize the reduction of the oxides and increase the efficiency of the processing. A second processing method focused on reducing the energy cost for making steel by using a hydrogen reduction process. Another example centered on hydrogen-based ironmaking, particularly the Hydrogen Breakthrough Ironmaking Technology initiative in Sweden [34], that replaces coal-based processes with a hydrogen-based process and the electric arc furnace. Thermodynamic predictions help elucidate the different reduction pathways of iron ore to iron depending on the various reducing gas combinations. Finally, new methods for recycling rare earth permanent magnets were highlighted, using optimized slags and separations processing guided by phase diagram calculations of the CaO-Al_2O_3-Nd_2O_3 slag system [35].

ICME approaches can improve sustainability in a variety of ways including optimizing materials to enhance durability and extend lifetimes, improving processing methods to reduce energy consumption and minimize waste, designing new processing methods for recycling valuable elements from waste by-products, incorporating near net-shape processing to reduce waste, and integrating life cycle assessment tools into the materials design process.

5.2. ICME Opportunities in the Automotive Industry

Some challenges and opportunities of integrating ICME approaches into aluminum recycling and sustainable manufacturing within the automotive industry were explored, with four primary goals outlined:

- Extend the use of materials and products through better designs
- Increase the use of recycled and reused products and materials
- Limit the use of primary clean production of raw materials
- Minimize the disposal of non-renewable materials

Within the automotive sector, end-of-life recycling of aluminum alloys for reuse in non-structural cast parts is well-established. However, the use of scrap Al for structural components produced via die-casting or wrought processing is limited due to the impurity content. One highlighted approach to overcoming this issue comes from work by Cinklic et al. [36], in which CALPHAD-based tools were used to develop processing-composition maps for effective iron/manganese ratios and cooling rates. This work aimed to avoid formation of the β-Al_5SiFe phase in the aluminum-magnesium-silicon-iron system, thereby enabling the development of low-cost recycled cast aluminum alloys with higher iron contents. Cinklic et al. used CALPHAD-based tools to develop processing-composition maps of effective iron/manganese ratios and cooling rates to avoid the formation of the β-Al_5SiFe phase, enabling the development of low-cost recycled cast aluminum alloys with high iron contents. The precipitate morphology can be further refined with small additions of strontium for improved properties [37]. These strategies have been used to develop new low-cost recycled aluminum alloys for die casting applications [38].

Extending the life of a part is an important element of increasing the sustainability of materials, and corrosion resistance is a critical property for extending the life of automotive parts. With the increasing use of aluminum scrap to produce structural aluminum alloy parts, understanding the role of impurities on the corrosion resistance will become increasingly important. Special emphasis was placed on the role of intermetallic precipitates (IMPs) in 6XXX-series aluminum alloys. The IMPs increase the localized corrosion, acting as either active sites for breaking down the passive film or as local cathodes that support anodic attack. Developing better methods to analyze the impact of these IMPs is essential, as highlighted by the work of Adapala et al [39].

The giga-casting process was identified as a key innovation for advancing automotive sustainability. The giga-casting process provides significant energy savings through part consolidation and reduces welding needs. However, determining the correct processing parameters to avoid defect formation for different alloys and parts can be challenging. There is a significant need for an aluminum-based processing-structure feedback control loops to increase processing efficiency. Novel research ongoing at Ohio State University is developing smaller-scale water analog experiments to simulate fluid flow in high-pressure die castings, enabling a better understanding of how to reduce air/gas entrapment and porosity [40].

Looking ahead, the integration of CALPHAD and other ICME tools with computer-aided design, and finite element analysis (FEA) tools was identified as a critical pathway forward. A new code, which couples process simulation with 3-D quantitative cellular automaton, has been developed to predict microstructure evolution in HPDC. In this approach, FEA software simulates HPDC thermal conditions which is used as input for temperature and grain size distribution~~s~~ predictions. These results are then used to model grain growth, porosity, precipitate formation, and inclusion distribution [41,42].

5.3. Data Needs

The continued development of data resources was emphasized as essential to accelerating sustainable materials design and processing. Several existing NIST data resources and tools were highlighted, including the Configurable Data Curation System (CDCS) [43], the Phasedata repository [44], the Additive Manufacturing Benchmark Test Series data repository[45], the Joint Automated Repository for Various Integrated Simulations (JARVIS) repository [46] and infrastructure, and the Interatomic Potential Repository [47]. One demonstration showcased how CDCS can be used in multiple ways to curate and disseminate data effectively.

The NIST Creating Helpful Incentives to Produce Semiconductors (CHIPS) Metrology Exchange to Innovate in Semiconductors (METIS) effort demonstrates how to integrate a variety of data user needs within a given system that includes management of sensitive data, metadata protocols and sematic models, Application Programing Interfaces to automate workflows and data ingest, persistent identifiers, and distribution services [48]. Complementary to this, a suite of data and design tools developed at the Pennsylvania State University through collaborative research efforts was described. These resources support data generation, processing, and alloy design for sustainable materials [49,50].

The discussion underscored the pressing need for improved multicomponent thermodynamic and kinetic models, especially with respect to impurity elements. Additionally, there is a growing demand for predictive tools that can estimate properties at both the individual phase level and with consideration of defects. A key challenge is to define the standards necessary for classifying recycled materials, particularly in terms of processing histories, composition, and expected performance.

