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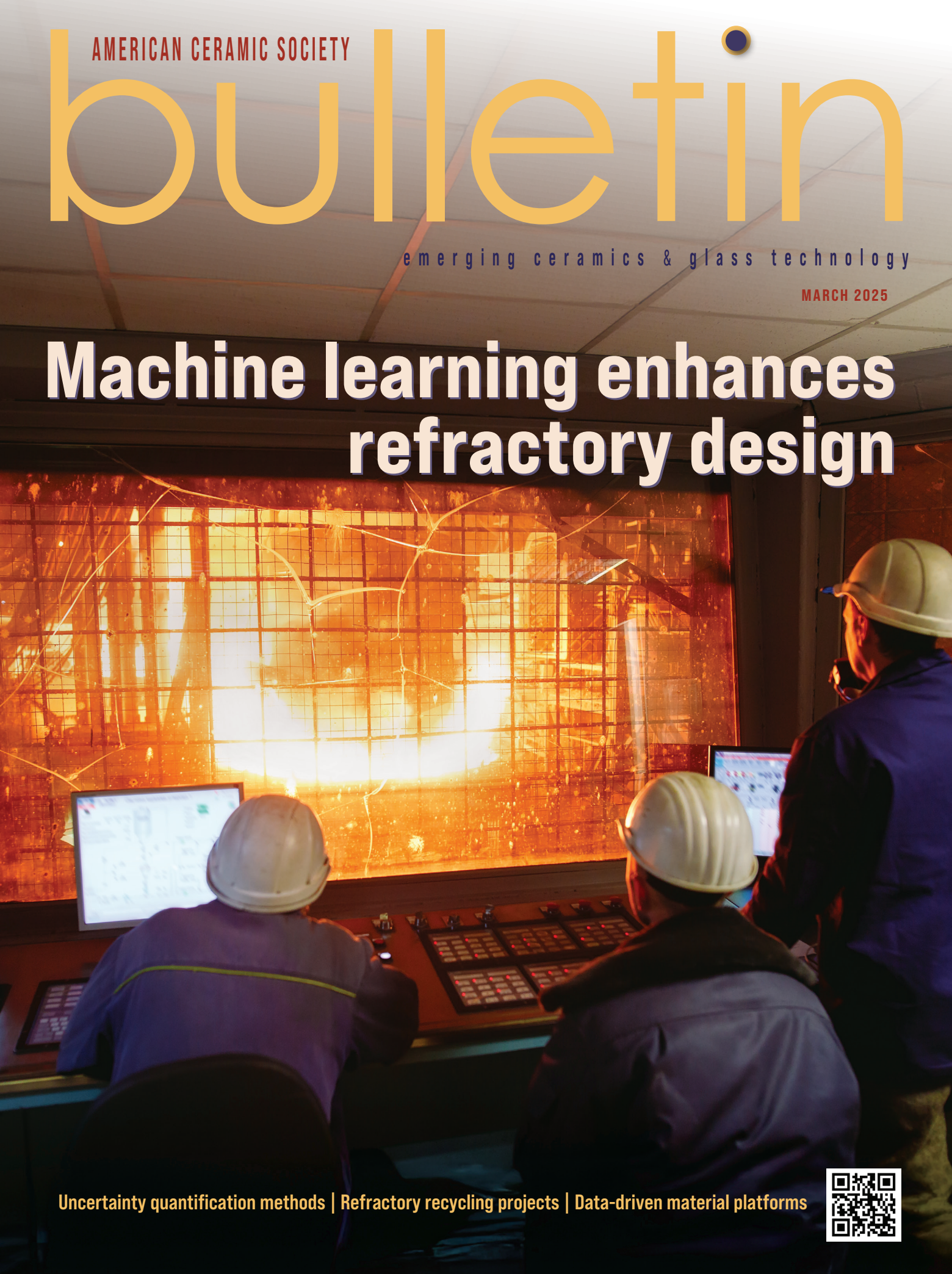
MARCH 2025

Machine learning enhances refractory design



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contents

March 2025 • Vol. 104 No.2

feature articles

departments

industry

columns

meetings

resources

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March 2025 • Vol. 104 No.2

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As seen on *Ceramic Tech Today*...

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Firebricks: A cost-effective alternative to battery energy storage for process heating

Thermal energy storage can be a more cost-effective approach to energy storage than batteries for industrial processes. Stanford University researchers investigated the potential impact of widespread use of firebrick-based thermal energy storage systems on global energy costs.

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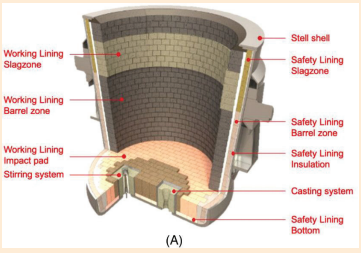

Credit: Gajjar et al., *ACT*

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ACSBA7, Vol. 104, No. 2, pp. 1–48. All feature articles are covered in Current Contents.

The Lobito Corridor: Inside the railway connecting mineral supply chains in Africa

As reported in the United States Geological Survey's Mineral Commodity Summaries 2024, the U.S. government has been hard at work supporting the launch of numerous mineral exploration and feasibility surveys as well as nascent mining projects in various states. But even if these projects are successful, the U.S. will still need to source some minerals from afar because of overwhelming demand for certain minerals and lack of local sources for others. In this regard, the U.S. government has involved itself with the Lobito Corridor initiative in sub-Saharan Africa.

Lobito Corridor: History and current status

The Lobito Corridor refers to a stretch of railway infrastructure that winds through mineral- and oil-rich parts of sub-Saharan Africa (Figure 1). It is viewed as a way to transport raw material quickly and efficiently from landlocked African mines to shipping ports, where it can be exported to refining hubs in other countries.

The rail route was established in the early 1900s and thrived until the mid-1970s, when damage sustained during the Angolan Civil War curtailed its use. It remained underutilized until the 2010s, when the Chinese government funded and conducted a nearly $2-billion rehabilitation effort to modernize the railway between 2006–2014.

Today, the railway is controlled by the Lobito Atlantic Railway company, a joint venture between Swiss commodities trader Trafigura, Portuguese construction company Mota-Engil, and Belgian private railway operator Vecturis. The company secured a 30-year concession in July 2023 to provide railway services on the condition that it would invest $455 million in Angola and $100 million in the Democratic Republic of the Congo.

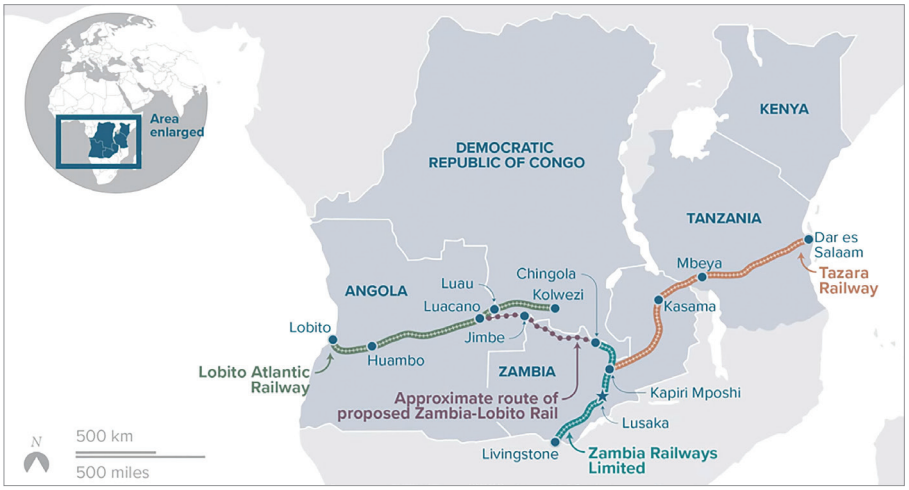

Figure 1. A map showing the main railway routes in sub-Saharan Africa. The U.S. and European Union are supporting the modification and expansion of the west section run by the Lobito Atlantic Railway company.

Development of the Lobito Corridor

In May 2023, during the G7 Summit in Japan, U.S. President Joe Biden announced the U.S. would support development of the Lobito Corridor as part of the Partnership for Global Infrastructure and Investment (PGII).

PGII is a collaborative effort by the intergovernmental Group of Seven. It aims to fund infrastructure projects in developing nations, and the Lobito Corridor is the first strategic economic corridor launched under the partnership.

In September 2023, the U.S. and European Union announced they had teamed up to support Lobito Corridor development, including launching feasibility studies for a new rail line from Angola through Zambia's Copperbelt region.

In October 2023, during the two-day Global Gateway Forum in Brussels, Belgium, delegates from the U.S., the European Union, the DRC, Zambia, Angola, African Development Bank, and Africa Finance Corporation signed a memorandum of understanding to cooperate on the Lobito Corridor development. This memorandum is on the back of a January 2023 agreement between the governments of Angola, the DRC, and Zambia to cooperate and harmonize relevant regulations.

Limitations of the Lobito Corridor

Though development of the Lobito Corridor will make transport of minerals within Africa easier, it may not secure critical mineral supply chains like the U.S. hopes, as explained in a *Harvard International Review* article by deputy managing editor Isabelle King.

The first limitation is that Chinese firms own 15 out of the 19 major mines in the DRC, and the remaining four often sell their raw material to China. So, "The mere existence of a Western-friendly railway with an Atlantic orientation does not directly lead to Western acquisition of the metal," King explains.

On top of that, even though the Lobito Atlantic Railway operates the rail lines, two Chinese firms won the public tender for the port of Lobito in 2022. These firms now hold the rights to operate the port for 20 years.

Finally, the Lobito Corridor is not the only mine-to-port railway in southern Africa. In February 2024, China announced plans to invest more than $1 billion to upgrade a rival set of tracks, the Tazara Railway, which runs eastward from the Zambian copper mines to the Indian Ocean port of Dar es Salaam.

Despite these limitations, on Jan. 23, 2025, the U.S. reaffirmed it will maintain its investments irrespective of the transition to the administration of President Donald Trump. ■

Corporate Partner news

Niterra announces partnership with Japan's largest class open innovation hub

Niterra Co., Ltd. announced that it will be serving as a partner company in Japan's largest class open innovation hub, STATION Ai. The goal is for Niterra, a manufacturer of spark plugs and sensors, to continue creating new businesses through this collaboration. STATION Ai opened in Nagoya, Japan, in October 2024. Read more: https://www.ngkntk.co.jp/english/news

Thermal Technology expands with new facilities

Thermal Technology LLC is expanding its current facilities in Nevada to accommodate two subsidiaries: Thermal Material Processing Company and Machinist Group. Thermal Technologies provides high-quality thermal processing equipment solutions. Read more: https://www.thermaltechnology.com/category/news

Höganäs-North American commits to reforestation in Germany

Höganäs teamed up with the State Forestry of Lower Saxony at the end of 2022 to plant trees in the Harz region, which is near Höganäs' site in Goslar, Germany. Höganäs planted the first 2,000 trees in 2023 and an additional 2,000 in 2024. Read more: https://www.hoganas.com/en/news-and-events/#news

JADCO Manufacturing receives ISO 9001 certification

JADCO Manufacturing, which is known for its alloy and abrasion-resistant steel products, achieved ISO 9001 certification. This certification demonstrates JADCO Manufacturing's commitment to international standards for quality management systems. It is distributed by the Performance Review Institute. Read more: https://jadcomfg.com/about-us/news ■

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Green hydrogen: Global markets

The global market for green hydrogen was valued at $4.4 billion in 2023 and is expected to grow at a compound annual growth rate (CAGR) of 48.7% to reach $38.1 billion by 2029.

Hydrogen does not produce carbon dioxide when burned, and so it is increasingly seen as an option for decarbonizing sectors where direct electrification or other low-carbon options may not be technologically or economically feasible, such as heavy industry and long-distance transport. The methods used to produce hydrogen, however, greatly determine its overall impact on the environment.

- **Grey hydrogen** is produced by steam methane reforming (SMR) of natural gas or coal gasification and uses methane or coal as feedstock.
- **Blue hydrogen** is produced by SMR of natural gas or coal with carbon capture and uses methane or coal as feedstock.
- **Turquoise hydrogen** is produced by pyrolysis and uses methane as feedstock.
- **Pink hydrogen** is produced by water electrolysis, using nuclear energy as feedstock.
- **Green hydrogen** is produced by water electrolysis, using renewable energy as feedstock.

As of 2024, green hydrogen occupies less than a 1% share of global hydrogen demand. But it is expected to increase to about 15% by 2030 as industries and governments shift toward low-emission fuels to achieve their net-zero emission targets in various sectors (Table 1).

Most green hydrogen is produced using alkaline and PEM electrolyzers. Other technologies, such as solid oxide electrolyzers and anion exchange membranes, are gaining traction but have not yet been fully commercialized.

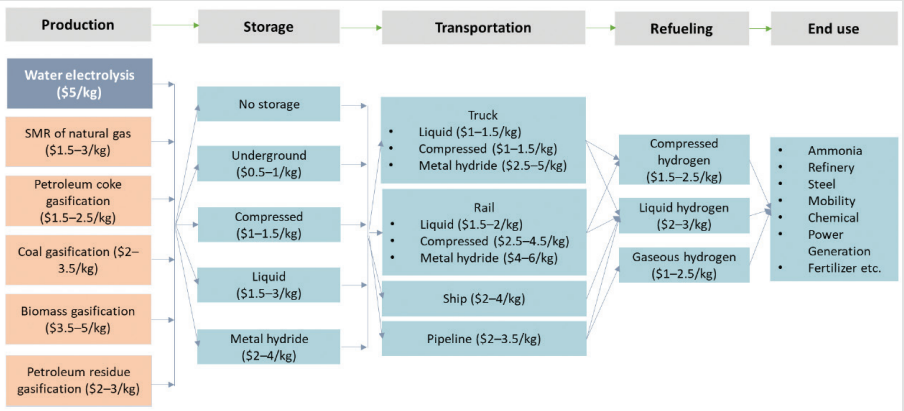

Figure 1. Value chain analysis of the green hydrogen market. The prices given in the figure are based on the year 2024.

The final cost of using green hydrogen is significantly influenced by the costs associated with purification, storage, distribution, and conversion, which vary depending on the specific value chain path. Figure 1 provides a detailed overview of a typical green hydrogen value chain along with cost analysis.

Europe holds by far the largest share of the global market for green hydrogen, with 57.0% in 2023. The Asia–Pacific region is a distant second, with 28% of the market in 2023. However, its share is expected to grow to 31.0% through 2029 due to rising investments by Chinese manufacturers to scale up renewable and electrolyzer manufacturing capacity and increasing interest by Western companies in the region's green hydrogen sector through joint ventures.

About the author

BCC Publishing Staff provides comprehensive analyses of global market sizing, forecasting, and industry intelligence, covering markets where advances in science and technology are improving the quality, standard, and sustainability of businesses, economies, and lives. Contact the staff at Helia.Jalili@bccresearch.com.

Resource

BCC Publishing Staff, "Green hydrogen: Global markets," BCC Research Report ENV060B, December 2024. https://bit.ly/BCC-December-2024-green-hydrogen ■

Table 1. Global market for green hydrogen, by end-use industry, through 2029 ($ millions)

End-use industry	2023	2024	2029	CAGR % (2024–2029)
Chemicals and petrochemicals	2,366.6	2,764.4	17,031.4	43.9
Mobility	939.9	1,201.4	12,471.9	59.7
Power	357.5	470.4	5,146.6	61.4
Other industries	701.0	798.7	3,420.1	33.8
Total	4,365.0	5,234.9	38,070.0	48.7

By Daniel Llaguno
Guest columnist

Sustainability meets intelligence—shaping the future of refractories at UNITECR 2025

In the age of the Fourth Industrial Revolution,[1] the refractory industry continues to make great strides toward adopting sustainable practices.

