JOURNAL OF CHEMICAL EDUCATION
Commentary
Cite This: J. Chem. Educ. 2019, 96, 2682−2688
pubs.acs.org/jchemeduc

Reimagining the Materials Tetrahedron

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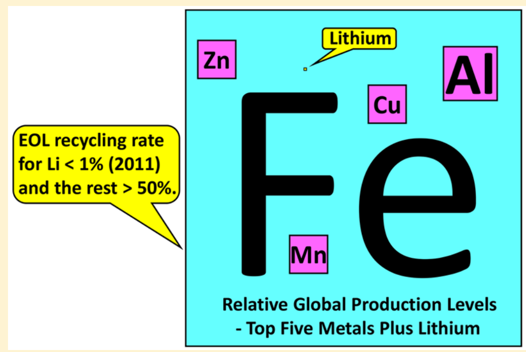
Supporting Information

ABSTRACT: In this commentary, the materials tetrahedron is critiqued, and an alternative format is proposed: a materials square pyramid. By examining the materials tetrahedron in the context of the life cycle of a metal in the anthroposphere, it is observed that the materials tetrahedron addresses only the middle portion of the life cycle, namely, the fabrication and manufacturing and the use component of the life cycle. The materials tetrahedron omits the beginning and end of the life cycle, namely, production of the metal and the disposal or recycling of the metal at end-of-life. The materials square pyramid retains the concepts of processing, structure, properties, and performance found in the materials tetrahedron, but adds a sustainability/criticality component, which constitutes the base of the square pyramid. Drawing from the field of industrial ecology, trends in metals usage are briefly delineated along with potential reasons for raw material supply shortages and price volatility. Criticality is defined, and its usefulness is illustrated in the context of this discussion. The utility of the materials tetrahedron versus that of the materials square pyramid is compared using three examples: lead solder, cobalt in lithium ion batteries, and rare earth elements in permanent magnets. The use of the materials square pyramid to critique these applications potentially raises red flags, either in the area of environmental impact or in supply risk−vulnerability to supply risk, which the materials tetrahedron misses or ignores.



KEYWORDS: *Systems Thinking, Sustainability, First-Year Undergraduate/General, General Public, Environmental Chemistry, Public Understanding/Outreach, Problem Solving/Decision Making, Materials Science, Metals*

INTRODUCTION

In this commentary, I argue for a modification of the traditional materials tetrahedron (see Figure 1). The materials tetrahedron can be found in the introductory chapters of textbooks on materials chemistry and materials science engineering.[1−3] Located at the four vertices of the tetrahedron are *processing*, *structure*, *properties*, and *performance*. This tetrahedron has been labeled the central paradigm of materials science engineering.[3] These four components have also been presented as a linear chain to emphasize the cause and effect relationships among these concepts, that is, that processing determines structure, structure determines properties, and properties determine performance (see Figure 2).[2,3] The problem with the perspective communicated by the materials tetrahedron and its linear companion is that it does not address the entire life cycle of the material; that is, sustainability issues are ignored because a systems perspective to materials usage is

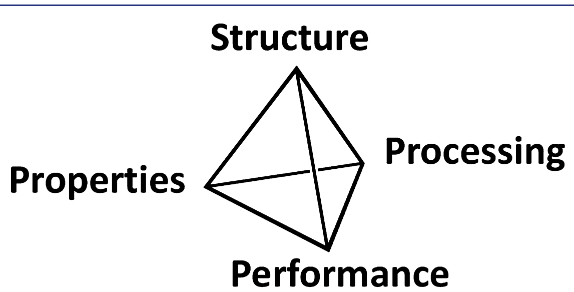


Figure 1. Traditional presentation of the materials tetrahedron.