6. Steel

Sustainable steel is a broad topic that encompasses innovations aimed at improving energy efficiency, enabling sustainability, and optimizing material performance across the steel lifecycle. The sustainable steel session highlighted research and technology in electrochemical ironmaking, microwave-assisted biomass reduction, and microstructural engineering. It also emphasized the need for coordinated research and infrastructure development to accelerate the deployment of sustainable steel technologies.

At the workshop, the Association for Iron and Steel Technology (AIST) presented a summary of the "Roadmap for Iron and Steel Manufacturing: Revolutionizing U.S. Global Leadership for a Sustainable Industrial Supply Chain" [51]. The roadmap was funded by the NIST Office of Advanced Manufacturing in 2022. Within this presentation, several technology themes were outlined. Accordingly, this section is organized to reflect three of these thematic areas: electrification of iron and steel processes, alternative reductants and energy sources, and materials and energy optimization. This section summarizes the workshop presentations and discussions focused on sustainable steel.

6.1. Electrification of Iron and Steel Processes

Presentations and discussions highlighted the potential impact of electrification as an impactful pathway for sustainable iron and steelmaking. In the U.S., the electric arc furnace (EAF) process already accounts for over 70 % of steel production [51]. In addition, the EAF leverages recycled scrap as feedstock over traditional blast furnace-basic oxygen furnace routes. However, limitations in scrap quality and availability require further innovation. Electrification of ironmaking, particularly using novel electrochemical and high-temperature electric processes, has the potential to close this gap while providing more energy-efficient pathways for producing primary iron and high-quality steels.

Boston Metal's molten oxide electrolysis (MOE) technology is an example of an electrochemical-based ironmaking process. MOE uses electricity to reduce iron ore directly into molten iron, eliminating the need for coke or other carbon-based reductants, and this process is compatible with a wide range of iron ore grades. The byproduct of MOE is oxygen, which makes it a low-emission iron production pathway, especially when it is powered by renewable electricity. Boston Metal is currently scaling up MOE with support from commercial and government partners. These efforts include a demonstration plant in the U.S. and a commercial facility in Brazil, which aim to extract high-value metals from mining waste. The combination of steel production and metal recovery in the MOE process illustrates the potential for electrification processes to advance both sustainability and resource efficiency in primary metal production.

Complementing industry efforts, the U.S. DOE Advanced Research Projects Agency - Energy (ARPA-E) Revolutionizing Ore-to-Steel to Impact Emissions (ROSIE) program seeks to advance innovative technologies that expand domestic iron and steel production to strengthen U.S. manufacturing capabilities. Launched in June 2023 with $35 million in funding across 13 projects, ROSIE supports diverse approaches including low-temperature electrolysis, microwave hydrogen plasma reduction, ammonia-based reduction, and laser furnaces. Notable projects include

Argonne National Laboratory's microwave hydrogen plasma rotary kiln, Tufts University's ammonia-based reduction of ore concentrates, and Worcester Polytechnic Institute's low-temperature electrolysis for high-efficiency iron powder production. These projects aim to advance novel iron making processes while achieving costs on par with traditional blast furnaces. The program also seeks to address broader challenges such as reductant availability, energy price uncertainty, and feedstock diversity, supporting the rapid de-risking and scaling of transformative technologies to support the future of sustainable steel.

6.2. Alternative Reductants and Energy Sources

Sustainable iron and steel production depends heavily on the deployment of alternative reductants and alternative energy sources to replace the legacy use of coal and coke [51]. This transition includes the use of hydrogen, biomass, electricity, electrochemical, and emerging plasma-based technologies [51]. Traditional blast furnace systems, which rely on carbon-intensive reductants and dominate global ironmaking, emit 2.0 tons to 2.4 tons of CO_2 per ton of steel [51]. Alternatives such as natural gas, hydrogen, and electrified heat sources like plasma torches are being explored for their potential to reduce carbon intensity while preserving process performance and economic viability. However, challenges such as hydrogen infrastructure, energy costs, and iron ore quality remain key barriers to widespread adoption.

Rio Tinto presented their BioIron™ technology, which is an alternative reduction pathway tailored to low grade iron ores. This process uses raw biomass as the primary reductant and microwave energy as the heating source. BioIron™ eliminates the need for coke or sintering by compacting biomass and iron ore into briquettes that are preheated and then metallized via microwave-assisted reduction. This approach has demonstrated over 95 % metallization with rapid energy absorption efficiency and CO_2 reductions of up to 95 % compared to the blast furnace route when using sustainable biomass and clean energy. With a successful small-scale pilot facility already completed, Rio Tinto is building a one-ton-per-hour pilot facility. By optimizing biomass feedstocks and leveraging efficient microwave heating, BioIron™ offers a potential solution for low grade ores that could be a scalable and adaptable alternative to conventional reduction technologies.

The U.S. DOE ARPA-E ROSIE program complements these developments by funding a diverse portfolio of early-stage technologies focused on alternative reductant ironmaking. Several ROSIE projects explore unconventional reductants and novel energy forms, including the University of Minnesota's microwave hydrogen plasma reduction. These methods bypass fossil fuel inputs and aim to use renewable electricity, hydrogen, or reactive nitrogen species as clean reductants. ROSIE projects are specifically targeting scalable, cost-competitive solutions, paving the way for a sustainable steel industry while broadening the feedstock and energy options for next-generation processes.