As most refractories are extracted from natural materials, developing environmentally friendly mining practices remains vital to the industry. Additionally, the high temperatures required during refractory manufacturing use significant energy from fossil fuels, which can contribute to greenhouse gas emissions. Common refractory materials also contain carbonate minerals that release CO_2 when heated during processing, which makes it challenging to immediately reduce greenhouse gases in this sector.[2]

Despite some of the challenges that come with fostering a sustainable future in the refractory industry, there are also many opportunities on the horizon. For example, the carbon footprint of the refractory industry can be reduced by using renewable energy to power industrial processes, implementing water waste management and storage protocols, and reusing mining waste.[3]

Also, methods to recycle, reuse, and responsibly source refractory raw materials have gained traction. In 2023, the European Union adopted the Critical Raw Materials Act (CRMA), with one goal being to increase the EU's domestic ability to extract, process, and recycle critical raw materials by 2030.[4] In June 2023, the EU announced proposals to emphasize this aspect of the CRMA, with goals to raise the level of processing capacity to 50% and recycling capacity to 20%.[5]

Looking ahead, emerging technologies such as artificial intelligence (AI) and machine learning (ML) can help support sustainability through better mining, manufacturing, and use of refractory materials. For example, from an equipment maintenance perspective, AI and ML algorithms can recognize patterns in data, effectively minimizing energy consumption. Digital sensors in kilns can keep track of conditions in real time, while predictive algorithms can anticipate equipment malfunctions or refractory corrosion through analyzing historical equipment data.[6]

These technologies can also minimize risk to employees and improve safety measures in the workplace. Due to the high temperatures used in blast furnaces, it is nearly impossible to predict the state of the inner refractory lining without shutting down the machine for human assessment.[1] AI and ML technologies may also affect areas such as thermal efficiencies, pollution mitigation, and waste reduction, which all have strong impacts on sustainability.

In recognition of the refractory industry's sustainability efforts, the theme for this year's Unified International Technical Conference on Refractories (UNITECR) is "Sustainability Meets Intelligence – Shaping the Future of Refractories." The goal is to spark conversations around sustainability in the refractory industry through collaborating with all types of refractory industry sectors, including extraction, processing, manufacture, deployment, maintenance, and recycling.

UNITECR 2025, which will take place in Cancun, Mexico, on Oct. 27–30, 2025, invites everyone with an interest in these topics to join the conversation and push boundaries in an enlightening atmosphere. Visit https://unitecr2025.com to register for UNITECR 2025 and learn even more about sustainability in the refractory industry.

About the author

Daniel Llaguno is president of ALAFAR and UNITECR 2025. Contact Llaguno at daniel@unitecr2025.com.

About UNITECR

The first Unified International Technical Conference on Refractories (UNITECR) took place in Tokyo, Japan, in 1987. Founding members include The American Ceramic Society, Latin American Association of Refractories Manufacturers, German Refractories Association, and Technical Association of Refractories, Japan.

Since its inception, the biennial conference has served as an influential forum for the international refractories community to exchange industry ideas and knowledge. This year, the organization of UNITECR is led by president Daniel Llaguno and vice president Jessica Fernández. ■

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By David Holthaus
Industry reporter

Refractory recycling: A potential key to meeting sustainability goals

Makers of refractories, like other manufacturers around the world, are under pressure to manage their impact on the environment as the threats related to global warming become more evident. Shareholders, customers, local and national governments, and advocacy organizations are, in many cases, holding manufacturers accountable for meeting sustainability goals.

Many industrial manufacturers, such as France-based multinational group Imerys S.A.,[1] have established sustainability programs at their companies to research and implement new practices, materials, and systems that reduce their environmental impact.

Among the various strategies to manage environmental impact, recycling offers both environmental and economic benefits for refractory manufacturers. On the environmental side, replacing primary raw material sources with a recycled mineral could potentially reduce the carbon footprint of mixed refractory linings by almost 60%, with a nearly 90% reduction possible for monolithic refractories.[2] On the economic side, recycling refractories helps manufacturers reduce their reliance on refractory raw material supply chains, which currently are caught up in tense geopolitical dynamics.[3]

One of the world's largest refractory manufacturers, Austria-based RHI Magnesita, has committed to ramping up its recycling strategy. The effort is seen as playing a key part in reducing both carbon emissions and landfill waste, as including 10% recycled material in its refractory products can prevent approximately 150,000 metric tons of material from going to landfills, according to the company.

RHI's recycling strategy includes establishing onsite recycling solutions for used refractories at customer sites; setting up recycling facilities at its own production sites; and developing formulas that include recycled content in a range of its products.

Credit: RHI Magnesita

At RHI Magnesita's plant in York, Pa., a team examines crushed material that can be used as recycled secondary raw material in production.

"For us, it is not only being able to reclaim materials, but we also have a business model where we're supporting the customers directly with our onsite solutions for recycling," says Craig Powell, RHI's regional president of North America, in an interview. "It's a value-added service that we are willing and excited to provide to our customers."

Implementing these strategies has not been without challenges. For example, though the executive leadership of RHI's customers may view progress in sustainability as a key goal, at the plant level, sometimes there is resistance to using recycled materials. However, year by year, the data shows that the company is successfully gaining support for its recycling initiatives, according to Nicole Sweet, RHI's head of end-to-end recycling in North America.

"In 2022, the overall percentage of raw materials that came from recycled sources in North America grew from 5.5% to 12.7%," Sweet says in an interview. "Our overall target globally in 2024 was 13.8%, and we came in at 14.2%."

The company plans to continue expanding its recycling programs, and the acquisition of Pittsburgh-based Resco Group will further that goal, Powell says.

Currently, about half of RHI Magnesita's U.S. sales are not produced in the country. The acquisition of Resco Group, which produces a wide range of refractories, will increase local production in North America by transferring significant volumes from non-U.S. plants to the seven Resco plants and two raw material sites in the U.S. That will expand recycling opportunities as well as reduce production lead times and improve supply chain security, the company says in a press release.

Recycling is also part of the overall sustainability strategy of Calderys, the multinational Paris-based refractories maker. According to Aurelie de Chassey-Hayot, Calderys' global vice president of communications and sustainability, the company is working to develop circular

economy business models starting from the design stage.

This approach allows for the incorporation of systems to reduce the consumption of virgin raw materials and increase the use of reclaimed minerals. For example, Calderys works with third-party processors at customer facilities to sort and process the spent material, and it handles some processing at its own facilities to create material that can be reintroduced into products.

"These processes help our customers reduce landfill use, reduce inventory, and free up space," de Chassey-Hayot says. "For us, it's a great material to recycle and reuse in our products."

As an example of these processes, Calderys developed a closed-loop program in North America for its MagCarbon product line used in iron and steel production and cement manufacturing. Calderys obtains spent refractory from its customers and processes it, making sure product performance is preserved. The company is working to expand the effort into other portfolio areas in the U.S.

Calderys has similar projects globally. In its two facilities in Türkiye, about 7.5% of the materials used in production were recycled materials in 2023. Some of the materials came from its customers, and some were purchased on the market. Calderys plans to expand the program into other countries, including India and Taiwan, says de Chassey-Hayot.

Ultimately, the market for refractory recycling is prime for growth. As more manufacturers adopt initiatives similar to RHI Magnesita and Calderys, the market for recycled materials could become a leading "refractory mineral resource."[4]

About the author

David Holthaus is an award-winning journalist based in Cincinnati, Ohio, who covers business and technology. Contact Holthaus at dholthaus@ceramics.org.

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SOCIETY DIVISION SECTION CHAPTER NEWS

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Northern California Section hosts Teacher Training Workshop for Materials Science Classroom Kits

The ACerS Northern California Section (NorCal), in collaboration with the Ceramic and Glass Industry Foundation (CGIF), Manufacturing Enterprise Solutions Association (MESA), and National Science Foundation, hosted a Teacher Training Workshop at the University of California, Davis on Oct. 27, 2024.

The goal of the event was to train 11 high school teachers from different high schools in the Sacramento area, in addition to nine MESA staff, how to use the ACerS Materials Science Classroom Kits. Twelve kits were donated to each of the high schools and MESA staff through the support of the CGIF.

The event was led by ACerS NorCal chair Scott McCormack (UC Davis) and his graduate students Fox Thorpe and Nicole O'Shea. The MESA team included Carla Thompson and Catherine Sencion, who identified the teachers and coordinated the meeting venue.

In total, the event attracted 20 participants. Three teachers returned from last year, who were allowed to present their experiences using the kits in the classroom with the students. The Section intends to expand this event in 2025 to include 20 schools in the Sacramento area. ■

Participants in the Teacher Training Workshop held at the University of California, Davis. First row (left to right): Catt Sencion, Carla Thompson, Maria Aguilar, Nicole O'Shea, Scott McCormack, Toyin Malomo, Carmen Wright, Tessa Heavlin-Martinez, Katie Blackwood, and Miguel Ramerez.
Second row (left to right): Lissette Rodriguez, Jason Turner, Erika Ruiz, Raith Orellana, Scarlet Coronel, Pravel Martinez, Eddie Salazar, Ciro Cervantes, Jeremy Heavlin-Martinez, Miguel Moreno, Fox Thorpe, Ronald Peters, and Marty Hall.

FOR MORE INFORMATION:

ceramics.org/spotlight

Dayton/Cincinnati/Northern Kentucky Section holds Section meeting

The ACerS Dayton/Cincinnati/Northern Kentucky Section members had a Section meeting on Dec. 13, 2024, at Shank Conference Room in Wright Memorial Public Library to elect new leadership for 2025:

- Chair: **Hyunjun Kim**, BlueHalo
- Secretary: **Patricia Loughney**, Air Force Research Laboratory
- Treasurer: **Charis Lin**, BlueHalo
- Social/outreach chair: **Donglu Shi**, University of Cincinnati ■

The 2025 leadership team of the ACerS Dayton/Cincinnati/Northern Kentucky Section. From left: Charis Lin, Donglu Shi, Hyunjun Kim, and Patricia Loughney.

ACerS International Türkiye Chapter hosts 'MA Guide: Alumni—Decide Your Way in the Industry'

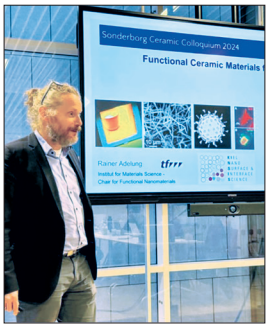
The ACerS Material Advantage Chapter at Eskişehir Technical University in Türkiye worked with the ACerS International Türkiye Chapter to organize an event called "MA Guide: Alumni—Decide Your Way in the Industry." This event, held on Dec. 22, 2024, brought together several alumni to share their career journeys and insights with current students:

- **Betül Özcan**, quality control and R&D engineer at Metko Hüttenes-Albertus
- **Ali Şanlı**, research and development executive at Kümaş
- **Uğur Cengiz**, general manager at Bilecik Demir Çelik ■

Attendees at the ACerS International Türkiye Chapter event "MA Guide: Alumni—Decide Your Way in the Industry."

ACerS International Nordic Chapter hosts roundtable on smart ceramics

The ACerS International Nordic Chapter hosted a roundtable about smart ceramic materials at the University of Southern Denmark on Dec. 10, 2024. The roundtable discussed new horizons in ceramics, including material development, properties, and applications. ■



Left: Attendees at the ACerS International Nordic Chapter roundtable event.

Right: Rainer Adelung, chair of the Functional Nanomaterials group at the Institute for Materials Science, CAU Kiel, shares the research taking place in his group during the roundtable event.

WEBINARS TO WATCH

Check out these recent additions to the ACerS Webinar Archives:

COMPUTER-AIDED SUSTAINABLE CEMENT MANUFACTURING AND MATERIALS: MODELING, VIRTUAL DESIGN, AND OPTIMIZATION
Original air date: Dec. 11, 2024
Hosted by: Cements Division
Featured speaker: Chengcheng Tao

BRIDGING THE GAP IN MATERIALS SCIENCE: EMPOWERING ECRS AND INSPIRING STEAM CAREERS THROUGH PODCASTING AND SCIENTIFIC OUTREACH FOR KIDS AND ADOLESCENTS
Original air date: Dec. 16, 2024
Hosted by: ACerS International Italy Chapter
Featured speaker: Erika Iveth Cedillo-González

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Volunteer Spotlight: Amjad Almansour and Sepideh Akhbarifar

ACerS Volunteer Spotlight profiles members who demonstrate outstanding service to the Society.

Amjad S. Almansour is materials research engineer in the Ceramic and Polymer Composites Branch of the Materials and Structures Division at the NASA Glenn Research Center in Cleveland, Ohio. He has made significant contributions in several research areas, including the design, processing, modeling, and characterization of ceramic matrix composites for advanced propulsion systems; lightweight composite conductors; high-power and energy-dense 3D-printed batteries; and battery thermal management systems.

Almansour has been the lead organizer of several symposia at the ICACC and PACRIM conferences and previously served as chair of the Awards Committee. He is currently chair-elect of the Engineering Ceramics Division and program chair for ICACC 2025. He has received the ECD Global Young Investigator Award, Global Star Award, Richard M. Fulrath Award, and Global Ambassador Award.

Sepideh Akhbarifar is research scientist in the Vitreous State Laboratory and assistant professor of mechanical engineering at The Catholic University of America in Washington, D.C. She leads research on thermoelectric phenomena in bulk oxide ceramics, metal–insulator transitions, quantum physical processes, materials synthesis, multiscale characterization, and statistical modeling. She also conducts research on CO-reducing geopolymer materials and high-efficiency dust removal systems.

Akhbarifar has actively contributed to organizing symposiums and sessions at major materials science conferences, including MRS and MS&T, focusing on thermoelectric materials. She currently serves as program chair of the Energy Materials and Systems Division and is outgoing chair of the D.C./Maryland/Virgina Section.

We extend our deep appreciation to Almansour and Akhbarifar for their service to our Society! ■

ACerStudent Engagement: Rajat Durgesh Ramteke

Rajat Durgesh Ramteke is a Ph.D. student in materials engineering at the University of Alabama at Birmingham. He is an active member of ACerS Global Graduate Researcher Network (GGRN) and has been recognized with an award from The Refractories Institute.

"Being a part of ACerS GGRN and the Refractory Ceramics Division has provided me with valuable opportunities to engage with professionals and peers. Through these affiliations, I have attended the annual Refractories Symposium and presented my research at the 2024 Pan American Ceramics Congress and Ferroelectrics Meeting of the Americas."

You can take advantage of these opportunities as well by becoming a student member of ACerS. Visit https://ceramics.org/membership/types-of-membership to learn more. ■

Names in the News

Members—Would you like to be included in the Bulletin's Names in the News? Please send a current head shot along with the link to the article to mmartin@ceramics.org.

Bikramjit Basu, FACerS, full professor at Indian Institute of Science, Bangalore, was appointed director of the Central Glass & Ceramic Research Institute in Kolkata, India.

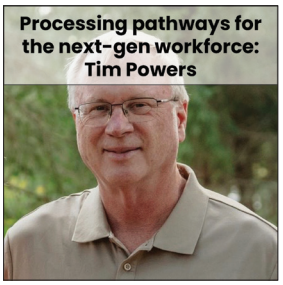
Richard Brow, FACerS, DLM, Curators' Distinguished Professor of materials science and engineering at Missouri S&T, and **Shibin Jiang**, FACerS, president and CEO of AdValue Photonics Inc., were inducted into the National Academy of Inventors 2024 Class of Fellows. ■

more MEMBER HIGHLIGHTS

Ceramic Tech Chat: Perena Gouma and Tim Powers

Hosted by ACerS Bulletin editors, Ceramic Tech Chat talks with ACerS members to learn about their unique and personal stories of how they found their way to careers in ceramics. New episodes publish the third Wednesday of each month.

In the November 2024 episode of Ceramic Tech Chat, **Perena Gouma**, the Edward Orton Jr., Chair in ceramic engineering at The Ohio State University, describes how she became interested in breath and gas-based diagnostic tools, explains how electrospinning can be used to fabricate components for these devices, and shares her passion for educating students and the public about these discoveries.



In the December 2024 episode of Ceramic Tech Chat, **Tim Powers**, retired engineering design lead at Owens Corning, shares his personal experiences working on some of the most well-known products produced by Corning and Owens Corning and describes how he is now supporting the next generation of the ceramic and glass workforce through the Ceramic and Glass Industry Foundation.

Listen to Gouma's and Powers' whole interviews—and all our other Ceramic Tech Chat episodes—at https://ceramictechchat.ceramics.org/974767. ■

IN MEMORIAM

Burton Brubaker

Arthur Waugh

AWARDS AND DEADLINES

Nomination deadlines for Division awards: May 15, 2025

Contact: **Vicki Evans | vevans@ceramics.org**

Division	Award	Deadline	Contacts	Description
GOMD	Alfred R. Cooper Scholars Award	May 15	Steve Martin swmartin@iastate.edu	Recognizes undergraduate students who demonstrated excellence in research, engineering, and/or study in glass science or technology.
ED	Edward C. Henry Award	May 15	Christina Rost cmrost@vt.edu	Recognizes an outstanding paper reporting original work in the *Journal of the American Ceramic Society* or the *Bulletin* during the previous calendar year on a subject related to electronic ceramics.
ED	Lewis C. Hoffman Scholarship	May 15	Christina Rost cmrost@vt.edu	Recognizes academic interest and excellence among undergraduate students in ceramics/materials science and engineering.