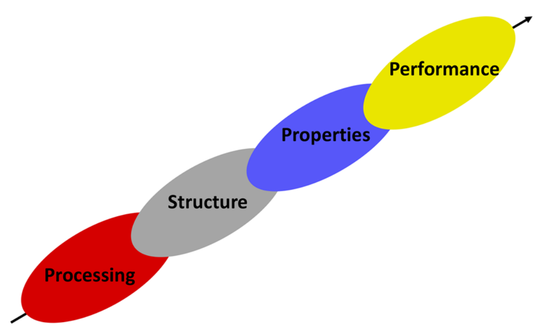


Figure 2. Traditional materials tetrahedron presented as a linear chain.

Special Issue: Reimagining Chemistry Education: Systems Thinking, and Green and Sustainable Chemistry

Received: January 7, 2019
Revised: May 28, 2019
Published: July 8, 2019

DOI: 10.1021/acs.jchemed.9b00016
J. Chem. Educ. 2019, 96, 2682−2688

absent. Here, I confine my focus to metals, a key component in the world of materials.

Big Picture View of Metals

Globally when all the materials that are extracted from the lithosphere, biosphere, hydrosphere, and atmosphere are considered, two roughly equal size categories can be defined: (1) materials that are extracted and used dissipatively (e.g., fossil fuels used to generate thermal energy and biomass used as a fuel and as a source of food for humans and livestock) and (2) materials used by humanity as manufactured capital. The first category of materials are quickly consumed and converted to carbon dioxide and other waste products (e.g., solid waste and air pollutants). The second category of materials are transformed into long-lived material stocks (e.g., buildings, mechanized modes of transportation, infrastructure, appliances, and other artifacts).[4] Our use of metals falls into this second category. Roughly 85% of the mass of manufactured capital is accounted for by aggregate, bricks, asphalt, and most importantly concrete. Of the remaining 15% of the mass of the manufactured capital, approximately half is due to plastics, paper, and solidwood, and the other half is contributed by metals, which is dominated by iron and steel. On a mass basis, the contribution of all other metals is minute.[5] Aluminum and copper come in at a very distant second and third (see Figure 3). However, metals play a central and crucial role in every

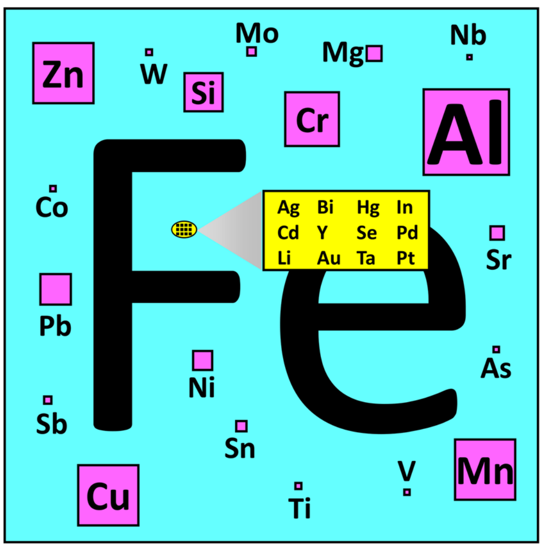


Figure 3. Rough approximation of the levels of the global production of metals. The production level of Fe is represented by the entire blue square. The production levels of the other metals in the pink and yellow squares are represented by the areas of the squares. Data used for the creation of this figure came from ref 6.

aspect of our modern society, and consequently, we need to be cognizant of how we use these precious resources and their fates in products containing them at the end-of-life.

Life Cycle of a Metal in the Anthroposphere

For there to be a sustainable perspective to modern society's use of metals, the entire life cycle of a metal in a product must be considered. This type of cycle is labeled an anthropogenic cycle. It has been described as the "quantitative characterization of the flows of a specific material into, within, and from a given system".[7] Graedel and co-workers have identified four key stages in the life cycle of a metal: (1) production, (2) fabrication and manufacturing, (3) use, and (4) waste management and recycling.[7] Figure 4 provides a schematic