6.3. Materials and Optimization

Materials development and process optimization are central to improving the sustainability and performance of steel. As the AIST Technical Roadmap outlines, future steel design must increasingly address extending material lifecycle and improving mechanical performance [51]. This design concept is also referred to as “indirect sustainability”, or sustainability achieved though material property or performance optimization [52]. Several examples of materials and optimization were presented during the workshop, emphasizing the importance of process-microstructure-property relationships in enabling indirect sustainability. For example, improved corrosion resistance can extend the service life of metallic materials, thereby contributing to more sustainable performance.

Colorado School of Mines presentation demonstrated how materials optimization can contribute to sustainability. Recent work conducted in collaboration with NIST revealed that intercritically rolled and tempered X65 pipeline steel possesses significantly improved performance in corrosive environments. By tempering the steel, researchers achieved a marked reduction in hydrogen-induced cracking susceptibility, and an increased impact toughness and yield strength. These improvements were attributed to the decomposition of martensite/austenite constituents, the formation of cementite, and a reduction in dislocation density [53]. This study highlights how process-microstructure-property relationships not only improves material properties but also can extend component service life, optimizing the material to aligning with sustainability goals.

6.4. Research and Development Needs

Economic viability, infrastructure limitations, and technology readiness remain key hurdles for both electrification and alternate reductants. The transition to circular steelmaking is complicated by scrap quality and the need for materials engineered to perform under new processing and service conditions. Workshop attendees called for targeted R&D with collaboration among government, academia, and the private sector. Additionally, workshop participants discussed that the growth of sustainable steel requires supportive regulatory and financial frameworks. With coordinated action and continued innovation, steel can be sustainable, resilient, and globally competitive.

7. Sustainable Manufacturing

Life Cycle Assessment (LCA) has emerged as a tool to support sustainable manufacturing, offering a quantitative method to evaluate energy consumption and environmental impacts associated with the manufacturing processes. LCA can help identify both direct sustainability measures, such as decarbonizing primary metal production, and indirect sustainability opportunities, including lifetime extension, remanufacturing, and lightweighting. This section captures the sustainable manufacturing presentations and discussions held at the workshop.

7.1. Life Cycle Assessments to Support Sustainable Manufacturing

LCAs are being used to drive carbon neutrality strategies, guide supplier practices, and inform engineering decisions across the vehicle lifecycle. These analyses show that while automotive electrification can reduce tailpipe emissions, it may also increase the carbon footprint of materials and manufacturing [54]. International Organization for Standardization (ISO)-compliant LCA methodologies / tools, like Argonne National Lab's Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET) model [55], and commercial software packages are being used across various manufacturing processes. Such tools enable engineers to evaluate energy and emissions throughout the lifecycle, ensuring sustainability principles can be embedded into the various stages of product manufacturing.

LCA was discussed as essential for identifying both direct and indirect sustainability opportunities throughout manufacturing processes. Direct measures typically target energy, emissions, and resource consumption at the point of production. In contrast, indirect measures, such as product lightweighting, lifetime extension, or reuse, often produce benefits downstream [56].

7.2. Direct Sustainability Measures in Automotive Manufacturing

Ford highlighted that using LCA methodologies, metal production tends to be identified as the highest contributor to emissions within their metallic manufacturing processes. For example, from 1900 to 2015, cumulative emissions from blast furnace operations alone were estimated at 58 Gt, which is considerably higher compared to downstream processes such as plate (1.2 Gt), strip (4.3 Gt), rod/bar (5.0 Gt), and cold rolling mills (7.7 Gt) [57]. This finding is consistent with reporting from Ford, who ranked mining and ore reduction as the highest emission contributor in metal vehicle manufacturing processes, followed by melting, alloying / casting, mill processing, finishing, and stamping. From this, decarbonization of primary metal production and maximizing recycled contents were identified as the most promising opportunities to decarbonize vehicle manufacturing processes.

These strategies are reflected in recent investments across the broader automotive industry. While not discussed at the workshop but relevant to this topic, Toyota recently acquired Radius Recycling, which operates over 100 facilities across North America, specializing in vehicle recycling and having EAF steelmaking capacity [58]. Additionally, Hyundai Steel Company is investing in an EAF facility with a DRI (Direct Reduced Iron) component in Louisiana. The planned facility is expected to produce 2.7 million tons of steel annually, primarily for automotive applications [59]. By investing in recycling infrastructure and adopting lower-emission steel production technologies, automotive companies are taking steps toward achieving sustainability goals through their manufacturing processes.

While steel has historically been the dominant metal within vehicles, more aluminum is being incorporated, a trend expected to continue. In 2020, the average vehicle had approximately 9 % aluminum by mass with projections to rise to 25 % by 2040 [60]. The incorporation of aluminum in vehicles presents open-loop recycling challenges. As discussed in an earlier section, a major hurdle lies in sorting the various alloys of aluminum, particularly between 5XXX and 6XXX series. Mixing these alloys during recycling can degrade mechanical properties and limit reuse in structural applications. End-of-life vehicle scrap is especially difficult to manage due to its heterogeneity and impurity accumulation, specifically iron and copper, which reduce the ductility of recycled aluminum [61]. However, Ford identified closed-loop recycling as a viable direct sustainability approach to minimize aluminum scrap contamination, because the scrap is recycled back into the same product system, which minimizes the introduction of impurities. Closed-loop recycling of aluminum is promising because it reduces energy consumption and the environmental impact associated with primary metal production [62].

Presentations and discussions highlighted expanding the use of recycled scrap into structural high pressure die castings. Using an ICME framework and virtual manufacturing programs, this approach has accelerated new material attributes/performance and optimization with plans to expand this framework to include other processes and alloys to improve the sustainability of vehicle manufacturing.