Ceramic and Glass Industry Foundation welcomes new program manager

Growing up in rural northeast Ohio, Danielle Wilmot did not know about all the career opportunities that exist in science—which is one reason why she looks forward to serving as the new program manager for the Ceramic and Glass Industry Foundation (CGIF).

Wilmot has a background in both teaching and nonprofits, specifically with a focus on legal education. She hopes to bring a unique perspective to the CGIF as someone who has worked in education not only inside the classroom but outside of it, too.

"When I was a young student, I didn't know all the opportunities that existed in the legal community for people, and similarly, we really didn't have a lot of STEM programming at my school," Wilmot says. "I really am excited about the opportunity to share those things, because who knows if I would have pursued a career in STEM or law if I hadn't discovered they existed."

Looking ahead, she is excited to dive into the CGIF's programs and spread awareness about the opportunities that ceramic and glass science can provide to students and their teachers.

Given her background in education regarding the law, Wilmot also looks forward to programs such as Congressional Visits Day, when Material Advantage students meet with legislators and congressional staff to educate Congress on the importance of research in materials science.

"I think that is an exciting concept, of being able to take students and show them you also have the voice for change," she says. "You're really the next generation of people who we want to be, and you can get people to pay attention and make sure our representatives are aware of the importance of materials science."

Wilmot is also passionate about reaching rural communities such as the one she grew up in, and she hopes to spread awareness about ceramic and glass materials science to those areas in her role as program manager. She feels grateful for the ability to leave a positive impact on students from a role outside of the classroom.

"Part of the reason I went into teaching is I just had some really amazing teachers. I think that amazing teachers make all the difference," she says.

Outside of her professional life, Wilmot enjoys reading and exploring Columbus with her husband and their dog.

Visit https://foundation.ceramics.org/about/programs for a complete list of CGIF program offerings. ■

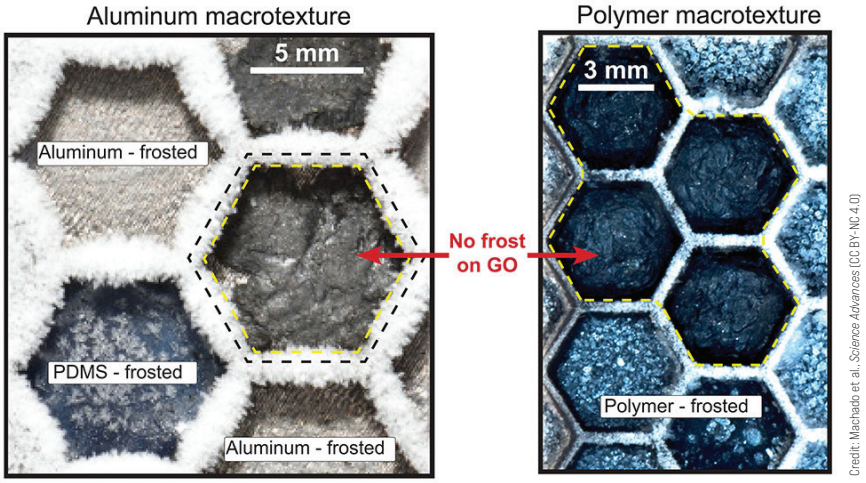
Frost-free surfaces: Leaf-inspired technique offers scalable, robust frost prevention

Researchers at Northwestern University in Illinois developed a hybrid technique to achieve stable and scalable frost protection using graphene oxide-coated textured surfaces.

Unwanted frost accumulation is a major concern across industrial, residential, and government sectors. Heaters and wind machines can help actively prevent frost formation, but passive mechanisms are needed as well to achieve widespread low-cost, low-energy protection.

Current passive methods for frost resistance generally involve either 1) altering a surface's chemistry and topography to generate nonwetting surfaces or 2) infusing the surface with lubricants to delay the onset of frosting. However, many nonwetting surfaces are vulnerable to damage of the micro/nanotextures, which leads to a marked increase in ice adhesion. Meanwhile, lubricant-infused surfaces lose their function as the lubricating layer depletes.

The Northwestern University researchers achieved stable and scalable frost-free regions by building on previous research from 2020. At that time, they showed that a leaf-inspired, millimeter-scale surface structure could theoretically reduce frost formation by up to 80%. In the new study, they coated the textured surface with a thin layer of graphene oxide.



Credit: Machado et al., *Science Advances* (CC BY-NC 4.0)

By coating a leaf-inspired textured surface with graphene oxide, frost formation can be prevented on various materials for long periods.

Graphene oxide is hygroscopic, meaning it tends to absorb moisture from the air. As a result, "the graphene oxide layer acts like a container to prevent water vapor from freezing," says senior author Kyoo-Chul Kenneth Park, assistant professor of mechanical engineering, in a Northwestern press release.

The graphene oxide layer was only 600 microns thick, but it resulted in a surface that resisted all frost formation for 160 hours. Additionally, the graphene oxide still worked effectively when scratched, cracked, and contaminated, though "work remains to fully characterize the durability with a broad variety of contaminants," the authors write in the paper.

Notably, the graphene oxide coated only the "valley" (flat) portion of the textured surface, not the peaks. The authors suggest combining the coated surface with a deicing mechanism to remove sacrificial frost from the peaks.

The open-access paper, published in *Science Advances*, is "Robust hybrid diffusion control for long-term scalable frost prevention" (DOI: 10.1126/sciadv.adq8525). ■

Materials in the news

3D architected materials that adapt and protect

Researchers from California Institute of Technology developed a new material called PAM (for polycatenated architected materials) that could have uses in areas ranging from helmets and other protective gear to biomedical devices and robotics. PAMs are made up of a variety of shapes linked together to form 3D patterns, which allows the particles to move freely relative to one another. The material thus shows a characteristic transition between fluid and solid-like behavior. Experiments with microscale PAMs have shown that they will expand or contract in response to applied electrical charges as well as physical forces. For more information, visit https://www.caltech.edu/about/news/reimagining-chain-mail.

Compact comb lights the way for next-gen photonics

Researchers at Ecole Polytechnique Fédérale de Lausanne, Colorado School of Mines, and China Academy of Science created a new ultrabroadband electro-optic comb generator that achieves an unprecedented 450 nm spectral coverage with more than 2,000 comb lines. The device consists of microwave and optical circuits on a newly developed lithium tantalate platform. Compared with lithium niobate, the lithium tantalate features 17 times lower intrinsic birefringence, which allowed for a compact design (1x1 cm^2). The device also reduces microwave power requirements almost 20-fold compared to previous designs. For more information, visit https://actu.epfl.ch/news/compact-comb-lights-the-way-for-next-gen-photonics. ■

New predictive formula offers facile estimation of ceramic armor ballistic efficacy

Jake Ganor, founder and CEO of Adept Armor (Tulsa, Okla.), proposed a new formula for predicting ballistic efficacy of ceramic materials, which he devised based on insights gleaned from developing silicon carbide and boron carbide armor systems.

In the open-access paper, Ganor explains that he noticed 7.8-mm sintered SiC performs as well as 8.3-mm sintered B_4C against steel-cored armor piercing ammunition when used in conjunction with an energy-absorbing backing layer made of ultrahigh-molecular-weight polyethylene. Thus, material density "cannot be the only thing that matters [to ballistic efficacy]," he writes, as suggested by the pioneering work of M.L. Wilkins and his associates at Lawrence Livermore National Laboratory on ceramic armor systems in the late 1960s and early 1970s.

To determine which other material properties contribute to ballistic efficacy, Ganor laid out the mechanical properties of several ceramic armor materials and then construed a series of downstream relations that linked those properties to their performance characteristics. Fitting these results to existing experimental data in an iterative process, Ganor derived the following equation:

$$BE = 1.677 \times D + 5 \times ((T \times D)/D) + 0.003 \times CS + 0.005 \times H$$

where BE is ballistic efficacy, D is density (g/cm^3), CS is compressive strength (MPa), T is thickness (mm), and H is Vickers hardness. The constants—1.677, 0.003, and 0.005—were derived from regression analysis.

Notably, quasi-static rather than dynamic compressive strength is used in this equation because previous studies showed that quasi-static strength is predictive of dynamic strength in ceramic armor materials.

Ganor validated the equation using in-house test data, historical experimental data from Wilkins' work at Lawrence Livermore National Laboratory, as well as separate test data provided by Erik Carton's group at TNO, the Dutch Organization for Applied Scientific Research.

Following this validation, Ganor states that "this new formula addresses the inaccuracies associated with previous equations, accurately and very rapidly assesses common armor ceramic types, and has sufficient explanatory power to resolve relations between materials that had seemed paradoxical."

The open-access paper, published in *International Journal of Ceramic Engineering & Science*, is "A facile method for the estimation of ceramic performance in light armor systems" (DOI: 10.1002/ces2.10227). ■

advances in nanomaterials

Salt-stabilized MXenes may find use in hypersonics

Purdue University researchers showed alkali cations can be used to improve MXene phase stability by filling in structural defects.

MXenes are an ever-expanding field of 2D transition metal carbides and nitrides. These materials demonstrate a wide range of chemical and structural diversity, including the ability to form ultrahigh-temperature nanolamellar structures that are highly stable in inert high-temperature environments (up to 1,500°C).

Of course, achieving this high-temperature stability is dependent on fabricating a pristine nanolamellar structure. But that can be difficult due to how MXenes are typically synthesized.

In contrast to other 2D materials, which are built up atom-by-atom from reactive gases, MXenes are produced via a top-down selective etching process. This process requires the use of harsh chemicals, such as hydrofluoric acid, which not only breaks the chemical bonds between layers but can also leave behind holes (defects) in the MXene structure.

"Because these materials are so small, when even the tiniest part of the MXene flakes away, it leaves an imperfect defective surface which significantly affects its stability. Every atom matters," says Brian Wyatt, a Ph.D. student at Purdue University, in a Purdue University press release.

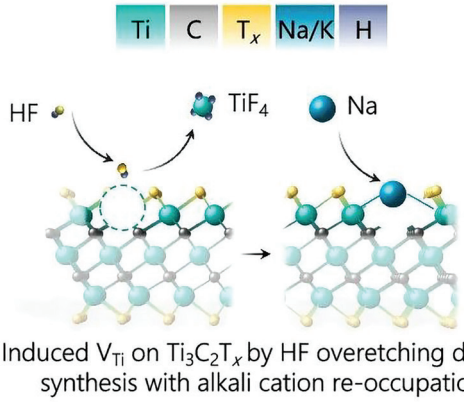
To address this challenge, Wyatt and others in the group of Babak Anasori, Reilly Rising Star associate professor of materials and mechanical engineering at Purdue University, investigated the possibility of using simple alkali chloride salts to fill in the holes caused by the acid etching process.

As explained in their open-access paper, the researchers knew from existing literature on MXene battery research that alkali cations can effectively shuttle between MXene interlayers and bind with the material's surface. However, exact interactions of these cations with the MXene surface—for example, if they prefer to bind with surface groups or occupy the transition metal atomic vacancy sites—were not fully understood.

To better understand these interactions, the Purdue researchers increased the acidity of the etching mixture to induce more defects in the resulting MXene. They then stirred the MXene in an alkali chloride salt solution and observed where the cations latched onto the MXene surface using dynamic atomic-resolution layer-by-layer secondary ion mass spectrometry.

The researchers discovered that the alkali cations preferred to occupy vacancy sites on the MXene surface rather than bind with the surface groups. This discovery led to experiments on the high-temperature phase behavior of the salt-filled MXenes, and these tests revealed that the cations did improve the MXene's structural stability.

The open-access paper, published in *Nature Communications*, is "Alkali cation stabilization of defects in 2D MXenes at ambient and elevated temperatures" (DOI: 10.1038/s41467-024-50713-2). ■



Credit: Wyatt et al., *Nature Communications* (CC BY-NC-ND 4.0)

Illustration showing the use of a highly acidic etching mixture to induce the formation of more defects in the MXene surface, after which alkali cations are used to fill the vacancy sites.

New material enters the 2D race: single-atom-thick sheets of gold

In April 2024, researchers at Linköping University announced they had finally developed a process for synthesizing true goldene, i.e., single-atom-thick gold sheets.

Gold atoms have a strong thermodynamic tendency to lump together, which complicates the production of single-atom-thick sheets. As such, previous work has only achieved gold monolayers confined on or inside templates.

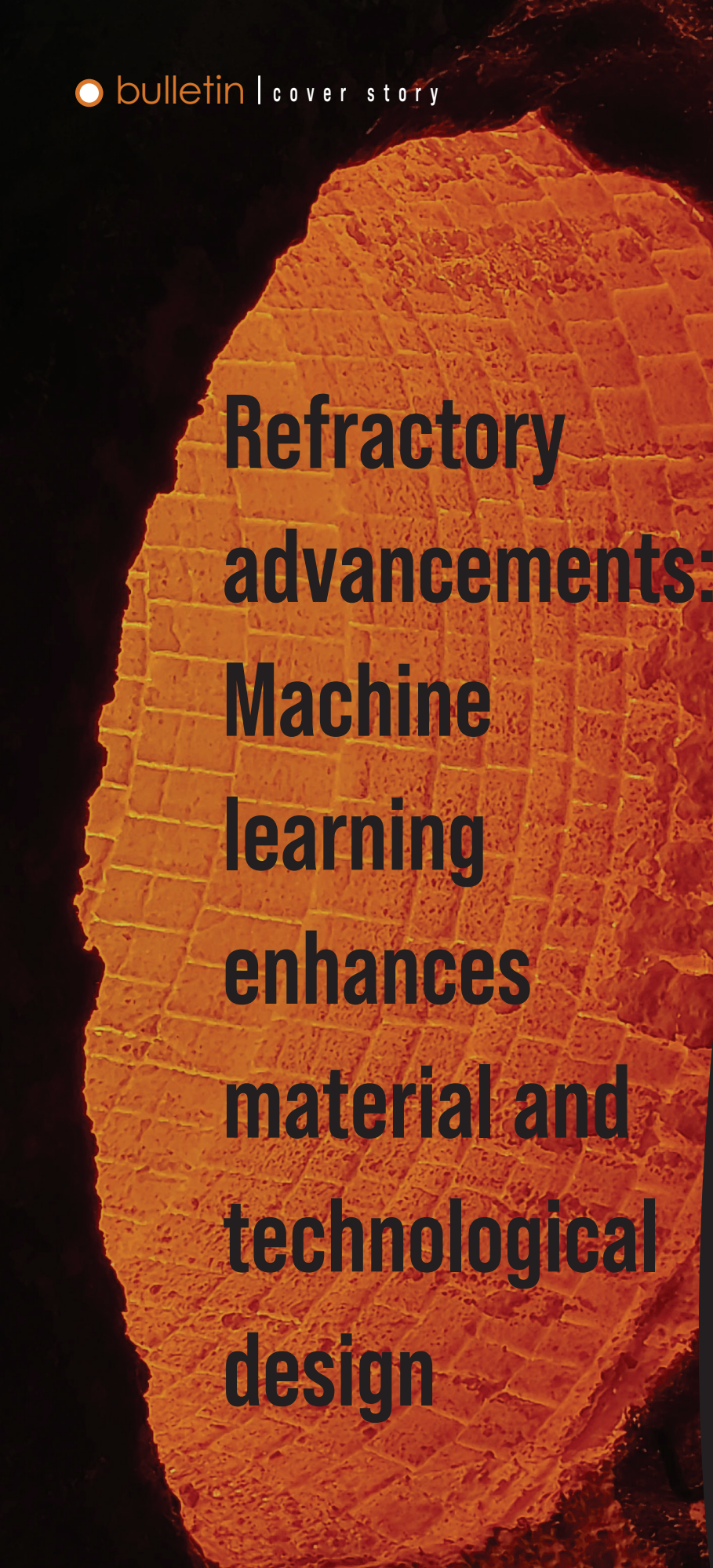
The method developed by the Linköping researchers mirrors the process used to create the well-known family of 2D transition metal carbides and nitrides called MXenes. They took the MAX phase Ti_3SiC_2 and swapped the silicon atoms for gold.

The researchers initially discovered this substitution process several years before, but they did not know how to extract the gold afterward. Now, though, they discovered they could borrow from a century-old Japanese knife production method, which uses an alkaline potassium ferricyanide solution called Murakami's reagent to remove carbon residue and change the color of steel.

They combined Murakami's reagent with a surfactant, either cetrimonium bromide or cysteine, to etch away Ti_3C_2 from the nanolaminated Ti_3AuC_2, thus leaving free-standing single-atom-thick gold sheets. Notably, this process was conducted in the dark because cyanide develops when the reaction takes place under light and subsequently dissolves the gold, according to the researchers.