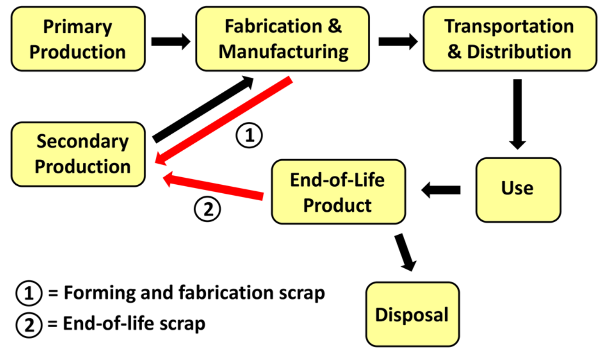


Figure 4. Life cycle of a metal in the anthroposphere.

diagram of the life cycle of a metal in the anthroposphere. This diagram is the author's creation but draws heavily from several sources, including Graedel's conception. In this conception, production is subdivided into primary and secondary production. Primary production means the metal is extracted from virgin metal ores found in the lithosphere. Secondary production means the metal is obtained from recycled material. This source of metal invariably has a smaller environmental impact than the metal obtained by the primary production route. Data substantiating this claim (based on a cradle-to-gate examination) for seven metals (Fe, Al, Cu, Zn, Pb, Ni, and Mn) is available.[8] Cumulative energy demand and greenhouse gas emissions per kilogram of produced metal are compared for primary production versus secondary production.

In Figure 4, use is followed by end-of-life product, which then leads to recycling or disposal. Scrap can be generated during several stages of the life cycle, as signified by the red arrows in Figure 4. The red arrow labeled 1 corresponds to scrap generated during forming and fabrication processes, whereas the red arrow labeled 2 corresponds to end-of-life scrap. The notion of scrap arising from several life stages has been highlighted by Allwood and Cullen.[9−11] They have created detailed Sankey diagrams describing the global flow of steel[9,11] and aluminum[10,11] from liquid metal to end-use goods. Figure 4 includes a fifth stage in the life cycle, that is, the transportation and distribution stage, which falls between fabrication and manufacturing and use. This is modeled after Ashby's approach.[12] A description of each of the stages found in Figure 4 is provided in the Supporting Information (Section S1).[13−16]

■ CRITIQUE OF THE MATERIALS TETRAHEDRON

When Figures 1 and 2 are compared with Figure 4, there are some overlapping concepts. In Figures 1 and 2, we begin with processing and end with performance. When considering these concepts in terms of Figure 4, we find ourselves in the middle of the life cycle. Processing falls in the fabrication and manufacturing stage, and performance equates with the use stage. The materials tetrahedron does not encompass the production or end-of-life stages, that is, the beginning and end of the life cycle of a metal. If we as a society want to act and live more sustainably and follow green chemistry[17] and green engineering[18] principles, the materials tetrahedron seems too narrowly focused. Put another way, the traditional materials tetrahedron does not embrace a systems approach to the

DOI: 10.1021/acs.jchemed.9b00016
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design, use, and disposal of products containing metals.[19] Holme and Hutchison have recently argued for an overarching central learning outcome for chemistry courses, namely, that chemicals have benefits and hazards, and these must be considered together.[20] I would argue that this axiom be expanded or applied to man-made or anthropogenic end products as well. Cell phones, automobiles, refrigerators, and other products have benefits and hazards, and these must be considered together.

Although the materials tetrahedron succinctly (and one might say brilliantly) describes the interconnections among processing, structure, properties, and performance, it completely ignores the energy and emissions costs involved in obtaining the metal to process and also totally ignores the fate of the product after its usefulness has ceased. This is not a sustainable way to conceive of, manufacture, use, and dispose of man-made objects.

■ MATERIALS TETRAHEDRON REIMAGINED

The proposed modification of the materials tetrahedron and its linear companion retains all the features of its original form but incorporates a sustainability/criticality component (see Figures 5 and 6). In Figure 5, the materials tetrahedron has been transformed into a materials square pyramid.