7.3. Indirect Sustainability Measures in Manufacturing

Indirect sustainability in manufacturing aims to reduce the energy and environmental impacts across the entire product lifecycle, rather than focusing on the point of production. Examples of indirect sustainability include component lifetime extension through material property or corrosion resistance improvements, reuse or remanufacturing, and material lightweighting. These measures can be used concurrently with one another and complement direct sustainability initiatives.

One indirect sustainability strategy presented/discussed at the workshop involves extending the service life of manufactured components through the improvement of material properties. Enhancements in fatigue, wear, and corrosion resistance can decrease the frequency of part replacement, thereby decreasing primary material consumption and associated energy and emissions. For example, the fatigue performance of medium carbon steels can be improved through the addition of silicon and vanadium followed by nitriding [63]. These material modifications extend component lifespan without changing the product’s function or use.

Remanufacturing is another indirect sustainability approach that returns end-of-life products back to a like-new condition. Unlike traditional recycling, which breaks materials down into raw feedstocks, remanufacturing preserves the embodied energy and structure of a component, making it a more resource and energy-efficient option. This process is particularly valuable for high-value large assemblies such as engines, transmissions, and industrial equipment. One U.S.

industry estimated that its remanufacturing processes result in 65 % to 87 % fewer emissions and 80 % to 90 % less raw material compared to primary manufacturing [64]. To capitalize on remanufacturing, materials and components must be designed for disassembly, inspection, and reassembly, and standards are needed to qualify the performance and safety of remanufactured parts. In addition to sustainability benefits, remanufacturing offers industries lower production costs and provides customers with a wider range of products [64].

Lightweighting, another indirect sustainability approach, reduces the mass of components without negatively impacting performance. Lightweighting strategies are frequently used within the automotive and transportation sectors. By lowering vehicle weight, manufacturers can improve the fuel economy or extend the driving range, thus reducing lifetime emissions and energy consumption. Vehicle lightweighting is frequently achieved by substituting steel with next-generation auto steel[3], high-strength aluminum, magnesium, or composites [60]. To support these efforts, programs like the NIST Center for Automotive Lightweighting (NCAL) were discussed. NCAL plays a critical role by advancing the measurement science needed to validate lightweight materials and ensure they meet industry standards for performance [65]. However, it was emphasized that lightweighting strategies must be balanced with recyclability. As previously discussed, when mixed material classes, such as steel and aluminum, are recycled and remelted for secondary life, the introduction of impurities can negatively impact the material performance. Additionally, lightweighting can be achieved through part consolidation enabled by advanced manufacturing methods like additive manufacturing [66].

7.4. Sustainable Large-Scale Additive Manufacturing

Metal additive manufacturing (AM) processes were introduced nearly a century ago [67] but have only recently matured enough to be adopted by industrial sectors. AM processes offer design complexity that cannot be achieved with conventional manufacturing methods, but AM parts are generally more expensive due to the initial capital costs of equipment and the high costs of powder feedstock materials. In both powder bed and powder blown processes, significant quantities of virgin material are introduced into the process that are not consolidated into the final part and are often collected after build completion. The collected powder material is typically considered waste, as the powder particles often deviate in morphology, chemistry, and flow properties when compared to the virgin feedstock.

WPI presented recent research that investigated approaches to reduce powder waste to make AM processes more sustainable. Their approach centered on understanding the factors that influence powder flowability, a critical parameter that affects build quality in metals-based AM processes [68]. WPI showed that powder flowability may be impacted by storage and environmental exposure conditions, such as time of environmental exposure and humidity [69]. The relative impacts of these factors appeared to vary among materials due to different powder attributes. The presentation emphasized that proper powder handling and storage practices are essential to maintain powder quality and reduce powder waste.

[3] Next-generation automotive steels, such as 3rd generation advanced high-strength steels and Transformation-Induced Plasticity (TRIP) steels, offer higher strength than conventional automotive steels. This enables the use of thinner gauge sections without compromising structural performance, contributing to vehicle lightweighting.

As discussed in earlier sections, recycling is an integral part of the sustainable manufacturing ecosystem, and using scrap metal to produce powder feedstock was also discussed in the WPI presentation. Commercially processed virgin titanium-based powder was used as a control, and powder characteristics were compared to powders atomized from a variety of recycled titanium alloys. Generally, the powders made from recycled materials had a comparable composition, microstructure, and hardness to virgin titanium-based powder materials [70]. These results demonstrated the use of scrap metal as a viable pathway for metal powder production. Similarly, the use of reclaimed powders from cold-spray for building parts was also discussed in detail. Preliminary results show that the reclaimed powder has many characteristics similar to the virgin powder, although this work is ongoing.

Additional aspects of the cold-spray process were presented, aside from material feedstock, that could help make the AM process more sustainable. These topics include optimizing the process to increase powder deposition efficiency, generating nitrogen carrier gas on-site from the atmosphere, developing alloys specifically for cold-spray AM with high printability, researching different carrier gases, and recovering expensive processing gases. All the approaches discussed aim to reduce material waste, reduce manufacturing costs, and enhance the sustainability of the cold-spray AM process.

8. Recycling and Reuse

Recycling and reuse were discussed as crucial aspects of sustainable metals processing. However, realizing the full potential within manufacturing industries requires addressing several challenges. Among the most pressing are the complexities of material separation, evolving scrap compositions, and the need for reliable standards to ensure that recycled content can meet industrial performance requirements. As manufacturers increasingly integrate recycled feedstocks into products, the development of qualification and certification protocols becomes critical. This section highlights presentations and discussions on metals recycling, including current challenges, the evolving role of material standards, and the growing importance of certification for products made with recycled content.