Adding a surfactant improved the stability of the sheets from curling up and forming blobs near the etched-free edges. The curling and blob formation was attributed to external factors related to the initial substitution of gold for silicon in the Ti_3SiC_2 MAX phase as well as interactions during the subsequent etching process.

The open-access paper, published in *Nature Synthesis*, is "Synthesis of goldene comprising single-atom layer gold" (DOI: 10.1038/s44160-024-00518-4). ■



Refractory advancements: Machine learning enhances material and technological design

By Sebastian Sado, Ilona Jastrzębska, Wiesław Zelik, and Jacek Szczerba

Machine learning has become one of the most transformative technologies of our time.

Machine learning (ML) is a field of study in artificial intelligence that uses algorithms and statistical models to analyze and draw inferences from patterns in data without following explicit instructions. This technology has enormous potential to solve complex and real-world problems, so it is no wonder that John Hopfield and Geoffrey Hinton, who laid the foundation for ML with artificial neural networks more than 40 years ago, were awarded the Noble Prize in Physics in 2024.[1]

In the past several years, ML algorithms have been increasingly employed in the refractory industry, which consumes a high amount of exhaustible natural resources. Thanks to big data collection in metallurgical plants, ML algorithms can be readily applied to the development of more durable, cost-effective, and energy-efficient refractory materials and technologies.

There are several dominant aims of using ML in the refractory industry: predicting refractory lifetime in a service environment, optimizing industrial processes to extend this lifetime, tracking the pattern of wear to reduce failure risk, and optimizing refractory compositions. All these avenues of investigation can contribute to the transformation of the refractory and

metallurgical industry to be more environmentally friendly and resource efficient.

Although the benefits of using artificial intelligence tools are unquestionably groundbreaking, the complexity and large number of parameters influencing refractory materials in high-temperature and corrosive industrial processing environments require manufacturers to possess extraordinary insight, a critical approach, and reasonableness. Many manufacturers are willing to put in the work, as demonstrated by the panel "Modeling and Digitalization," which was held at the 2023 Unified International Technical Conference on Refractories in Frankfurt, Germany.[2]

During this panel, numerous manufacturers and researchers described how they used computational techniques to improve different aspects of refractory operations. For example, recently published works confirm the usefulness of ML to predict the wear of refractory linings in high-temperature metallurgical environments. The work by Arostegi and Manjarrés is particularly noteworthy because it implements ML for the biggest refractory consumer: steel metallurgy.[3] The authors applied several ML techniques to predict the number of remaining heats for a ladle and the wear of the most critical areas. The ML models were developed based on real metallurgical data, and as a result, deviation between the validated and predicted values was small. Such slight variances prove the applicability of the ML models.

Manufacturers must be careful when choosing data to build the ML model, though. For example, Gil et al. highlighted the selection of data from a wide range of accessible metallurgical data across the steel ladle campaign.[4] By showing the resultant overfitted ML model based on linear regression and a random forest algorithm, they concluded that failure of ML models can derive from inaccuracies in 3D laser measurements, leading to incorrect residual thickness measurements, too many data points, or missing critical data. So, numerous factors impact the reliability of the ML model.

Determining a reasonable scope for the question to be answered by the ML model can help manufacturers control the impact of too many variables. For example, in the work by Vermeulen et al.,[5] they disregarded other process parameters and focused only on maintenance strategy when using linear regression methods to predict the wear and lifetime of converter refractory linings. The study also suggested the use of fixed laser scanners in each converter as more appropriate to improve scan accuracy.

The 3D laser scanner method employed by Vermeulen et al.[5] may be useful to other refractory manufacturers because it allows control of the refractory lining condition during operation; however, it may also lead to several misunderstandings, as noted in the work by Gil et al.[4] The first step when making laser scans is to prepare a high-quality reference based on the refractory lining thickness before converter operations commence. This step is followed by scans after a specific number of heats throughout the campaign and again at the end of the campaign. However, the laser sometimes treats the slag layer that sticks to the refractory as a refractory lining, so recorded values of lining thickness may be incorrect. What is more, most steel plants do not regularly perform 3D laser scans because the scans require prolonged downtime of the converter, which raises production costs.

To enhance the use and efficiency of the 3D laser scanner method, manufacturers must pursue higher automation and the production of more accurate data. Once this data is collected, it can be used to develop refractory wear maps to inform ML models, which then can predict the wear of specific refractory linings in heating devices.

Thanks to these and other advancements in the application of ML methods, these methods are no longer limited to laboratory-scale experiments; they are starting to support refractory manufacturers in industrial-scale operations as well. For example, in recent work,[6] we validated the results of an earlier study on sustainable MgO-C refractory design by installing the refractory on a steel ladle in a Polish steel plant. The successful installation confirmed that the applied approach supports technologists in more effective optimization of mass-scale produced MgO-C refractories, contributing to a more sustainable production process.

In summary, ML has much to offer the refractory industry, and this potential is sure to be realized in the coming years. Learn more about the application of machine learning in refractory design and development on the following pages, which contain an excerpt from an open-access paper that we published in 2023.

About the authors

Sebastian Sado is technologist and product manager and Wiesław Zelik is chief technologist and head of the Research and Development Center at Zaklady Magnezytowe Ropczyce SA (Ropczyce, Poland). Ilona Jastrzębska is assistant professor and Jacek Szczerba is professor at AGH University of Krakow (Krakow, Poland). Contact Sado at sebastian.sado@ropczyce.com.pl and Jastrzębska at ijastrz@agh.edu.pl.

References

[1]"The Nobel Prize in Physics 2024," Royal Swedish Academy of Sciences. Published 8 Oct. 2024. Accessed 14 Jan. 2025. https://www.nobelprize.org/prizes/physics/2024/press-release

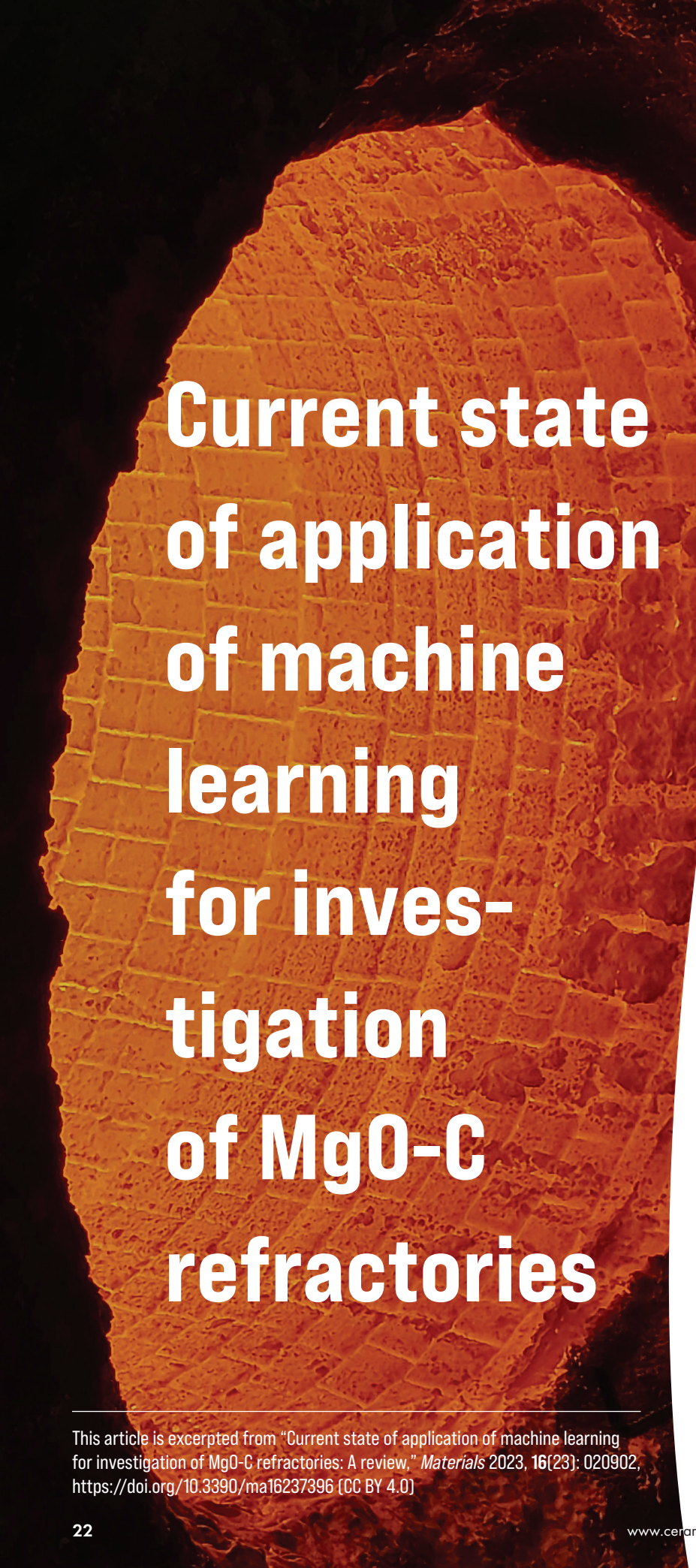
[2]Unified International Technical Conference on Refractories, 18th Biennial Worldwide Congress on Refractories, 26–29 Sept. 2023, Frankfurt, Germany. https://www.ecref.eu/de/unitecr2023-proceedings

[3]M. Arostegi, D. Manjarés, "Remaining useful life and wear estimation of the refractory bricks of the ladle lining by artificial intelligence," *UNITECR 2023: Conference Proceedings*, 642–645.

[4]A. Gil, W. Tesselaar, E. Gisolf, "Into the unknown: Explaining and predicting slag line wear based on process parameters," *UNITECR 2023: Conference Proceedings*, 662–665.

[5]F. Vermeulen, W. Tesselaar, E. Gisolf, "Converter on life support: A structured approach to determine the governing parameters of refractory wear to stabilize and prolong the lining lifetime," *UNITECR 2023: Conference Proceedings*, 658–661.

[6]S.Sado, I. Jastrzębska, W. Zelik, J. Szczerba, "Self-organizing maps as a tool to assess possible substitution of fused by sintered MgO aggregates in MgO-C refractories," *Ceram. Int.* 2024, **50**(9): 14996–15012. ■



Current state of application of machine learning for investigation of MgO-C refractories

By Sebastian Sado, Ilona Jastrzębska, Wiesław Zelik, and Jacek Szczerba

Magnesia–carbon refractories (MgO-C) belong to the most significant type of refractories for steel and iron industry operations. They thermally protect basic oxygen furnaces, steel ladles, and electric arc furnaces, and they are used in the production of special products, such as purging shapes and taphole sleeves.

The wear of MgO-C refractories is caused mainly by attack of metallurgical slag, oxidation of carbon in the refractory by oxygen or other oxidizing compounds, and interaction with CO/CO_2, which occurs at temperatures of 1,600–1,750°C. Also, thermomechanical impact, associated with thermal shocks and the turbulent flow of hot metal, significantly influences MgO-C refractory service time.[1]

Although MgO-C refractories have been used since 1950 in steel and refining plants,[2] their service periods are still being extended owing to progressing research efforts. One of the main research directions in MgO-C improvement is the application of various metallic and nonmetallic additions (e.g., aluminum, magnesium, silicon, silicon carbide, aluminum–magnesium alloys, iron) as well as the development of new ones (e.g., c-ZrN nanopowder, Ti_3AlC_2, Ti_3SiC_2, Cr_3C_2C, spinel micro-powder, YAG nanopowder, and other oxide composites). With the increased demand for widely understood decarbonization and sustainable development, much effort is also being put into the recycling of MgO-C materials.[3]

This article is excerpted from "Current state of application of machine learning for investigation of MgO-C refractories: A review," *Materials* 2023, **16**(23): 020902, https://doi.org/10.3390/ma16237396 (CC BY 4.0)

However, the commonality in all these experimental studies is that both the experiment and result interpretations are always conducted traditionally, with a relatively low quantity of data taken into consideration to interpret and draw conclusions. Simultaneously, researchers have to face multiple data types.[4] For this reason, the refractory industry should take the opportunity of the available data and introduce techniques that allow for their better usage.

Recently, more companies have become interested in collecting data to find relationships between metallurgical factors and refractories' wear rate to optimize the metallurgical process, making it more efficient and environmentally friendly. An invaluable tool is machine learning (ML), the outstanding performance of which has so far been reported in numerous materials science studies.[5]

ML algorithms refer to computational systems that can be trained to perform specific tasks, with no need to implement any explicit programming. Moreover, the performance quality of these algorithms improves with extended experience.

Interest in using ML techniques is constantly growing. The Web of Science database, when searched with the keyword "machine learning" 10 years ago (2014), showed 10,065 papers, while in 2023 and 2024, it revealed 85,062 and 124,310 papers, respectively. This 46% increase in the number of publications over the two last years and the more than 12-fold rise over the last 10 years permits the prediction of a forthcoming boom in ML utilization.

Taking into account the relatively newly applied ML techniques in the refractories field and their vast innovation potential, this work aims to evaluate the most important published works on the application of various ML techniques in the investigation of MgO-C refractories.

ML algorithms: An overview

ML is a subset of artificial intelligence. Algorithms are dedicated to building computational tools that make decisions without explicit coding. One of the main aims of the application of ML algorithms is taking the historical data and training the algorithms to further use these data in the prediction of specific features.

The main advantage of ML algorithms is their powerful performance and speed of data processing compared to hand-coding. ML algorithms have proven their performance and utility in a variety of fields, such as speech recognition, text mining, medicine, data analysis, aeronautics, data analysis, stock market analysis, and many others. This wide range of applications is possible due to a variety of existing algorithms, which are presented in Figure 1 (the graph does not exhaust all currently used algorithms).[6–10]

ML investigations of refractories

Oxidation of MgO-C refractories

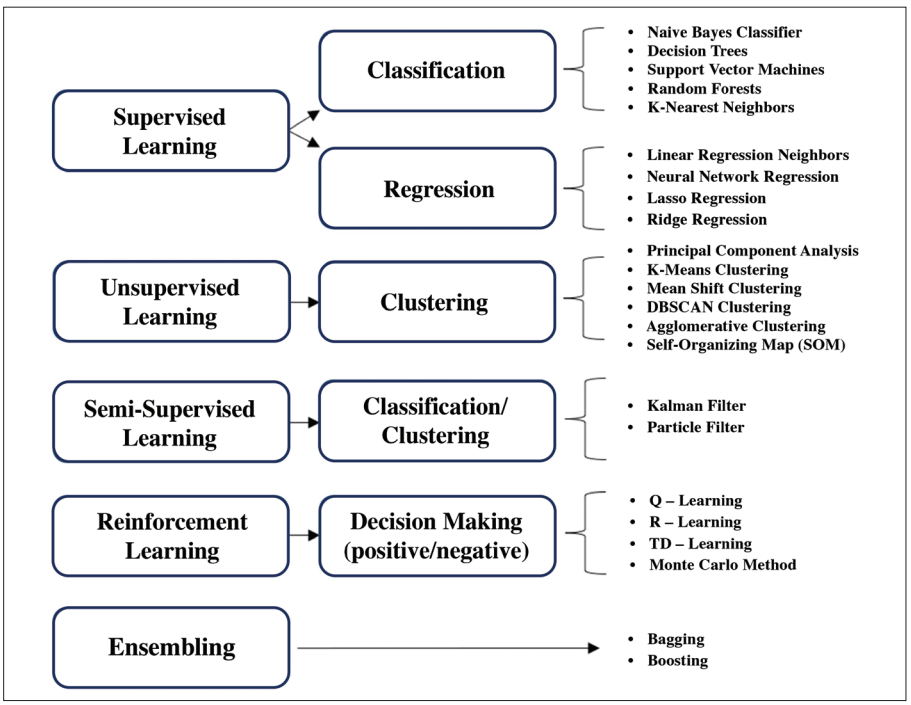
Oxidation of carbon in MgO-C refractories, especially below 1,400°C, is one of the main problems in the application of these materials. The decarburized part of the refractory is loose and porous; thus, the slag and hot metal can easily penetrate the refractory matrix.

Artificial neural networks (ANN), which represent one of the supervised ML techniques, were used by Nemati et al. to predict the oxidation behavior of MgO-C materials.[11] The model was developed using a standard feed-forward backpropagation network with one hidden layer.

Oxidation of carbon in MgO-C refractories was found to be driven mainly by the diffusion of oxygen to the MgO-C material's matrix. The ANN model was also used to predict the effective diffusion coefficient at different temperatures. The obtained results showed good quality of fit, expressed by the determination coefficient R^2 in the range 0.986–0.999.