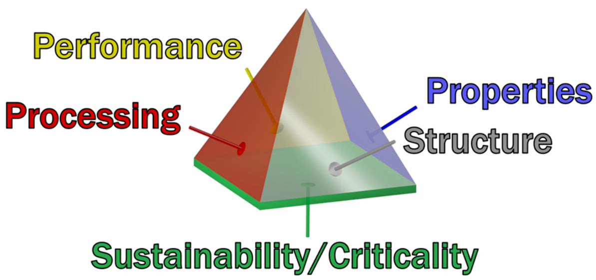

Figure 5. Materials square pyramid.

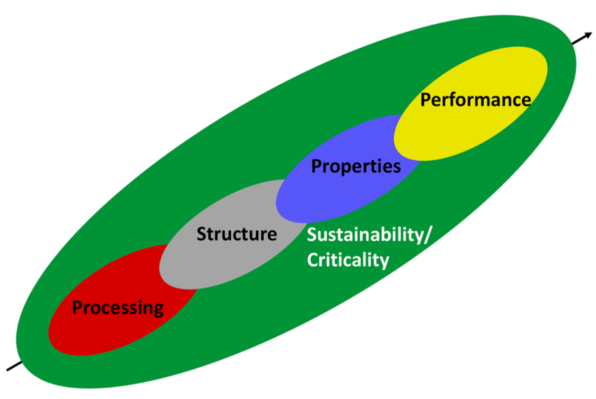

Figure 6. Linear approach with sustainability/criticality component.

The four pillars of materials science, processing, structure, properties, and performance, now occupy the four triangular faces of the square pyramid. Their importance and their interrelationships are retained in this depiction, but now these four pillars rest on a base that requires that sustainability and criticality issues be considered. The incorporation of a sustainability component into the materials polyhedron ensures the entire life cycle of the metal is considered, and the incorporation of the criticality component (described below) into the materials polyhedron addresses the issues of supply and demand challenges for the metal in question.

In Figure 6, an alternative presentation to the materials square pyramid is provided. It modifies the linear conception found in Figure 2. It retains the linear progression from processing through performance, but they are now surrounded (encapsulated) by a region labeled sustainability/criticality.

Is the reimagining of the materials tetrahedron really necessary and justified? Additionally, what is the meaning of criticality? To attempt to answer these questions, the next sections draw from research findings and observations advanced by the industrial ecology community. A brief introduction to the field of industrial ecology is provided in the Supporting Information (Section S2).[7,21−25]

Trends in Metal Usage and Recycling Rates

Research performed by the industrial ecology community allows the following trends in metal usage and recycling rates to be highlighted. The trends highlighted below are revealing. They confirm that our millennia-long dependence on metals continues but at an accelerated rate. In addition, we have, because of our ingenuity and our ever-increasing technical knowledge, begun to rely on nearly every metal in the periodic table. We use and discard some metal products at an alarming rate, and our track record as regards recycling of metals, especially scarce and critical metals, is tenuous at best. From a sustainability perspective, these findings are troubling. Note the label "metal" as used by industrial ecologists often includes the metalloids.

- The amount of metal used by modern society has dramatically increased in the last century.[6,26,27]
- A larger number of metals are being used in products than ever before.[28,29]
- Unparalleled technical advances have yielded a multitude of new devices with shorter and shorter lifetimes, creating a monumental waste and recycling challenge.[30−33]
- The level of metal recycling rates varies considerably across a wide spectrum.[34]

A more in depth treatment including examples of each of these themes is provided in the Supporting Information (Section S3).