8.1. Challenges in Recycling of Metals

A presentation by the Recycled Materials Association (ReMA) highlighted the challenges associated with metals recycling. The presentation highlighted that approximately 137 million metric tons of materials are recycled and processed in the U.S. annually as of 2022, including ferrous and non-ferrous alloys, paper and fiber, plastics, and electronics [71]. The impact of recycled materials on the economy was discussed. As of 2021, with $117 billion in economic impact, approximately 500,000 direct and indirect jobs, and about $12.3 billion generated in combined federal, state, and local taxes [71]. Iron, aluminum, and copper alloys, account for about 56 % of the 137 million metric tons [71], largely because end-of-life vehicles serve as the primary source of recycled materials in the U.S. by mass.

It was emphasized that recycling rates and efficiency depend on market demand, since recycled material can only be utilized when a need arises from manufacturers and producers of goods. The demand for recycled materials depends on a variety of conditions that vary across manufacturing industries. Conditions that generally favor the uptake of recycled material include sufficient quality and supply of the recycled material, cost-effective recycling technologies, efficient material logistics, good markets for the materials, and favorable policies, laws, and regulations. Workshop discussions highlighted that recycling should be driven by market forces, materials should move freely, fees and mandates should be temporary and only be imposed by government in special circumstances, and that manufacturers should consider end-of-use and recycling in the design process of manufactured products.

Materials separation was highlighted as a key component of the recycling process that has a large impact on the feasibility and quality of recycled material. Recycling of products varies in complexity depending on the type and number of dissimilar materials contained within. Simple products, such as steel or aluminum cans, often contain one or two alloys and can be readily recycled and reused to produce the same products. Complex products, like automobiles, laptops, or appliances, are comprised of many different alloys and non-metallic parts. More intensive separation processes are required to recycle complex products, which ultimately increases the cost of recycling and makes the materials less likely to be recycled. Workshop discussions emphasized that sustainable manufacturing should consider end-of-life separation processes in product design to facilitate easier recycling.

Separation of materials is a process that can be performed both before and during the recycling process. Many end-of-life products are taken to industrial shredders, where mixed metals are shredded into finer pieces. Depending on the characteristics of each metal, different downstream separation techniques can be used to separate shredded products. Ferrous metals are typically separated from the shreds using magnets, which are in-line with the shredders, due to the ferromagnetic properties of many iron-based alloys. The remaining non-magnetic metals, such as aluminum, copper, zinc, or austenitic stainless steels, can be further separated using a variety of techniques including trommels, screens, eddy current separators, optical scanners, and other proprietary methods. The separated material can then often be sold as products, while the remaining residue is discarded as solid waste.

The need for high-quality scrap material that can be obtained from complex products containing many dissimilar components was emphasized. It was highlighted that better separation processes are needed to achieve desirable chemistries of the recycled materials while keeping the cost of production and energy requirements of recycling processes low. Meanwhile, technological and engineering advancements continuously change scrap streams due to the introduction of novel alloys and other high-strength materials. A particular example is the recycling of automobiles, which have been traditionally made with various types of steel grades. However, motivated by vehicle light-weighting, higher fractions of aluminum are being incorporated in addition to the traditional automotive steels. As of 2010, the average vehicle had 154 kg of aluminum content. By the year 2020, the fraction of aluminum had increased over 35 % to 208 kg. This trend is expected to continue, where in 2026 the average vehicle is projected to have 233 kg of aluminum, an increase of over 50 % from the 2010 levels [60]. Likely, more aluminum alloys, magnesium alloys, and composites will continue to be incorporated into automobiles, and recycling and separation processes will need to address the rapidly changing scrap streams of the future.

8.2. Qualification, Certification, and Standards for Materials with Recycled Contents

Industrial participants at the workshop highlighted that successfully integrating recycled materials into manufacturing requires ensuring that recycled-content products meet established performance criteria. However, as discussed in previous sections, recycled metallic materials can exhibit greater variability in composition and properties compared to primary materials. This variability can present challenges to meeting product specifications. It was emphasized that the incorporation of materials with high levels of recycled content created a need for internal material requalification. More specifically, any change in the supply chain, such as the incorporation of recycled or sustainable materials, requires internal requalification and/or recertification, a time-consuming and costly endeavor for industry.

The workshop attendees challenged standardization bodies to consider recycled inputs. This effort is critical to build confidence with manufacturers that products are made from secondary or sustainable feedstocks to meet the same quality / performance as those made from primary materials. While specifications from recycling industry trade groups provide some consistency and quality metrics, they lack the connection to downstream performance. Open-loop recycling processes may utilize complex, blended, or non-homogeneous feedstocks that meet recycling industry trade group specifications. However, as discussed at the workshop, guidance is needed for testing and certifying recycled materials, such that they can be more readily in compliance with final material performance requirements.

9. Potential Activities to Facilitate a Sustainable Metals Industry

A sustainable, resilient, and circular U.S. metals industry can be enabled by addressing measurement science gaps, supporting the technical basis for standards development, and advancing modeling and data tools. Drawing on the insights throughout this report and the discussions with the workshop participants, the following sections describe potential action items.