Finally, the three-layer backpropagation ANN model was used to predict the oxidation kinetics of MgO-C materials based on their weight loss at different temperatures of heating. The authors developed reliable models with excellent fit of experimental with calculated data. The oxygen diffusion was reported as responsible for carbon oxidation in MgO-C refractories.

The oxygen diffusion mechanism in MgO-C composites was also investigated by A. Nemati et al. with the use of the ANN approach.[12] The authors developed models that enabled the prediction of the effective diffusion coefficient of oxygen in an MgO-C refractory with an R^2 coefficient in the range of 0.986–0.999, depending on the carbon content and temperature of the test.



Credit: Sado et al., *Materials* (CC BY 4.0)

Figure 1. Commonly used machine learning algorithms, based on References 6–10.

The authors confirmed that predicted data are comparable with experimental data obtained by other authors.[13–15] It was also confirmed that oxygen diffusion through the material's pores is the most significant factor controlling the oxidation intensity of the MgO-C refractory.

In the two works described above, the authors conducted advanced calculations to predict the oxidation kinetic parameters of MgO-C samples depending on the carbon content and test temperatures. However, it is necessary to extend this research and find if it is possible to apply ML techniques for predicting the oxidation behavior of MgO-C bricks by applying additional parameters, such as the compactness of the bricks, as far more factors affect the decarburization of MgO-C bricks.

Optimization of carbon content in MgO-C refractories

Graphite is a main source of carbon in MgO-C refractories, which, due to its poor wettability by slag and low thermal expansion coefficient, provides high slag corrosion resistance and good thermal shock resistance, respectively. However, too much carbon in the MgO-C composition leads to heat loss during operation due to the raised conductivity of the MgO-C refractory lining. Also, greater amounts of carbon in the MgO-C composition decrease the hot strength and oxidation resistance of MgO-C materials.[16] Therefore, the optimization of graphite content in MgO-C bricks is crucial.

Mazloom et al. used an ANN model to optimize graphite content in MgO-C refractories.[17] The work aimed to find the optimal ratio of graphite to resin to provide the highest possible compressive strength and minimize the apparent porosity of the materials. In total, 100 specimens were prepared (four specimens for each of 25 formulations) for experimental testing.

According to the obtained results, it was found that replacing magnesia powder with graphite decreases the compressive strength of MgO-C materials up to 10% graphite content. If the graphite content was raised up to 12.5%, the compressive strength was raised, but a further increase of graphite content to 15% and 17% caused a compressive strength drop. The experimental results also showed that an increase in the amount of synthetic resin in the refractory always raises its cold compressive strength.

For ML model development, backpropagation of training error and a three-layer network for training were used. Two variables were selected as input data, namely, resin and graphite content, while the output variables were ultimate compressive strength and apparent porosity of 100 specimens prepared experimentally. Approximately 250 cycles of training were conducted with the use of different numbers of neurons to find the best model.

Based on the ANN model, it was reported that a refractory formulation of 13.5% graphite and 3.0% synthetic resin provides the highest ultimate compressive strength and lowest apparent porosity. The model was validated experimentally on seven specimens, based on the ANN-proposed formulation.

The ultimate cold compressive strength predicted by the ANN model was 365.16 MPa while the experimental value was 376.47 MPa, which means 1.3% error. The ANN model predicted apparent porosity at 7.08% while the experimental porosity was 7.11%, which gives 0.35% error. So, the authors concluded that a reliable and accurate model can be developed using ANN to predict the MgO-C material's properties.

Corrosion resistance of MgO-C refractories

The corrosion resistance of refractory materials is widely studied due to its exceptional importance for the service life of heating devices. Corrosion of MgO-C refractories limits the duration of a device campaign, which increases maintenance costs for refractory end-users.

Optimization of MgO-C refractories composition for improved corrosion resistance was studied with unsupervised learning techniques using clustering algorithms.[18] A total of 20 different variants of MgO-C materials were prepared based on four different main raw materials. From each of the variants, eight industrially produced MgO-C bricks were selected for further examination. Principal component analysis (PCA) and the K-medoids algorithm were applied to develop a model that clusters MgO-C materials into groups of comparable properties. PCA analysis showed that it is possible to use two variables (instead of eight) to characterize the prepared MgO-C materials.

A new variable PC1 was obtained, which explained approximately 81% of the variability in the dataset and referred to the basic properties of MgO-C materials. The second variable PC2 explained about 12.3% of the data variability and referred to the values of pressure used for shaping the materials. Using the K-medoids algorithm with partitioning around medoids (PAM), PC1 and PC2 were used as input variables.

The algorithm distinguished nine groups with materials of considerably comparable properties. It was assumed that materials assigned to the same clusters by the PAM algorithm had comparable corrosion resistance. Experimental tests of corrosion resistance were conducted with the use of an induction furnace to verify the obtained ML results.

The algorithm indicated that a material consisting of fused magnesia of standard quality (shaped at 120 MPa) should perform similarly to a material consisting of 65% sintered and 12% fused magnesia of the highest quality (shaped at 180 MPa). Moreover, the algorithm suggested that materials composed of fused magnesia of standard quality and 27% sintered magnesia but shaped at higher pressure of 180 MPa should perform similarly at high temperatures to test materials containing 65% sintered magnesia and 12% of the highest-quality fused magnesia.

With a statistical Wilcoxon test applied to the measured wear rates after corrosion tests, it was confirmed that the described material variants were located in the same cluster indicated by the PAM algorithm and performed similarly after being exposed to slag attack at high temperature. Therefore, the algorithms properly indicated materials of comparable corrosion resistance.

This research revealed an extremely important issue in terms of the sustainable development of refractories, as the production of fused magnesia demands about 15 times more energy than the production of sintered magnesia aggregates.[19]

Even if the corrosion of MgO-C refractories is widely described in the literature, scarce information can be found regarding the comparison of high-temperature properties of MgO-C materials based on different magnesia raw materials.

Thermomechanical properties of MgO-C refractories

MgO-C refractories are exposed to extreme thermal, mechanical, and chemical stresses during operation in steel plants. The highest thermal stresses occur during the preheating stage of the heating device and the tapping of the hot molten steel into the ladle, where the refractory lining suffers mostly from a high-temperature gradient (from about 300°C at the steel shell to 1,600–1,700°C at the lining). For some applications, MgO-C materials have to withstand additional mechanical stresses, such as the rocking of the basic oxygen furnace vessel during preheating.[20,21]

An advanced investigation of the thermomechanical behavior of different lining concepts in steel ladles was conducted by Hou et al.[22] ANNs were used to predict the thermal and thermomechanical responses of refractory lining during operation.

Overall, 160 different configurations of lining were investigated. The finite element method was used to obtain the input data for the ANN architecture design. For the experiment and calculation, 10 different variables were used assuming various steel shell thicknesses and refractory lining thicknesses (insulation, permanent, and working lining) together with its thermal conductivity and Young's modulus. Three-layer backpropagation ANN was used for prediction. Hyperbolic tangent sigmoid was selected as an activation function.

Three tests were used to establish the optimal ANN architecture. In the first test, all 160 samples were selected for the training, in which gradient descent with the adaptive learning rate backpropagation algorithm was used. In the second test, the data set was divided into three groups (96, 126, and 160 samples) to find the minimum sample size for the study. In the third test, eight different algorithms were used to find the most favorable one for the steel ladle.

Table 1. Predicted thermomechanical response based on ANN using CFG and BR algorithms,* based on Reference 22.

	End temperature [°C]		Maximum tensile stress [MPa]		Maximum compressive stress [MPa]	
Used algorithm	CFG	BR	CFG	BR	CFG	BR
RE_MAX [%]	7.15	7.15	16.62	12.43	3.12	4.09
MRE [%]	1.02	1.76	2.43	2.37	0.93	0.78
B	0.9967	0.9908	0.9279	0.9348	0.9963	0.9966

**RE_MAX, MRE, and B coefficients evaluate the error between the results of the two used algorithms CFG and BR.*

The model assessment was conducted with the use of various errors: maximum relative error (RE_MAX), mean relative error (MRE), relative root-mean-squared error (RRMSE), and coefficient of determination (B). Out of eight algorithms, two were selected (CFG—conjugate gradient backpropagation with Fletcher–Reeves updating and BR—Bayesian regularization backpropagation) as the most suitable for calculations. ANN was then built to compare the performance of the selected algorithms in the prediction of the end temperature (the temperature at the cold end of the steel shell), maximum tensile stress, and maximum compressive stress.

The comparison results are shown in Table 1. Low values of RE_MAX and MRE and high B values are desirable. For the maximum tensile strength and maximum compressive strength, the BR model performed more efficiently than the CFG model (for BR: higher values of the coefficient of determination B, lower values of MRE, and a lower value of RE_MAX for tensile strength). Based on the obtained results, a neural network model with BR was utilized for final calculations.

The optimal ANN architecture was found for seven nodes in the hidden layer and Bayesian regularization with 160 samples for training. Two insulation lining concepts were then compared using the optimized ANN architecture.

The results confirmed that ANN performed outstandingly. The predicted values of selected properties (steel shell temperature, maximum tensile stress, maximum compressive stress) were close to the finite element-simulated ones. The presented model was also reported as promising for material recipe improvements and steel production optimization.

Application of ML in industrial-scale examinations

From the industrial point of view, the most important thing is to provide the longest possible service time for refractories in heating devices, which allows for the optimization of the cost-to-service time ratio. The service time of refractories is affected by several factors, including metallurgical conditions, refractory brick quality, and the periodic maintenance of devices, among others. The service time is difficult to assess and precisely predict. However, it seems to have become more feasible with the implementation of computational technologies.

Borges et al. applied self-organizing maps (SOMs), which is one of the unsupervised algorithms, to identify the main factor influencing the wear rate of MgO-C materials at the slag lines of the steel ladles.[23] The authors compared the results of the traditional statistical approach with the SOM results.

Approximately 23 metallurgical parameters were investigated. The SOMs showed the relations between ladle service time and hot metal treatment with the following technological parameters: CaSi, argon bubbling without CaSi, argon bubbling with CaSi, steel permanence time, steel temperature after tapping, steel weight, and type of product (thick plates, hot strips, and boards for sale). At each step of the analysis, the results were verified with the use of typical regression and correlation analysis.

Based on the SOM results, the authors indicated the numerous reasons

responsible for the premature or intense wear of MgO-C materials in steel ladles, including the number of chemical additions (such as nepheline and CaSi), the interaction between the desulphurization route, the intensity of ladle furnace use, and the extended contact time of the refractories with slag.

The important fact in this work is that the authors verified the calculation results versus traditional statistics and post-mortem results for selected MgO-C bricks. The ML algorithm results agreed with traditional statistics calculations. SOMs are considered a useful tool not only to indicate the parameters affecting ladle service time but, thanks to the applied technique, direct recommendations may be allocated for steelmakers to improve the production process and extend the ladles' work. Considering the industrial practice, it would be valuable to investigate not only the metallurgical factors but also the type of ladle maintenance techniques, e.g., using gunning mixes or other protection techniques.

Yemelyanov et al. proposed the use of ANN to diagnose lining conditions based on thermograms of refractory lining.[24] The input parameters were as follows: the mass centers of the thermograms, distance matrixes defining the borders of specific lining zones, and colors spotted on thermograms.

ANN was used to classify the burnout zones of the lining. The training of the network was conducted in two steps. The first step was the typical training of the network with data sampling. In the second step, only experimental data were utilized for training.

The authors tested 22 neural networks to find the optimal architecture. The obtained results enabled the implementation of specialized software in the steel plant that inspects the lining conditions.

It is worth emphasizing that the authors used unprecedented real thermograms of the lining collected at the steel plant. In total, 480 standard thermograms and 620 collected experimentally were used, which made it possible to obtain a reliable model with low values of classification error (0.258–0.443). The model performance was satisfactory and was the basis for developing software for monitoring the refractory lining condition. The major advantage of this work is that its results were positively implemented in industry. Moreover, it seems that the model is flexible and can be used successfully in various types of devices, such as steel ladles and torpedo ladles.

The works of Zelik et al.[25] and Sado et al.[26] describe the application of different ML techniques for the prediction of the wear rates of MgO-C materials in basic oxygen converters using metallurgical parameters collected during hot metal treatment. The authors obtained models of different qualities. Among the used techniques, ANN and the boosted trees algorithm were reported as providing the most accurate results.

Even though the works carry practical meaning, the model performance needs to be improved through better quality of data. First of all, in both works, the residual thickness of the MgO-C refractory lining thickness in the slag spout zone was used as an output variable. Unfortunately, due to the specific work of the steel plant, only about 20 laser-scanned results for lining thickness were obtained during the campaign. Such a low amount of data in the campaign (which lasted more than 2,000 heats) affects the quality of the ML model.

Industrial data are often not prepared appropriately and contain missing or invalid values (e.g., hot metal content exceeding the device's capacity). Collecting quantitative data on the gunning mixes used for sidewall protection would also enhance the models' quality.

Benefits and limitations of using ML techniques to investigate MgO-C refractories

Although the number of publications on the application of ML is growing rapidly, it is still very low when it comes to ML applications in the refractory industry. Nevertheless, the presented articles prove that ML algorithms are highly useful in the development and industrial application of MgO-C materials.

Currently, ML techniques have obvious limitations because the quality of data collected in the industry is still not satisfactory. Thus, it is necessary and highly recommended to improve the process of data registration in industry, especially data involving steel production processes, to avoid missing data, unreal values, or mistakes due to hand typing. Using data of unsatisfactory quality may lead to inaccurate or misleading conclusions, making ML models useless or ambiguous.

Another important limitation is related to laboratory experiments and the fact that ML algorithms are trained on data collected from specific, highly advanced examinations influenced by specific operational conditions. It might be difficult, or even inappropriate, to apply external data to such models and obtain reliable results, especially if one—allegedly insignificant—factor is changed.

Despite these limitations, implementing ML in the refractory industry can still speed up innovation, and so interest in using ML will continue growing as the digitalization of industrial data is very desired. The possibility of predicting the wear rate of refractories depending on various processing parameters shall be especially encouraging for refractory end-users. They should be conscious of the need to improve data collection in order to develop highly predictive models that will serve them in industrial practice and help make the steel process more sustainable and thus more economical.

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Participants in the "Uncertainty Quantification of Materials Processing for Ultrahigh-Temperature Materials" workshop. Credit: ACerS

Uncertainty quantification of materials processing for ultrahigh-temperature materials

By Soumya Sridar, Wei Xiong, Hessam Babaee, William Fahrenholtz, and Scott J. McCormack

Throughout humanity, materials have defined the ages: Access to new materials creates novel paradigms for tool design.

One of the most engineered materials today is steel, with concrete and aluminum being close behind. Our understanding of steel process–structure–property relationships is so advanced that we can design new formulations predominantly from computation (with a few experiments for validation and tuning). Examples of steel products designed this way by QuesTek include Ferrium C61 for automotive applications,[1] Ferrium C64 for rotor blades,[2] and Ferrium M54 for airplane landing gears,[3] among others.

If we can design steel predominantly from computation, then can we use the same principles to address the needs of ultrahigh-temperature materials for the leading edges of next-generation reentry vehicles? While the answer is "yes" theoretically, currently we do not have the necessary data for this approach.

According to "Digital Science – Dimensions,"[4] there are about 6,500,000 publications on steel, with the oldest in the database dating back to 1665. By comparison, there are only about 27,000 publications on a key hypersonic material, zirconium diboride (ZrB_2), with the oldest in the database dating back to 1905. While it is clear that Digital Science is missing some of humanity's knowledge on steels and ZrB_2, as humans have been working with steel and iron–carbon derivates since the Roman era and before,[5] it still highlights that our understanding of steel is vast in comparison to ultrahigh-temperature materials.

For the development of future material systems such as ZrB_2 and its composites, we must increase our comparative knowledge of ultrahigh-temperature materials. Statistical tools can help researchers design targeted experiments that increase the amount of data on these materials in a cost-effective and rapid manner. But first we must quantify the uncertainty of existing data so frameworks can be built that reduce uncertainty, thus allowing new materials systems to be developed more reliably.

The need to develop new tools for uncertainty quantification led researchers to organize the "Uncertainty Quantification of Materials Processing for Ultrahigh-Temperature Materials" symposium session and a workshop at ACerS Annual Meeting at MS&T24 in Pittsburgh, Pa. The goal for this session and workshop was to bring together computational, mathematical, and experimental experts to discuss several topics: (i) state-of-the-art uncertainty quantification, (ii) database development, (iii) statistics in data-poor regimes, and (iv) robust microstructure descriptors. These discussions were incorporated into the workshop designed for undergraduate and graduate-level students, which welcomed about 20 participants, and the symposium session targeted at researchers and professors, which attracted about 80 attendees.