There are several reasons for these trends: unparalleled urbanization and industrialization over the last 100−150 years,[35,36] concomitant world population growth (the global human population grew from 1.6 billion people in 1900 to 7.6 billion today),[37] and an increase in the standard of living for a larger fraction of the world's population leading to higher production and consumption rates of manufactured goods.[38] One measure of this progress is the prediction that the planet's economic middle class is expected to grow from 3 billion to over 5 billion by 2030.[39]

Causes for Raw Material Supply Shortages and Price Volatility

The aforementioned trends in metal usage have increased concerns regarding raw material supply shortages and price volatility of metals. The industrial ecology community with their systems approach to the life cycle of a metal has also examined these issues.[40−54] Insights into these challenges include:

- Some metals exhibit low natural abundance in the Earth's crust.[40]

DOI: 10.1021/acs.jchemed.9b00016
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- For some metals, the ore deposits are located in just a few countries (that might be geopolitical adversaries or might be experiencing political unrest).[41−44]
- Some metals previously little used are now in high demand because of the development of new high tech applications for the metal.[45]
- Some metals are obtained partially or exclusively as byproducts of the recovery of another metal.[46,47]
- A significant shift of resources from the lithosphere to the anthroposphere is occurring.[48−52]
- Changing geopolitics, new regulatory guidelines, and social perspectives can affect the availability and prices of resources.[53,54]

A more in depth treatment including examples of each of these themes is provided in the Supporting Information (Section S4).

Metal Criticality

Criticality, included in the proposed materials square pyramid, is a technical term developed by the industrial ecology community. Here, I embrace the definition and methodology for criticality developed by T. E. Graedel and his colleagues at the Center for Industrial Ecology at Yale University. Their methodology assesses the criticality of a metal along three dimensions: supply risk, environmental implications (i.e., impact on human health and ecosystems), and vulnerability to supply risk.[25] Criticality periodic tables have been published: one for supply risk, one for environmental implications, and one for vulnerability to supply risk.[55,56] Another payoff to this approach is the generation of criticality space maps, which have been published for >60 elements.[55,57−61] A more in depth treatment of criticality is provided in the Supporting Information (Section S5).[62−64]

Materials Tetrahedron versus Materials Square Pyramid: Three Examples

Replacing the materials tetrahedron with the materials square pyramid removes the blinders from the traditional symbol of the materials science engineering paradigm.

Lead Solder. Lead solder (i.e., 60/40 tin−lead solder) was the solder of choice in the electronics industry and other industries for many decades. Its performance characteristics are impressive.[65] One might even say it could be the poster child for the materials tetrahedron. However, it was eventually abandoned by the electronics industry because it posed a serious hazard to human health and the environment. Use of the materials tetrahedron championed 60/40 tin−lead solder. On the other hand, use of the materials square pyramid would raise a red flag, because criticality considerations in the environmental implications domain are factored into the analysis of the suitability of this metal alloy.

Cobalt in Lithium-Ion Batteries. In a recent Sponsored Content article appearing in C&EN, the statement was made that "for electric vehicles to move forward, cobalt must be left behind".[66] Lithium cobalt oxide, $LiCoO_2$, was the original intercalation cathode material used in Li-ion batteries and debuted in 1991. Now, however, the goal is to eliminate the use of cobalt as much as possible because "cobalt is a limited and expensive component". The United States imports three-quarters of the cobalt it uses.[44] Only 15% of the cobalt is obtained from cobalt minerals; 50% is obtained as a byproduct from nickel ores, and the remaining 35% is obtained as a byproduct from copper ores.[46] Fifty-eight percent of global cobalt production originates from the Congo.[44] Use of the materials square pyramid would highlight the issues of supply risk and vulnerability to supply risk, whereas the materials tetrahedron does not.

Rare Earth Elements (REE) in Magnets. Although electric vehicles account for only 0.3% of the over 1 billion cars on the road today, this number is expected to increase dramatically over the next two decades, from 3.1 million vehicles in 2017 to 157 million vehicles by 2030.[66−68] This has led to concerns on the part of the automakers about the availability and cost of metals such as lithium, cobalt, and the rare earth elements (REEs). Electric vehicles depend on electric motors. Electric motors, in turn, depend on permanent magnets that are invariably composed of REEs and more specifically neodymium in the form of $Nd_2Fe_{14}B$. Fearing the availability of REEs will decrease and their cost will increase, Toyota has set about reducing its reliance on REEs in the permanent magnets that it depends on.[68] It has already eliminated its use of terbium (Tb) and dysprosium (Dy), used to improve the heat resistance of the neodymium magnets, and is reducing the amount of neodymium in its magnets by replacing it with low-cost lanthanum and cerium. This reflects the use of the concepts of criticality and substitutability[56] in their choice of magnets, concepts incorporated in the materials square pyramid but not the materials tetrahedron.