9.1. Advance Measurement Science for Sustainable Metallurgy and Manufacturing

The transition to sustainable metal processing can be accelerated by developing and disseminating measurement methods for:

- Identification and quantification of impurities within recycled metal feedstocks.
- Characterization of alloys with recycled content to understand the impact of impurities on performance.
- In-process monitoring of additive and primary metal manufacturing processes to enhance efficiency and performance.
- Advance in-line alloy identification, sorting, and separation techniques to enhance the quality and purity of recycled materials.
- Assessment of energy consumption and impacts across metal life cycles with a particular focus on extraction and refining.
- De-risking emerging technologies that are promising for advancing sustainable metals processing (e.g., hydrogen-based reduction, electrification).

9.2. Develop the Technical Basis to Support Standards Development

Accelerating the industrial adoption of a sustainable metals industry necessitates the development and adoption of standards rooted in sound technical foundations. Specific action items in support of this include:

- Generation of data to enable the creation and/or revision of performance-based standards for recycled-content metals, such as aluminum and steel alloys with higher impurity tolerances.
- Measurement science and technical validation to enable specifications for feedstock variability in additive manufacturing using reclaimed powders.
- Methodology development and generation of reference data to facilitate sustainability criteria such as identifying recycled content, energy intensity, and environmental impact across the metals and manufacturing supply chains.

9.3. Enable Integrated Data Infrastructure and Modeling Tools

Support the development of modeling tools and data infrastructures that are essential for materials design, lifecycle tracking, and decision-making:

- Expand thermodynamic and kinetic databases and assessments for recycled and impurity-tolerant alloys.
- Develop predictive models linking impurity levels, microstructure, and material performance in high recycled-content metals.
- Facilitate benchmarking and integration of LCA data into alloy and process design platforms.
- Develop methods and tools that integrate sustainability considerations, such as recycled content, supply risk, and end-of-life recoverability, into alloy design, materials qualification, and procurement processes.

9.4. Promote Workforce Development and Educational Revitalization

To address critical skill gaps in sustainable metallurgy and sustainable manufacturing, investments are needed to:

- Create partnerships between universities, national laboratories, industry, and federal/state entities to inform extractive metallurgy and ICME curricula with sustainability-focused modules.
- Establish training programs such as internships, undergraduate and graduate research pathways, and post-doctoral programs focused on data-driven sustainable materials science and circular economy practices in metallurgy and manufacturing.
- Facilitate industrial-focused workshops to share and promote sustainability and circularity practices within the metals and manufacturing industries.

9.5. Convene Stakeholders and Coordinate Strategy

To drive progress in sustainable metal production and recycling, diverse stakeholders should establish collaborations that foster knowledge sharing, innovation, and collective action, including:

- Multi-sector workshops and formation of consortia focused on circular metals innovation.
- Roadmap development for sustainable aluminum, steel, and critical materials supply chains.
- Mechanisms to align measurement needs with regulatory and market drivers.
- Coordination with relevant federal initiatives on critical materials security, manufacturing innovation, and the circular economy.

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Appendix A. Workshop Agenda and Speakers

NIST	**Material Challenges in Developing a Sustainable Metal Processing Infrastructure** Tuesday, July 30th, 2024	NIST
8:00 am – 8:45 am	**Arrival / Check in**	
8:45 am – 9:00 am	**Mark VanLandingham**, Ph.D., Division Chief, Materials Science and Engineering, NIST	**Opening Remarks**
9:00 am – 9:30 am	**Mike Molnar**, Director of the U.S. Advanced Manufacturing National Program Office	**Sustainability and Recycling in Advanced Manufacturing Strategy**
9:30 am – 9:45 am	**Discussion**	
	Critical Materials Session Chair: James Zuback, NIST	
9:45 am – 10:15 am	**Diane Bauer**, Ph.D., Deputy Director, Advanced Materials and Manufacturing Technologies Office, DOE	**DOE's 2023 Critical Materials Assessment**
10:15 am – 10:45 am	**Elisa Alonso**, Ph.D., U.S. Geological Survey	**Challenges in Processing Infrastructure for Mineral Commodities and how it Impacts Criticality**
10:45 am – 11:15 am	**Discussion/Break**	
	Sustainable Extractive Metallurgy Session Chair: Andrew Iams, NIST	
11:15 am – 11:45 pm	**Brajendra Mishra**, Ph.D., Director, Metal Processing Institute & Center for Resource Recovery and Recycling, WPI	**Sustainability of Aluminum Production: Environmental Management of Bauxite Residue**
11:45 am – 12:15 pm	**Corby Anderson**, Ph.D., Director, Kroll Institute for Extractive Metallurgy, Colorado School of Mines	**The Kroll Institute for Extractive Metallurgy - 50 Years of Success**
12:15 pm– 12:30 pm	**Discussion**	
12:30 pm – 1:45 pm	**Lunch**	
	Aluminum Session Chair: Samantha Webster, NIST	
1:45 pm – 2:15 pm	**Marshall Jinlong Wang**, Manager of Sustainability Programs, The Aluminum Association	**Pathway to Net Zero: A Decarbonization Roadmap for the North American Aluminum Industry**
2:15 pm – 2:45 pm	**Robert Sanders**, Ph.D., Senior Technical Advisor, Novelis Global Research and Technology	**Barriers to Raising Recycled Content in Wrought Aluminum Alloys**
2:45 pm – 3:15 pm	**Alex Plotkowski**, Ph.D., Senior R&D Staff, Oak Ridge National Lab	**Sustainable Alloy Design for Aluminum High Pressure Die Casting**
3:15 pm – 3:30 pm	**Discussion**	
3:30 pm – 3:45 pm	**Break**	
	Integrated Computational Materials Engineering (ICME) for Sustainable Material Design Session Chair: Mark Stoudt, NIST	
3:45 pm – 4:15 pm	**Alan Luo**, Ph.D., The Donald D. Glower Chair in Engineering, Ohio State University	**Development of Recycled Aluminum Alloys and Sustainable Manufacturing Processes: The role of ICME**
4:15 pm – 4:45 pm	**Paul Mason**, President, Thermo-Calc Software Inc.	**The Role of CALPHAD-Based Tools in Developing a Sustainable Metal Processing Infrastructure**
4:45 pm – 5:00 pm	**Zi-Kui Liu**, Ph.D., Professor, Materials Science and Engineering, Pennsylvania State University	**Data to Support Sustainable Manufacturing**
5:00 pm – 5:15 pm	**Carelyn Campbell**, Ph.D., Group Leader, Thermodynamics and Kinetics, NIST	**NIST Data and Tools to Support sustainable Metals Processing**
5:15 pm – 5:30 pm	**Discussion**	
5:30 pm	**Adjourn**	