This article provides a snapshot of the workshop and the symposium session along with our perspective on the current state-of-the-art uncertainty quantification methods, limitations and next steps to improve these methods, and commentary on the development of a ZrB_2 process–structure–property database. In particular, the article highlights two presenters whose work is at the nexus of these challenges: Noah Paulson at Argonne National Laboratory, who discussed Bayesian methods in computational thermodynamics, and Jeremy Mason at the University of California, Davis, who discussed microstructure classification and the microstructure state space.

Workshop overview

The workshop began with an overview of hypersonic platforms, including the origins of aerodynamic heating and a brief history of hypersonic materials.[6] The role of ZrB_2 as a matrix material for next-generation ceramic matrix composites was then discussed, which led into discussion of an in-development process–structure–property database for ZrB_2 that currently contains 82 publications from 1950–2024 (~143 data entries).

Three key insights stand out when reviewing this database. The first is that chemical composition is the least populated of the entries. This finding means that, in general, impurities in ZrB_2 have not been well characterized, which highlights the importance of having statistical tools to help handle the uncertainty in ZrB_2 impurities and their resulting effects on properties. The second is that 2D microstructure entries are well populated while 3D microstructure characterization is rare. 3D microstructure characterization is difficult but will be required to understand microstructure evolution and failure mechanisms, especially when expanding to ceramic matrix composites. The third is that properties are clustered, i.e., samples are measured for a single property, such as thermal conductivity or flexural strength, but rarely characterized for multiple properties on the same sample. This finding highlights the need for more diverse materials characterization studies to build statistics.

From these insights, the workshop discussion then turned to statistical tools that can be implemented in data-limited regimes. Two core statistical/machine learning techniques were discussed: (i) multifidelity surrogate modeling and (ii) matrix completion. Surrogate modeling involves developing a complex mathematical model to describe the behavior of a complex system. This technique is widely used in materials science and engineering for applications such as optimization, digital twins, and uncertainty quantification. On the other hand, matrix completion involves estimating missing entries in a matrix based on the available data. This technique has a wide range of applications in materials science and engineering, such as predicating unreported or unmeasured quantities and supporting surrogate modeling efforts.

Currently, many questions involving ultrahigh-temperature materials involve a large number of input variables with limited data. While matrix completion can help predict gaps in the data, there are still significant challenges to building surrogate models with such scarce data. To overcome this challenge, a multifidelity surrogate model was used at this workshop. This model used Gaussian process regression to combine high-fidelity, scarce-labeled data with many low-fidelity samples to minimize the need for high-fidelity labeled data points.

While this approach minimizes the need for high-fidelity data, comprehensive data collection is still a crucial part of reliable uncertainty quantification. Storing the collected data in a structured manner that can be retrieved easily—along with advanced search capabilities to screen through them—is beneficial. Making the collected data freely available would encourage sharing among different users in the scientific community as well.

For this purpose, the workshop introduced the National Institute of Technology's Materials Data Curation System (MDCS),[7] which is developed within the broader Configurable Data Curation System (CDCS).[8] CDCS is a family of systems for structuring, searching, and sharing data based on extensible markup language (XML). XML is utilized as it is a robust, proven standard written as plain text and can be shared and converted into other formats easily. The purpose of MDCS and CDCS is to (i) increase the availability and quality of scientific data for higher community standards, (ii) increase the integration of scientific data among different platforms for federated searches, and (iii) support the development of FAIR (Findable, Accessible, Interoperable, Reusable) data communities.

Symposium session overview

The symposium session presentations were categorized into three broad themes: (i) uncertainty quantification of thermochemical data, (ii) uncertainty quantification of microstructural data, and (iii) applications of uncertainty quantification in ultrahigh-temperature material systems.

Discussions on thermochemical data were led by Noah Paulson (Argonne National Laboratory), Theresa Davey (Bangor University), and Raymundo Arroyave (Texas A&M). Current research efforts in this area involve developing protocols that use Bayesian methods for uncertainty quantification (UQ) and uncertainty propagation (UP) within the CALPHAD (CALculation of PHAse Diagrams) framework. These methodologies address the intrinsic uncertainties present in experimental data and model parameters, which significantly influence the reliability of predictions. By explic-

itly accounting for these uncertainties, UQ and UP enable more accurate and robust decision-making in materials design and optimization. Regarding the in-development ZrB_2 database, these UQ and UP methodologies will help address the sparsity in chemical composition and will help identify optimum experimental plans to remedy this challenge.

Discussions on microstructural data were led by Jeremy Mason (University of California, Davis). Historically, microstructures have been characterized based on features defined from human observations. With the advent of computers and statistics, new and more objective metrics for defining microstructures are being proposed.

For example, new methods involve breaking down material microstructures into smaller regions or "windows." Conceptually, materials can be compared by sampling many windows from each microstructure and finding the best possible matching between the two window sets. While two materials with identical processing conditions will not have identical microstructures, it is very likely that the windows in one set could be matched with similar windows in the other set. Notably, this matching ability is not true for materials with different processing conditions. This idea can be formalized by defining an underlying probability distribution of windows that would be sampled from random locations for each microstructure and then comparing the probability distributions of windows for two materials of interest.

Regarding the in-development ZrB_2 database, these novel microstructure characterization techniques well help better characterize and understand uncertainty within the already existing microstructures, thus allowing for more precise development of new microstructures. In addition, it will assist in the analysis of more complicated 3D microstructures.

In terms of ultrahigh-temperature material systems, a variety of statistical tools can be applied to high-temperature material manufacturing challenges. Tenfei Luo of the University of Notre Dame presented a probabilistic physics-integrated neural differential modeling framework for accurately predicting outcomes of the isothermal chemical vapor infiltration process,[9] a complex manufacturing method essential for producing high-temperature-resistant carbon composite materials.[10,11] Meanwhile, Soumya Sirdar of the University of Pittsburgh presented a CALPHAD model to predict the effective thermal conductivity, including porosity and impurities for ZrB_2.

Highlighted presenters

Bayesian methods in computational thermodynamics

Noah Paulson, Argonne National Laboratory

Computational thermodynamics is an essential tool in the design and deployment of materials for extreme environments. However, while CALPHAD databases span an enormous compositional space, data is sparse, which leads to potentially unreliable predictions for multicomponent materials.

In recent years, researchers have prioritized the development of uncertainty quantification approaches for CALPHAD modeling to provide useful uncertainties. At Argonne National Laboratory, we have explored the potential of Bayesian methods for uncertainty quantification, with particular attention to parameter inference, uncertainty quantification and propagation (UQ&P), and automated dataset weighting.

Bayes theorem describes how the probability distribution of a model's parameters, contingent on observed data, is proportional to the data likelihood, which describes the probability of observing data in the context of a specific model and its associated parameters, and the prior distribution, which describes the probability distribution of the model parameters before observing the data. The probability distribution is typically specified via mathematical or physical constraints and expert insights. Marginalizing the data likelihood and prior distributions over the entire parameter space yields the marginal likelihood, which describes the probability of the data given a choice of model.

For two models with equal prior probabilities of describing anticipated data observations, the ratio of marginal likelihoods (i.e., the Bayes' Factor) expresses the Bayesian degree of preference for one model over another. Analytical solutions for the posterior are not tractable for many choices of model, data likelihood, and prior distribution. Consequently, we have turned to approximate Monte Carlo inference methods, which also enable efficient estimation of the marginal likelihood.

The discrete nature of the posterior representation obtained from these Monte Carlo methods lends itself to numerical uncertainty propagation. In this case, uncertainty intervals on the model prediction are obtained by evaluating the model on a representative sample of parameter sets from the converged posterior distribution; percentile bounds are then calculated on these sampled model predictions. In the paper by Low et al.,[12] we employed these approximate methods to develop thermodynamic descriptions of monoclinic and tetragonal HfO_2 from 0 up to 3000 K based on first principles calculations.

Careful specification of the data likelihood and prior distributions enable diverse modeling capabilities. For example, in Paulson et al.,[13] instead of directly employing reported uncertainties for experimental datasets in the likelihood definition, the uncertainties were treated as potentially inaccurate. So, they were rescaled with a per-dataset hyperparameter that was included in the inference procedure alongside the model parameters.

This simple modification to the likelihood definition enabled more robust model selection, parameter inference, and UQ&P by giving the model the freedom to identify dataset weightings. This robustness led to thermodynamic consistency across specific heat and enthalpy

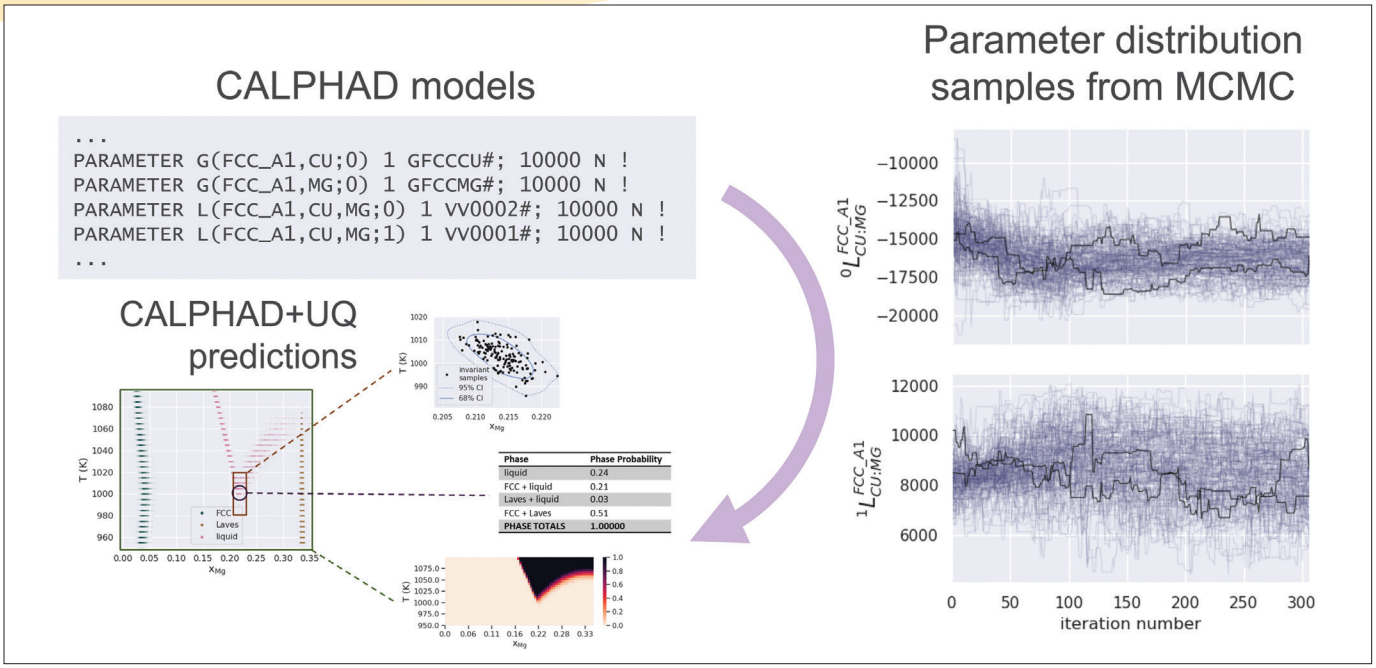


Figure 1. Schematic representation of Bayesian inference in CALPHAD for the copper–magnesium (Cu–Mg) binary thermodynamic description, which leads to UQ&P capabilities spanning those common in deterministic CALPHAD methods. Adapted from Reference 14.

measurements for elemental hafnium, and in the paper by Gabriel et al.,[14] for aluminum considering both atomistic and experimental datasets.

Bayesian methods were also explored for binary systems with two distinct species. In the work by Paulson et al.,[15] the open-source ESPEI python package[16] was leveraged to perform Bayesian inference for the copper–magnesium binary system. As illustrated in Figure 1, this approach involved first identifying inferable parameters from the traditional database file, then performing numerical Bayesian inference via ESPEI, and finally performing UQ&P analyses for standard CALPHAD prediction outputs.

The novelty of this work was in the final stage, where the previously described numerical uncertainty propagation approaches were applied to diverse CALPHAD predictions, including the base thermodynamic quantities, the overall phase diagram, invariant points, and phase fractions at any composition, temperature, and pressure.

Most recently,[17] we explored a question at the core of CALPHAD—how can we efficiently propagate uncertainties from unary systems to binary systems and beyond? The simplest approach would be to include the parameters for the thermodynamic descriptions of the individual species alongside the parameters of the binary phase descriptions. Unfortunately, this approach would not scale to practical thermodynamic databases with dozens of species and potentially thousands of parameters due to the computational limitations of numerical Bayesian inference.

Instead, we proposed performing inference on the thermodynamic descriptions of the individual species first and then numerically propagating these uncertainties during inference for the parameters of the binary phases. While phase diagrams and uncertainties were not identical between these two approaches for the copper–magnesium system, the results were comparable, indicating that this propagation approach was worth further investigation.

The ultimate goal of our work is to enable UQ&P for multicomponent thermodynamic databases, in turn enabling accelerated materials development and deployment. In a 2023 workshop, we examined three core areas of development required to reach this goal: (i) improving access to data and models, (ii) core UQ&P methodology development, and (iii) automated tools to aid CALPHAD assessment. Ultimately, progress in CALPHAD will inspire progress in the greater materials science field.

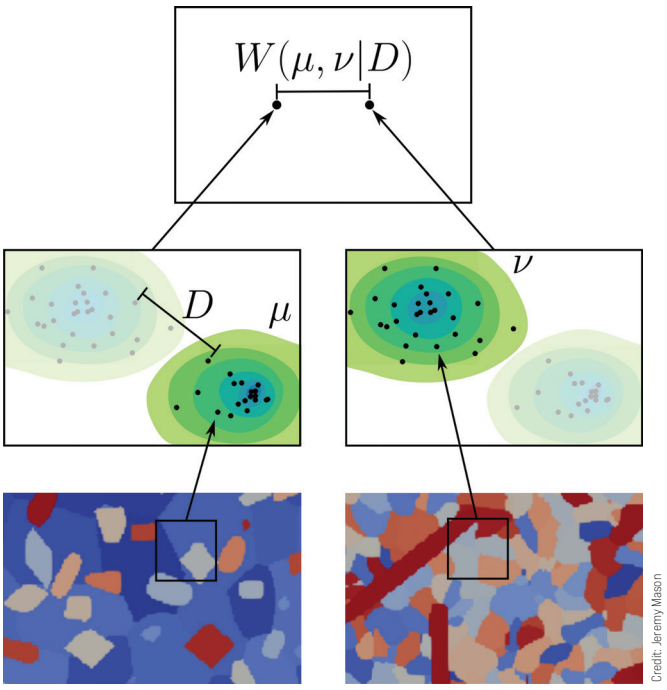
Microstructure classification and the microstructure state space

Jeremy Mason, University of California, Davis

Advances in processing methods enable increased control of material microstructures and thereby material properties. Consequently, the development of integrated computational materials engineering (ICME)[18] systems requires a canonical description of material microstructures.

The ideal microstructure state space for ICME systems would have the following properties:

1. Any microstructure can be represented as a point in the state space.
2. The state space specifies enough microstructural information to constrain the material properties.
3. Increasing the statistical similarity of two microstructures reduces the distance between the corresponding points in the state space.



Credit: Jeremy Mason

Figure 2. Schematic showing the various concepts involved in the construction of the microstructure state space.

The availability of such a microstructure state space would have widespread and significant implications for materials science. For example, material standards could be defined by means of the similarity of a produced microstructure to a reference one, thus allowing manufacturers to use any processing procedure provided the microstructure conforms to the specification. Furthermore, a materials database constructed on this state space could allow the properties of a proposed material to be interpolated by a distance-weighted average of properties of known materials. Processing routes to an arbitrary target microstructure could then be realized by an automated iterative process in which the next processing step is selected to most rapidly reduce the distance to the target microstructure.

Establishing such a microstructure state space is difficult, however. Regarding the first property, that any microstructure can be represented as a point in the state space, one subtlety is that many instances of nominally equivalent microstructures (e.g., all microstructures produced by a standardized processing procedure) should be identified with the same point up to statistical error. This decision requires a microstructure to be described as a probability distribution of small volume elements or "windows" at a user-specified length scale, effectively associating the material with a statistical volume element (SVE) that can be used to predict the material properties.[19]

The second property, that enough microstructural information be specified to usefully constrain material properties, requires that the representation of the SVE be explicit enough to allow property predictions. The SVE is fundamentally a probability distribution defined on a space that contains all possible windows. Given a distance function or other metric on the window space, the SVE can be approximated by a point cloud of windows sampled from experimental micrographs. The heterogeneity of such data means that the metric on the window space should be flexible enough to allow users to specify precisely what window features should be compared.