Critics of the proposed materials square pyramid might argue that if problems arise with the original formulation, the issue will be addressed and corrected as the three examples above illustrate. However, this view is reactionary: if a problem arises, we will fix it. On the other hand, the materials square pyramid provides a proactive approach to metals selection. It requires us to consider the entire life cycle of the metal and better allows us to anticipate problems and challenges. This is not unlike the shift in the chemical industry from pollution control and abatement to pollution prevention.[69]

Are our current rates of metal consumption sustainable? Graedel and Klee have proposed a four-step process for establishing an appropriate (i.e., sustainable) rate of use of resources and conclude that in the United States, the consumption of zinc and germanium (the two metals examined in the study) is unsustainable.[70] Henckens et al. have addressed metal scarcity and sustainability by dividing 42 metals into four categories. They highlight the following eight metals and metalloids as being the scarcest: antimony, bismuth, boron, copper, gold, molybdenum, rhenium, and zinc.[71] Again, the materials square pyramid seems better suited to address these challenges than the traditional materials tetrahedron.

■ CONCLUSION

In this commentary, I offer an infographic (the materials square pyramid and its linear companion) better suited to face the materials challenges of the 21st century. My inspiration for this infographic came from two decades of teaching a two-semester general chemistry sequence to undergraduate engineering students (using the theme of *Chemistry and the Automobile*, which emphasizes the topics of energy, materials, the environment, and sustainable practices).[72] The challenges highlighted here need to be addressed by the entire STEM community, not just engineers. I encourage the chemistry community to champion the sustainable production, use, and recycling of metals with the same fervor that we have tackled the issue of climate change. To quote T. E. Graedel and his co-workers, "the consideration of possible futures of metals is every bit as important as those of energy, water or climate."[73]

DOI: 10.1021/acs.jchemed.9b00016
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Every facet of our modern society depends on metals: transportation, housing, commerce, industry, and communications.

The issues emphasized here can be addressed in a variety of chemistry courses (e.g., general chemistry, inorganic chemistry, and special topics courses, among others). Suggestions on how the concepts presented in this commentary can be utilized in the chemistry curriculum are provided in the Supporting Information (Section S6).

I have had former engineering students who completed general chemistry with me and went on to complete an engineering course entitled *An Introduction to Materials Science and Engineering* read and comment on this article. They all acknowledge that sustainability was not a topic addressed in the aforementioned engineering course, and they support the notion that materials square pyramid would yield better design choices than the traditional materials tetrahedron.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.9b00016.

> Explanation of the different stages in the life cycle of a metal, as illustrated in Figure 4; brief introduction to the field of industrial ecology; trends in metal usage; causes for raw material supply shortages and price volatility; metal criticality as conceived by the Center for Industrial Ecology at Yale University; and suggestions on how to integrate the main concepts presented in this commentary into the chemistry classroom (PDF, DOCX)

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Notes

The author declares no competing financial interest.

■ ACKNOWLEDGMENTS

The author gratefully acknowledges the technical assistance of Liz McDowell, Director of UM-D's Science Learning Center, in the preparation of the figures and the graphical abstract.

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(23) Definition:

> *Industrial ecology is the study of the flows of materials and energy in industrial and consumer activities, of the effects of these flows on the environment, of the influences of economic, political, regulatory, and social factors on the flow, use and transformation of resources. The objective of industrial ecology is to understand better how we can integrate environmental concerns into our economic activities.*

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