NIST	**Material Challenges in Developing a Sustainable Metal Processing Infrastructure** Wednesday, July 31st, 2024	NIST
8:00 am – 8:45 am	**Arrival / Check in**	
Steel Session Chair: James Zuback, NIST		
8:45 am – 9:15 am	**Brian Bliss**, General Manager, Association of Iron and Steel Technologies (AIST)	**AIST Roadmap for Iron and Steel Manufacturing: Revolutionizing U.S. Global Leadership for a Sustainable Industrial Supply Chain - Overview and Status Update**
9:15 am – 9:45 am	**David Leigh,** General Manager, Steel Decarbonization, Rio Tinto	**BioIron™ – The Development of a Low CO_2 Emissions Ironmaking Process Utilizing Raw Biomass as a Reductant and Microwaves as an Energy Source**
9:45 am – 10:15 am	**Guillaume Lambotte**, Ph.D., Chief Scientist, Boston Metal	**Molten Oxide Electrolysis - How to Decarbonize Steelmaking and Transform How Metals Are Made**
10:15 am – 10:30 am	**Break**	
10:30 am – 11:00 am	**Elise Goldfine**, Ph.D., ARPA-e Fellow, DOE	**The ARPA-E ROSIE Program: Innovative Methods for Decarbonizing Iron and Steel Production**
11:00 am – 11:30 am	**Kip Findley**, Ph.D., Professor, Metallurgical and Materials Engineering, Colorado School of Mines	**The Role of Steel Research and Development on Sustainable Manufacturing**
11:30 am – 11:45 am	**Discussion**	
Industrial Panel Session Chair: Andrew Iams, NIST		
11:45 am – 12:15 pm	**Gordon Alanko**, Ph.D., Sr. Manager, ATI Specialty Alloys & Components **Zhuqing Wang**, Ph.D., Staff Engineer Materials Science, Kennametal Inc. ***More to be announced soon.***	**Topics: Innovations in Sustainable Metal Production, Strategies for Reducing Carbon Footprint in Metal Manufacturing, Circular Economy in Metals: Recycling and Reuse, Policy and Regulation Impact on Sustainable Metallurgy, Supply Chain Sustainability and Ethical Sourcing**
12:15 pm – 1:15 pm	**Lunch**	
Sustainable Manufacturing Session Chair: Samantha Webster, NIST		
1:15 pm – 1:45 pm	**George Luckey**, Ph.D., Manager, Advanced Metal Technology Research and Advanced Engineering, Ford	**Perspectives on Decarbonizing Automotive Grade Structural Metals**
1:45 pm – 2:15 pm	**Cody McIntyre**, Engineering Manager – Salvage Development Remanufacturing Division, Caterpillar Inc.	**Caterpillar Remanufacturing Division: Bringing Equipment Back to Life**
2:15 pm – 2:45 pm	**Discussion**	
2:45 pm – 3:00 pm	**Break**	
Recycling and Reuse Session Chair: Carelyn Campbell, NIST		
3:00 pm – 3:30 pm	**David L. Wagger**, Ph.D., Chief Scientist / Director of Environmental Management, Recycled Materials Association	**Recycling Ferrous and Non-Ferrous Metals: Challenges, Opportunities, and Potential Research Directions**
3:30 pm – 4:00 pm	**Danielle Cote**, Ph.D., Co-Director: Materials Reimagined, Sustainability of Metal AM Processes, WPI	**Approaches towards Sustainable Large Scale Metal Additive Manufacturing**
4:00 pm – 4:15 pm	**Discussion**	
4:15 pm	**Adjournment**	