The third property relates to the measurement of distances on the microstructure state space. Given that points on the state space define microstructures as window distributions, the desired metric is a function that measures the similarity of probability distributions on the window space. Of the many metrics that are suitable for this purpose and are already available in the literature, the Wasserstein metric effectively reduces to finding the best match between two populations of sampled windows, where the cost of matching a single pair of windows is equivalent to the distance between them on the window space.[20]

Figure 2 visually represents these ideas. Two micrographs of material microstructures appear on the bottom row, with windows of a consistent size sampled uniformly at random from the interiors of the micrographs. The windows are represented as points in the window space on the middle row, with the points distributed according to underlying probability distributions μ and ν. Distances between points in the window space are measured by a function D that quantifies the similarity of the corresponding windows. The window distributions are represented as two points in the microstructure state space on the top row. Distances between points in the state space are measured by the Wasserstein metric $W(\mu,\nu|D)$, which quantifies the similarity of the corresponding window distributions given the window metric D. That is, the statistical similarity of the two microstructures on the bottom row at the length scale of the windows is quantified by the distance between the corresponding points in the microstructure state space on the top row.

In a preprint,[21] we verified that such an approach is indeed possible for the restricted case of single-phase polycrystalline materials (or for general polycrystalline materials where only grain boundary geometry information is retained). One metric that allows the similarity of windows to be quantified is defined, and practical guidelines for the size of sampled windows, the number of sampled windows, and the area of the micrograph from which to sample are established. Pairwise distances are evaluated for a set of synthetic microstructures generated by the modeling software DREAM.3D, and a proof-of-concept microstructure database is constructed with a query capability whose computational cost is manageable. These efforts are not intended to be authoritative but merely to show that the vision described here could be realized in practice.

Conclusions

From the workshop and symposium session, it is clear that uncertainty quantification in materials processing for ultrahigh-temperature materials is an up-and-coming field that will grow in the future. Key areas will include the development of Bayesian methods for uncertainty quantification and uncertainty propagation in thermochemical data along with the CALPHAD method. These developments will be essential to understand where the next thermochemical measurements are required to effectively develop multicomponent elemental systems.

In addition, new statistical techniques to analyze microstructures, such as the microstructure state space, will be essential in quantifying the similarities and differences between two sets of microstructures. This ability will be critical to reduce uncertainty in materials whose properties are highly sensitive to microstructure, such as ceramics and other brittle systems.

Finally, novel statistical methods that can be applied in data-poor regimes will be essential in pushing the boundaries in new and emerging material systems. These ideas will enable new material technologies, such as ZrB_2 and its subsequent composites, to catch up much faster to the maturity of established systems, such as steel.

Future conferences

In 2026, the "Uncertainty Quantification of Materials Processing for Ultrahigh-Temperature Materials" session will expand to become a full symposium at MS&T26 in Pittsburgh, Pa.

Acknowledgments

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The workshop presenters include Scott J. McCormack (University of California, Davis) Soumya Sridar (University of Pittsburgh), and Hessam Babaee (University of Pittsburgh). The symposium session presenters include Noah Paulson (Argonne National Laboratory), Jeremy Mason (University of California, Davis), Tenfei Luo (University of Notre Dame), Raymundo Arroyave (Texas A&M), Theresa Davey (Bangor University), and Soumya Sridar (University of Pittsburgh).

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Predictive tools and data-driven insights to accelerate ceramics innovation


Credit: MaterialsZone

By Assaf Anderson

For ceramics manufacturers, consistently achieving high material quality while meeting specific functional needs is a key challenge.

The traditional way of achieving these objectives is through trial and error. But this approach is often time-consuming and expensive, leading to inefficiencies that cut productivity and profits. As the demand for high-performance materials grows—especially in the electronics, construction, and consumer goods sectors—manufacturers are under even more pressure to speed up production cycles and cut down on wasted resources.

Manufacturers can make the production process more efficient and cost-effective by leveraging data-driven insights and predictive tools. This article highlights one such platform for data-driven R&D, MaterialsZone, and describes how it can be used to support accelerated innovation in the ceramics industry.

The need for data-driven R&D

In materials science, many research and development teams rely heavily on trial-and-error methods, which can impede the ability to innovate quickly and respond to market needs.[1] On top of that, especially in the ceramics industry, traditional R&D methods often suffer from data silos, with key information dispersed across different systems and formats. Scattered data leads to gaps in knowledge and makes collaboration more difficult, resulting in a slower and less reliable research and development process. Additionally, there are increasing regulatory and environmental pressures to implement more sustainable and streamlined processes to reduce carbon emissions.[2]

Data-driven solutions are helping to address these challenges.[1] By providing a centralized platform for data, manufacturers can make informed, data-backed decisions that require fewer trial-and-error experiments to achieve material property optimization, resulting in products being brought to market faster and in a more cost-effective manner.

Benefits of data-driven insights in traditional ceramics industries

In the ceramics industry, manufacturing involves multiple processes applied at various steps, as well as complex formulations. So, the potential for data-driven solutions to positively impact the process is profound.

For example, European tile manufacturers have recently experienced heightened disruptions in clay sourcing due to geopolitical tensions, notably issues with clay imports from Ukraine.[3] Data-driven solutions can help these companies quickly adapt to the disruptions by analyzing alternative clay compositions and forecasting their effects on critical factors, such as shrinkage rates, thermal expansion, bonding strength, firing temperatures, dimensional stability, and the risk of defects such as cracking, crazing, warping, or delamination. This information allows manufacturers to minimize the production of grade B tiles, ensuring greater consistency and higher product quality while reducing the number of iterations needed to identify the right blend of materials and process conditions.

Another significant challenge for tile manufacturers is finding the right balance of whiteness, durability, and cost in glaze formulation. Data-driven tools evaluate a range of parameters, such as color management, gloss levels, and cost, which improves product quality and reduces production costs.

As the ceramics industry shifts to water-based inks in digital printing,[4] data-driven solutions address challenges such as maintaining solid concentrations and preventing printhead clogs. These tools help develop formulations that balance these requirements, making the printing process efficient and sustainable.

Data-driven solutions also support optimized kiln operations. By adjusting kiln parameters to accommodate alternative energy sources, such as green hydrogen,[5] these solutions support efforts to reduce carbon emissions, helping manufacturers adopt cleaner energy without sacrificing product quality.

MaterialsZone: A comprehensive solution for accelerated innovation

MaterialsZone is a cloud-hosted software as a service (SaaS) platform that specializes in materials informatics. It provides essential storage and AI-driven computing capabilities for companies and research organizations to allow streamlined optimization of material properties, improved production efficiency, and accelerated time-to-market.

MaterialsZone's comprehensive suite of tools is structured around four key components (Figure 1):

The **Materials Knowledge Center** provides one central source for all data by aggregating everything from procurement information to regulations, technical specifications, experimental results, and quality control (Figure 1a). Team members can then use the **Collaboration Hub** to share insights, leave comments, and track progress in real-time, thus making collaboration seamless and reducing redundancies.

The **Visual Analyzer** makes it easy to perform complex, multidimensional analyses (Figure 1b). Researchers can quickly extract meaningful insights from large datasets by visualizing correlations, sensitivities, and performance metrics, helping them make informed decisions that improve products.

The **Predictive Copilot** utilizes the organization's materials data and AI algorithms to guide researchers in their materials discovery and optimization (Figure 1c). This tool can be used to forecast experimental results. For example, it can help predict mechanical failures, drops in material stability, or tonality conformity issues before they occur. These predictions give teams time to mitigate the effects of these issues or even to avoid them altogether when planning and designing experiments.

The Predictive Copilot excels with data, but it is also designed to function without it. The **AI-Guided**

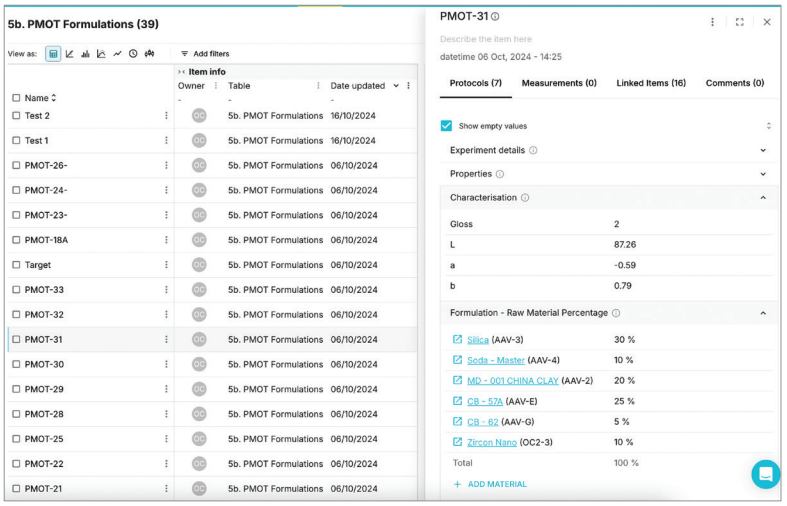

Figure 1a. The Materials Knowledge Center and Collaboration Hub allow the documentation of all experiments in a centralized database, thus making collaboration seamless and reducing redundancies.

Figure 1b. The Visual Analyzer helps researchers uncover trends and relationships that exist within their data, facilitating data-driven decision making and providing an up-to-date picture of progress and achievements.

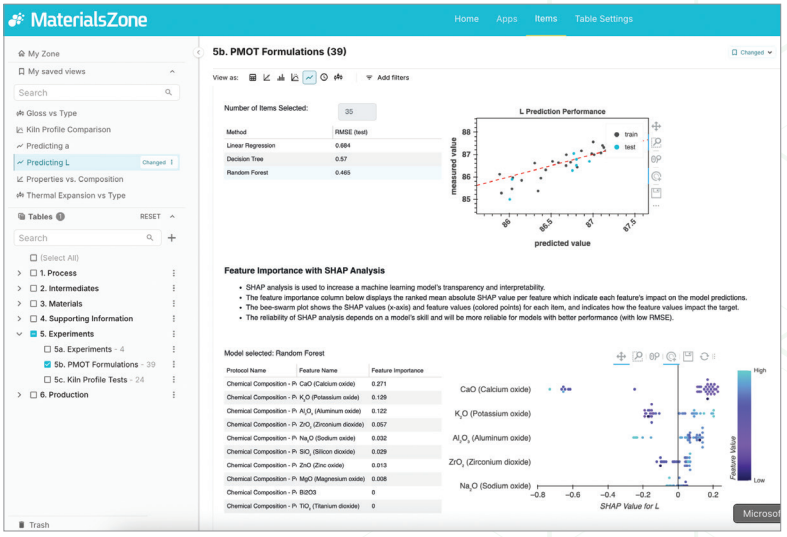

Figure 1c. The Predictive Copilot uses machine learning models to predict experimental outputs. In this screenshot, tonality L values based on glaze compositions are being predicted, and the importance of each glaze formulation component in the model's decision-making process is explained.

Predictive tools and data-driven insights to accelerate ceramics innovation

Product Development feature of the Predictive Copilot simplifies iterative AI modeling, empowering researchers and materials scientists to achieve faster and smarter innovation. For example, with direct access to AI-generated experiment suggestions, users can streamline development cycles seamlessly within their existing workflows. Where it is necessary to react to changes in the quality of supplied raw materials, process fluctuations, or customer specifications, the algorithm can suggest the next best course of action, with or without historical data. These suggestions drastically cut the valuable time and resources that go into trial-and-error iterations.

Case study: Ceramics for solid-state batteries

The benefits of MaterialsZone's suite of tools are not just applicable to traditional ceramics industries—they benefit advanced sectors as well, such as energy storage.

Ceramic materials have widespread uses in the energy sector,[6] including in the development of solid-state batteries. By replacing traditional liquid electrolytes with solid-state ceramic materials,[7] batteries become significantly less flammable, enhancing safety. Additionally, these batteries allow the use of metallic lithium, enabling a more compact and energy-dense design that translates to longer-lasting batteries and extended range for electric vehicles.

In collaboration with the U.S.–Israel Binational Industrial Research and Development Foundation,[8] MaterialsZone partnered with professors Eric Wachsman and Paul Albertus at the University of Maryland to advance the application of ceramic electrolytes in battery technologies. They are working to establish a comprehensive knowledge base on the performance of ceramic electrolyte materials in both lithium-based and sodium-based battery systems, benchmarking these insights against other battery technologies. This knowledge base will combine data, predictive models, and visualizations to deepen understanding of ceramic electrolyte performance in solid-state batteries, aiding the industry in making data-driven improvements.

More opportunities for data-driven ceramic innovation

By centralizing data, enhancing collaboration, and harnessing the power of artificial intelligence, data-driven solutions improve efficiency, reduce costs, and accelerate product development for materials-based companies. Whether optimizing glaze formulations for ceramic tiles or advancing battery safety and performance, this technology empowers traditional manufacturing processes and next-generation technologies to thrive in an increasingly competitive and environmentally conscious market.

About the author

Assaf Anderson is founder and chief technology officer of MaterialsZone (Tel Aviv, Israel). For more information, visit https://www.materials.zone or contact the MaterialsZone team at contact@materials.zone.

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MaterialsZone: Founding and future goals

Anderson

The idea for MaterialsZone took shape in 2015, when founder Assaf Anderson was researching oxide photovoltaics at Bar Ilan University, Israel. Recognizing the potential of data-driven tools to revolutionize high-throughput materials discovery, Anderson envisioned a centralized platform to transform raw data into actionable insights through advanced analytics and predictive capabilities.

Collaborating closely with professor Arie Zaban, a leading expert in energy materials and nanotechnology, Anderson laid the foundation for what would become the MaterialsZone platform. Together with a team of passionate scientists, engineers, and domain experts, they developed a comprehensive suite of tools designed to empower R&D teams and streamline innovation in materials science. In later years, Ori Yudilevich joined the team, bringing additional leadership and strategic expertise to scale the platform further.

Launched in 2018, MaterialsZone has since partnered with dozens of companies across diverse sectors. As the platform continues to evolve, the MaterialsZone team remains dedicated to refining its capabilities to meet the ever-changing needs of its users.

Future goals for MaterialsZone include integrating cutting-edge AI-driven solutions and broadening partnerships to support a wider array of materials and applications. By fostering a data-driven culture, MaterialsZone envisions a future where innovation is accelerated, sustainability is prioritized, and global manufacturing is transformed. ■

Jonathon Foreman
ACerS journals managing editor

Modeling opens new paths for research on refractory ceramics

Metal refining and steel manufacturing rely heavily on ceramic materials to contain the high-value products throughout the high-temperature processes while protecting workers and equipment.

Steel ladles are among the most demanding uses for refractory materials. Layers of refractory ceramics must contain liquid steel at temperatures approaching 1,600°C without reacting and while providing sufficient insulation to keep the outer shell cool for safe operations. Heating, cooling, filling, draining, and moving the ladles puts tremendous thermal and mechanical stresses on the refractories.

Measuring mechanical and thermal properties of the individual refractories that comprise ladles is relatively straightforward. However, experimentally ascertaining the interactions that occur in situ is very difficult and costly due to the ladles' considerable size. Thus, numerical modeling has become an important tool for improving performance and reducing purchase and operating expenses. Three recent articles in *International Journal of Applied Ceramic Technology* provide examples of the use of modeling for design and operational predictions.

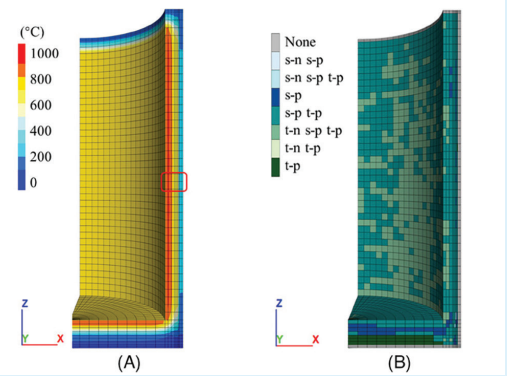
To approach full-scale testing, Gajjar et al. used numerical methods to develop a pilot-scale testing fixture.[1] They chose commonly used materials and construction techniques, with alumina spinel bricks for the working layer, bauxite for the safety layer, and low-density glass/fumed silica mat as insulation between these layers and the steel shell. Using commercially available modeling software, they determined the pilot-scale fixture size and refractory configurations that would provide data representative of full-scale ladles. The subsequent experimental temperature profiles followed trends predicted by the modeling. They also observed plastic deformation in the working layer bricks.