Appendix B. List of Registered Workshop Participants

First Name	Last Name	Role	Organization
Gordon	Alanko	Panelist	ATI Specialty Alloys & Components
Paul	Allison	Attendee	Baylor University
Elisa	Alonso	Speaker	U.S. Geological Survey
Corby	Anderson	Speaker	Colorado School of Mines
Erin	Barrick	Attendee	Sandia National Laboratories
Diana	Bauer	Speaker	Department of Energy
Brian	Bliss	Speaker	National Institute of Standards and Technology
John	Bonevich	Attendee	National Institute of Standards and Technology
Marissa	Brennan	Attendee	General Electric Aerospace
Carelyn	Campbell	Organizer/ Speaker	National Institute of Standards and Technology
Danielle	Cote	Speaker	Worcester Polytechnic Institute
Adam	Creuziger	Attendee	National Institute of Standards and Technology
Tyler	Del Rose	Attendee	U.S. Department of Energy
Martin	Detrois	Attendee	National Energy Technology Laboratory
Ram	Devanathan	Attendee	Pacific Northwest National Laboratory
Matthew	Draper	Attendee	Industrial Base Analysis and Sustainment, ICAM, OSD
Kip	Findley	Speaker	Colorado School of Mines
Brian	Gable	Attendee	Apple
Tao	Gao	Attendee	University of Utah
Thomas	Gardner	Attendee	HP Inc.
Elise	Goldfine	Speaker	ARPA-E
Glenn	Grant	Attendee	Pacific Northwest National Laboratory
Dale	Grigorenko	Attendee	Caterpillar Inc.
John	Hryn	Attendee	Argonne National Laboratory
Mark	Iadicola	Attendee	National Institute of Standards and Technology
Andrew	Iams	Organizer	National Institute of Standards and Technology
Kumar	Kandasamy	Attendee	Enabled Engineering
Helena	Khazdozian	Attendee	U.S. Department of Energy
Suhyeon	Kim	Attendee	Korea Institute of Materials Science
Guillaume	Lambotte	Speaker	Boston Metal
Darby	LaPlant	Attendee	HRL Laboratories, LLC
David	Leigh	Speaker	Rio Tinto
Zi-Kui	Liu	Speaker	Pennsylvania State University
George	Luckey	Speaker/ Panelist	Ford Motor Company
Alan	Luo	Speaker	Ohio State University
Paul	Mason	Speaker	Thermo-Calc Software Inc
Steven	Mates	Attendee	National Institute of Standards and Technology
Suveen	Mathaudhu	Attendee	Colorado School of Mines
Cody	McIntyre	Speaker	Caterpillar Reman

First Name	Last Name	Role	Organization
Brajendra	Mishra	Speaker	Worcester Polytechnic Institute
Mike	Molnar	Speaker	National Institute of Standards and Technology
Kil-Won	Moon	Attendee	National Institute of Standards and Technology
William	Moore	Attendee	Honda - Production Engineering Business Unit
Amin	Nozariasbmarz	Attendee	Rowan University
Chang Seok	Oh	Attendee	Korea Institute of Materials Science
Joshua	Orlicki	Attendee	DEVCOM - Army Research Laboratory
Todd	Palmer	Attendee	Pennsylvania State University
Jiwon	Park	Attendee	Korea Institute of Materials Science
Alexander	Plotkowski	Speaker	Oak Ridge National Laboratory
Robert	Sanders	Speaker	Sanders Aluminum Consulting LLC
Paul	Sanders	Attendee	Michigan Technological University
Michelle	Seitz	Attendee	U.S. Department of Energy - AMMTO
Dongwon	Shin	Attendee	Oak Ridge National Laboratory
Yongho	Sohn	Attendee	University of Central Florida
Daniel J. C.	Stewart	Attendee	U.S. Dept. of Energy (Energetics Contractor)
Mark	Stoudt	Organizer	National Institute of Standards and Technology
Mark	VanLandingham	Speaker	National Institute of Standards and Technology
Edgar	Vidal	Attendee	NobelClad and Colorado School of Mines
David	Wagger	Speaker	Recycled Materials Association (ReMA)
Jinlong	Wang	Speaker	The Aluminum Association
Zhuqing	Wang	Panelist	Kennametal
Bryan	Webler	Attendee	Carnegie Mellon University
Samantha	Webster	Organizer	National Institute of Standards and Technology
Matthew	White	Attendee	Edison Welding Institute
Eliza	Wirkijowski	Attendee	DARPA
Hang	Yu	Attendee	Virginia Tech
James	Zuback	Organizer	National Institute of Standards and Technology

Appendix C. Photo of Workshop Participants – July 31st, 2024

Appendix D. List of Acronyms

AM: Additive Manufacturing

AIST: Association for Iron and Steel Technology

ARPA-E: Advanced Research Projects Agency - Energy

CALPHAD: Calculation of Phase Diagrams

CDCS: Configurable Data Curation

CHIPS: Creating Helpful Incentives to Produce Semiconductors for America

CMI: Critical Materials Innovation Hub

CML: Critical Minerals List

CR^3: Center for Resource Recovery and Recycling

DOE: Department of Energy

DRI Direct Reduced Iron

DPA: Defense Production Act

EAF: Electric Arc Furnace

FEA: Finite Element Analysis

GREET: Greenhouse gases, Regulated Emissions, and Energy use in Transportation (model)

HEA: High-Entropy Alloy

HPDC: High-Pressure Die Casting

ICME: Integrated Computational Materials Engineering

IMPs: Intermetallic Precipitates

ISO: International Organization for Standardization

JARVIS: Joint Automated Repository for Various Integrated Simulations

LCA: Life Cycle Assessment

METIS: Materials and Emerging Technologies Integrated System (part of NIST CHIPS)

MOE: Molten Oxide Electrolysis

NCAL: NIST Center for Automotive Lightweighting

NIST: National Institute of Standards and Technology

ReMA: Recycled Materials Association

ROSIE: Revolutionizing Ore-to-Steel to Impact Emissions (ARPA-E Program)

R&D: Research and Development

USGS: United States Geological Survey

WPI: Worcester Polytechnic Institute