The method Gajjar et al. used to assemble the test fixture working layer—cutting and stacking the spinel blocks—is a labor-intensive process. In contrast, Dai et al. explored how using a cost-reducing method for fabricating the working layer would affect performance.[2] They simulated the effects of temperature dependencies of thermal conductivity, thermal expansion, and Young's modulus on thermal profiles and failure probabilities throughout all the layers of the ladle (Figure 1). Their model encompassed typical time–temperature schedules used for drying, firing, and operation.

As was observed in the Gajjar article, the model in the Dai study predicted permanent plastic deformation, particularly near the hot surface of the working layer. Furthermore, the stresses of thermal expansion were mitigated by the decrease in Young's modulus. Their sensitivity studies showed that temperature dependence is important for modeling damage, while thermal conductivity is the most critical because it leads to temperature variances that are then translated to variances in expansion and modulus.

The temperature profiles that result from using a variety of refractory materials and configurations was explored by Santos et al.[3] They showed the effects not only on the refractories but also on the contained steel. For example, they showed temperature changes that result from thermal energy retained within and released by the refractory materials.

Notably, they replaced the alumina–magnesia of the working layer with an insulating alumina foam. The insulating working layer decreased the temperature at the shell while simultaneously enabling higher temperatures within the contained steel, though it retained very little thermal energy. These results point to the potential for saving energy and expense.



Credit: Dai et al., *ACT*

Figure 1. Temperature distribution (A) and plasticity states (B) of the model after being heated for 55,800 seconds. None: no damage; s and t: shear and tensile failures; p: failure happened in past.

The authors performed their simulations using open-source modeling software and compared their results with those attained from commercially available software. The data from both programs agreed to within about +/–10°C throughout the experiment cycles and through the thickness of the refractory layers. This finding demonstrates the potential to bring modeling capabilities to researchers with limited budgets.

In conclusion, modeling has become an important tool for ceramics and glass research by allowing speedy determinations of composition–structure–property relationships in complex systems. Thus, it can lead to fast improvements in a rapidly changing world.

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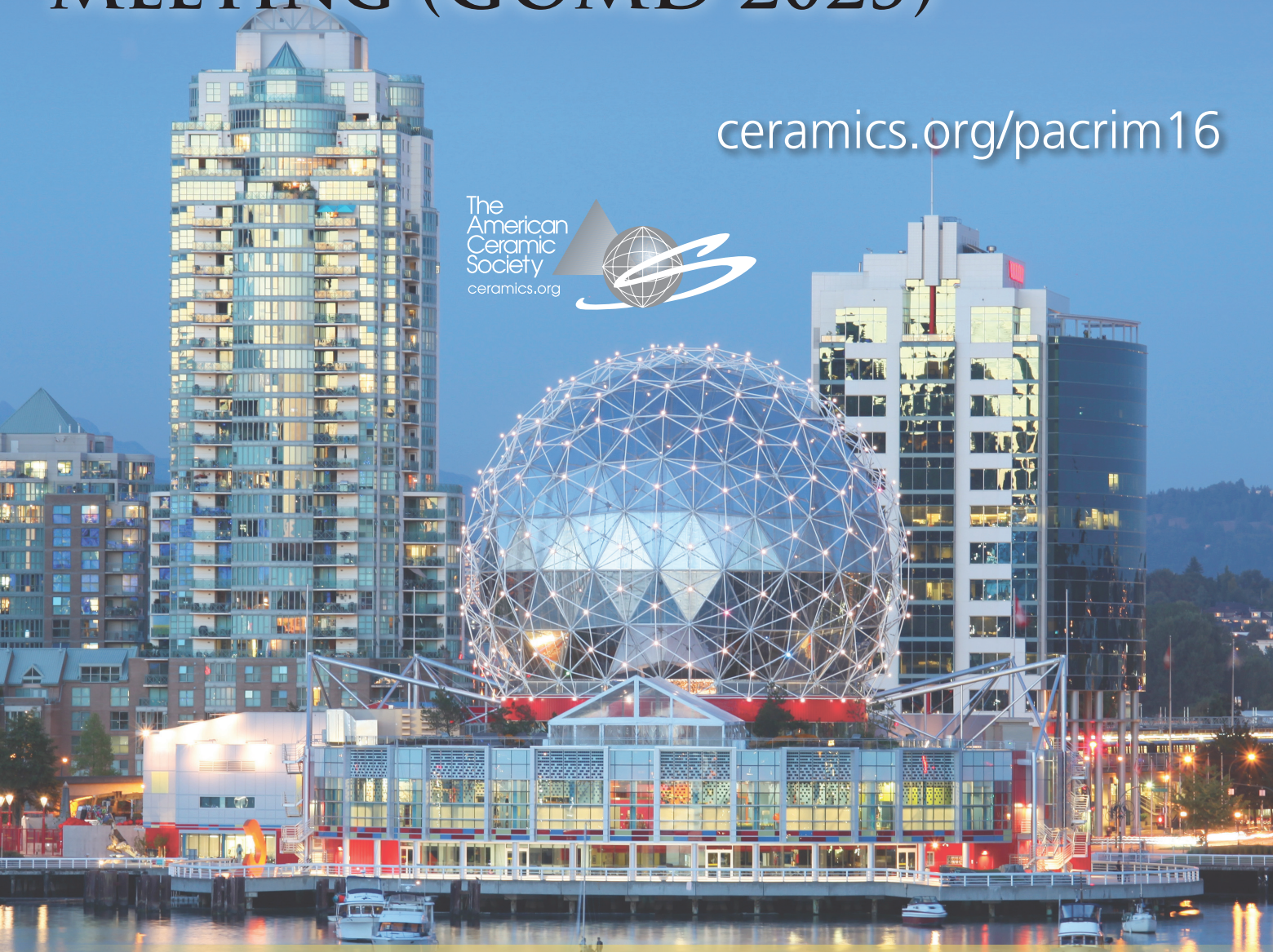

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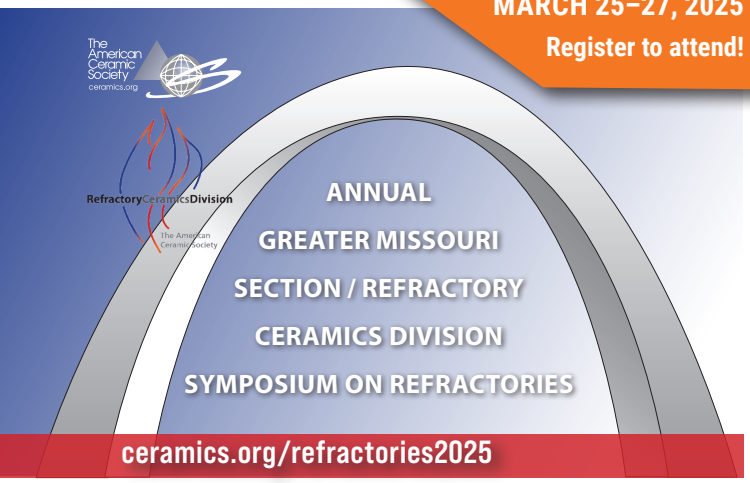

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28–Oct. 1 ACerS 127th Annual Meeting with Materials Science and Technology 2025 – Greater Columbus Convention Center, Columbus, Ohio; https://www.matscitech.org/MST25

October 2025

27–30 ➨ Unified International Technical Conference on Refractories – JW Marriott Cancún Resort & Spa, Cancún, Mexico; https://unitecr2025.com

January 2026

25–30 International Conference and Expo on Advanced Ceramics and Composites (ICACC 2026) – Hilton Daytona Beach Oceanfront Resort, Daytona, Fla.; https://ceramics.org/icacc2026

April 2026

12–16 ACerS Spring Meeting — Bellevue, Wash.; http://ceramics.org/acersspring

May 2026

31–June 5 12th International Conference on High Temperature Ceramic Matrix Composites (HTCMC 12) and Global Forum on Advanced Materials and Technologies for Sustainable Development (GFMAT 2026) – Sheraton San Diego Hotel & Marina, San Diego, Calif.; https://ceramics.org/htcmc12_gfmat2026

August 2026

31–Sept. 1 ➨ The International Conference on Sintering – Aachen, Germany; https://www.sintering2026.org/en

Dates in **RED** denote new event in this issue.

Entries in **BLUE** denote ACerS events.

➨ denotes meetings that ACerS cosponsors, endorses, or otherwise cooperates in organizing.

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By Rajat Durgesh Ramteke
Guest columnist

Potential and practical use of computational fluid dynamics in refractory design

Refractories are the backbone of numerous high-temperature manufacturing processes. These materials serve as the barrier between molten materials and the walls of the containing vessel, which exposes them to a complex variety of wear mechanisms that affect their durability.

Recent advancements in computer modeling and simulation techniques have helped shed light on refractory wear mechanisms.[1] Computational fluid dynamics (CFD) modeling specifically has found use in this field.

CFD modeling uses numerical methods to solve and analyze fluid flow and heat transfer within a given system. When applied to refractory design, CFD offers a platform for exploring the multifaceted mechanisms of wear, including thermal gradients, interfacial surface tension gradients, complex geometries, comprehensive parameters testing, and enhanced flow pattern visualizations.

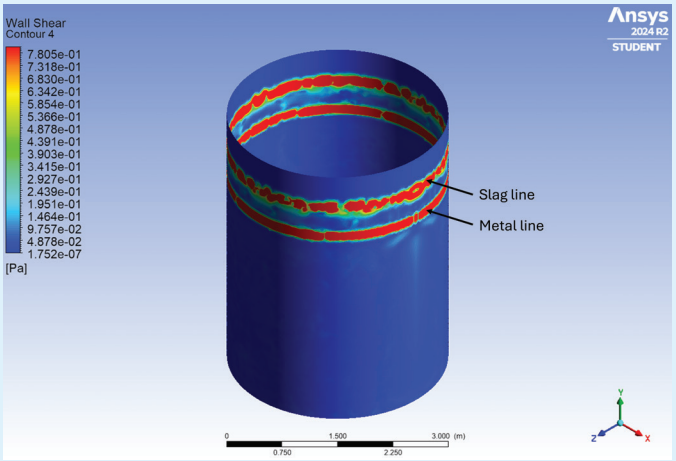
An example of how CFD modeling can support durable refractory design is understanding slag line and metal line wear in steel ladle operations. During steel processing, the ladle holding the molten steel will experience shear stresses due to temperature differences between the fluids (molten slag, molten steel, air) and the ladle walls. These viscosity and temperature gradients can result in complex wear phenomena, such as the Marangoni effect.[2]

The Marangoni effect describes the spontaneous motion of fluid interfaces driven by interfacial tension gradients.[2] In the context of refractory wear, these gradients arise from variations in chemical composition, temperature, and other factors at the interface between fluid phases. This interfacial motion can amplify stress at the triple points—the points where molten steel/molten slag/refractory wall and molten slag/air/refractory wall meet—resulting in accelerated wear.

Understanding these interconnected phenomena requires advanced modeling tools capable of capturing the intricate interplay of forces at work under these extreme working conditions. Addressing these challenges is where CFD modeling proves invaluable.

As part of my doctoral work at the University of Alabama at Birmingham, I used a CFD simulation to examine the shear stresses on the walls of a steel ladle (Figure 1). I focused on the effects of thermal gradients within the system, specifically the temperature difference between the fluids (molten slag, molten steel, air) and the ladle walls. Additionally, my analysis incorporated variations in the slag viscosity and thermal gradients to evaluate their influence on shear stress distribution.

Key findings from this simple study revealed that, despite minor variations caused by changes in viscosity and thermal



Credit: Rajat Durgesh Ramteke

Figure 1. CFD model of shear stresses on a ladle wall. Excessive stresses at triple points are depicted using a colormap, where blue represents low values and red indicates high values.

gradients, the triple points consistently showed excess shear stresses. Although these excess shear stresses may not be enough to cause erosion, these mechanical stresses facilitated and enhanced the corrosive wear, and so need to be studied.

These findings align with observations from the industry, showing that higher stress increases erosion rates while simultaneously enhancing corrosion by accelerating the transport and reaction of the corrosive species. It is important to note, however, that this case study is a simplified representation of the complex metal line and slag line wear phenomena.[3]

By understanding phenomena such as metal line and slag line wear at a fundamental level, industries can optimize ladle designs to minimize stress concentrations and develop refractory materials tailored to specific wear mechanisms. Fortunately, as this article shows, refractory modeling and simulation, particularly through CFD, offer unparalleled opportunities to address the challenges of high-temperature industrial processes.

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Rajat Durgesh Ramteke is a Ph.D. candidate at the University of Alabama at Birmingham. His research focuses on the corrosion resistance behavior of refractory ceramics against ironmaking and steelmaking slags. He spends his free time riding motorcycles. ■

WELCOMING NEW FACULTY

Myungkoo Kang, Ph.D.

Alfred University welcomes Dr. Myungkoo Kang as Assistant Professor of Ceramic Engineering. Dr. Kang leads the *Advanced Optical Glass-Ceramics & Correlative Metrology Laboratory.* His research team carries out the fabrication and characterization of novel chalcogenide glass and glass-ceramic materials for photonic applications, examining optical functionalities in bulk, planar, and three-dimensional forms. Specifically, his group focuses on the creative usage of irradiation processes to enable the seemingly destructive method to constructively form spatially modulated microstructures where their process-structure-property relationship is quantitatively established via multi-faceted cross-correlating in-situ microstructural-optical characterizations. Ultimately, his team aims to realize high figure-of-merit optical platforms such as next generation gradient refractive index lenses, reconfigurable photonic devices, and self-healing sensors. Dr. Kang has been actively engaged in scholarly activities, including serving as a former and current PI/co-PI/subcontractor of multiple government and industry-funded research programs (NSF, DARPA, AFOSR, and BAE Systems).

He has authored more than 60 peer-reviewed publications, numerous conference proceedings, and book chapters as well as multiple IPs related to these advances. His team's research has been covered on multiple press releases including Laser Focus World in 2024 (Self-healing chalcogenide glass?). He has received numerous international awards recognizing his contributions to both the optics and materials science fields, including Karl Schwartzwalder - Professional Achievement in Ceramic Engineering Award. He is a member of the American Ceramics Society (ACerS)'s Glass & Optical Materials (GOMD), Electronics (EDiv), and Basic Science (BSD) divisions.

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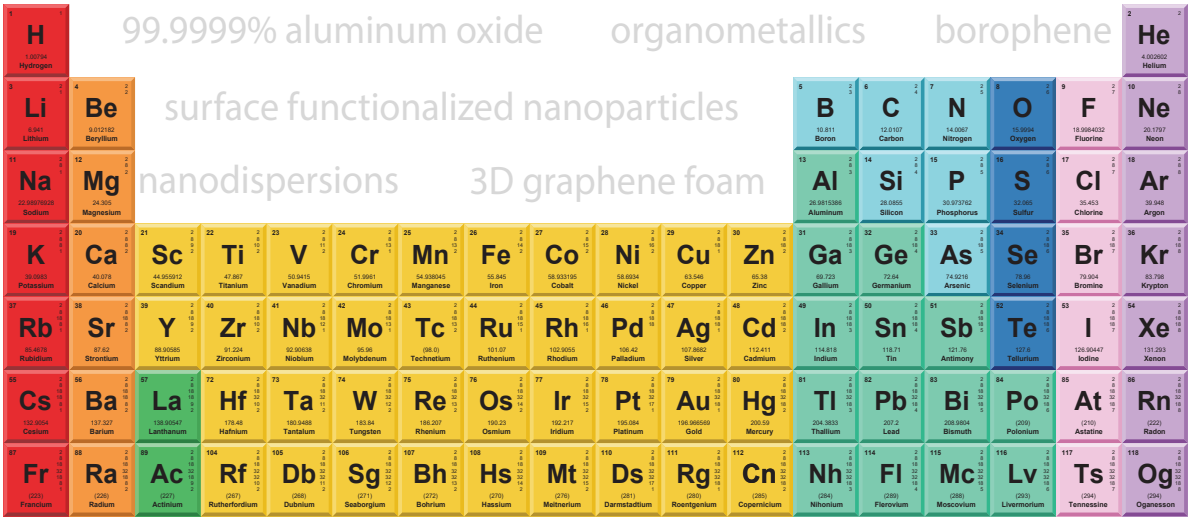

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