Materials for the energy transition: facilities that produce hydrogen, such as Linde AG's plant in Leuna, require new materials for efficient energy carrier storage and transportation.

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AI'S MATERIAL POWER

TEXT: TIM SCHRÖDER

As sustainability becomes ever more important, steel and other materials must meet increasingly demanding requirements: they need to be non-toxic, produced with minimal waste, and fully recyclable. There's also a push to reduce reliance on countries like China for raw materials. This makes it especially challenging to develop new materials and manufacturing methods. To tackle this, Jörg Neugebauer and Dierk Raabe from the Max Planck Institute for Sustainable Materials are now turning to artificial intelligence.

When the General Conference on Weights and Measures unveiled its new prototype for the meter on September 26, 1889, in Sèvres, near Paris, experts at metrology institutes around the world breathed a sigh of relief. After nearly a century, the scientific community had finally created a meter prototype that satisfied all demands for precision: a rod made of an alloy containing 90 percent platinum and 10 percent iridium. The rod featured a fine scale that allowed for exact measurements of one meter. The crucial factor, however, was that platinum-iridium alloys are nearly unaffected by the temperature fluctuations typical of temperate regions. Other metals expand significantly when heated and contract in the cold. Not so with the platinum-iridium alloy: under such conditions, the meter prototype remains virtually the same length at all times.

The International Bureau of Weights and Measures (IBWM) in Sèvres sent 30 copies of the meter prototype to metrology institutes in various countries. It wasn't long before experts realized that this would become quite expensive over time, as platinum was extremely costly, even back then. So, the IBWM tasked its in-house physicist, Charles Édouard Guillaume, with finding a more affordable alternative to the platinum-iridium alloy. Over the following months and years, Guillaume tested numerous material combinations. In 1896, he finally discovered the perfect mixture: an alloy of 64 percent iron and 36 percent nickel that, like platinum-irid- ⟶

ium, barely reacts to temperature fluctuations. The researcher had hit the jackpot. The alloy wasn't just a suitable alternative for the meter prototype, it was also perfect for other measuring and precision instruments, such as the tiny gears in pocket watches and wristwatches. These too must resist temperature fluctuations to ensure the mechanism doesn't seize up when it gets warmer. Guillaume named his alloy "Invar," meaning invariable, unchanging. In 1920, his groundbreaking discovery earned him the Nobel Prize.

Invar alloys for hydrogen infrastructure

Today, there is a wide range of Invar alloys, all of which maintain a stable volume within a specific temperature range. For instance, there are alloys used in cryogenic tanks that store liquefied natural gas (LNG) at minus 160 degrees Celsius. If the alloy contracted in the cold, cracks could form, bolts could loosen, and valves might start leaking. "Industry is constantly searching for new Invar alloys that neither shrink nor expand over a wider temperature range," says Dierk Raabe, a materials scientist and Director at the Max Planck Institute for Sustainable Materials in Düsseldorf. For instance, they are exploring alloys for hydrogen tanks, pipelines, and the global hydrogen infrastructure that will emerge in the coming years.

In general, there is currently a high demand for new alloys, as the sustainable transformation of the economy places significant demands on materials. "This goes far beyond the example of Invar," says Dierk Raabe. For instance, the European Union aims to reduce its dependence on individual countries for raw materials by 2030 with its Critical Raw Materials Act – particularly for rare earth metals, which today are predominantly sourced from China. One solution would be to design alloys using chemical elements that can be easily recovered during recycling. This would reduce the need for imports. Alternatively, the metal industry could shift from critical materials like rare earth metals to alternatives that do not rely on a small number of dominant suppliers. Another goal is to ensure that chemical elements that harm the environment or pose health risks are eliminated from alloys. "The challenge is that you can't simply replace elements in alloys with others, as this usually results in fundamental changes to the material's properties," adds Jörg Neugebauer, a physicist and Director at the Max Planck Institute for Sustainable Materials.

Materials science currently faces the challenge of developing a wide range of new alloys within just a few years. "This can't be accomplished with experience, scientific intuition, and laboratory experiments alone," says Dierk Raabe. That's why researchers in Düsseldorf have been relying on artificial intelligence for some time now, or to be specific: on machine learning. The algorithms help them identify new alloys for everyday applications more quickly.

SUMMARY

Artificial intelligence, specifically machine learning, can uncover patterns in large datasets that remain hidden from humans. This ability can be used to identify alloys with desired properties from among countless possibilities.

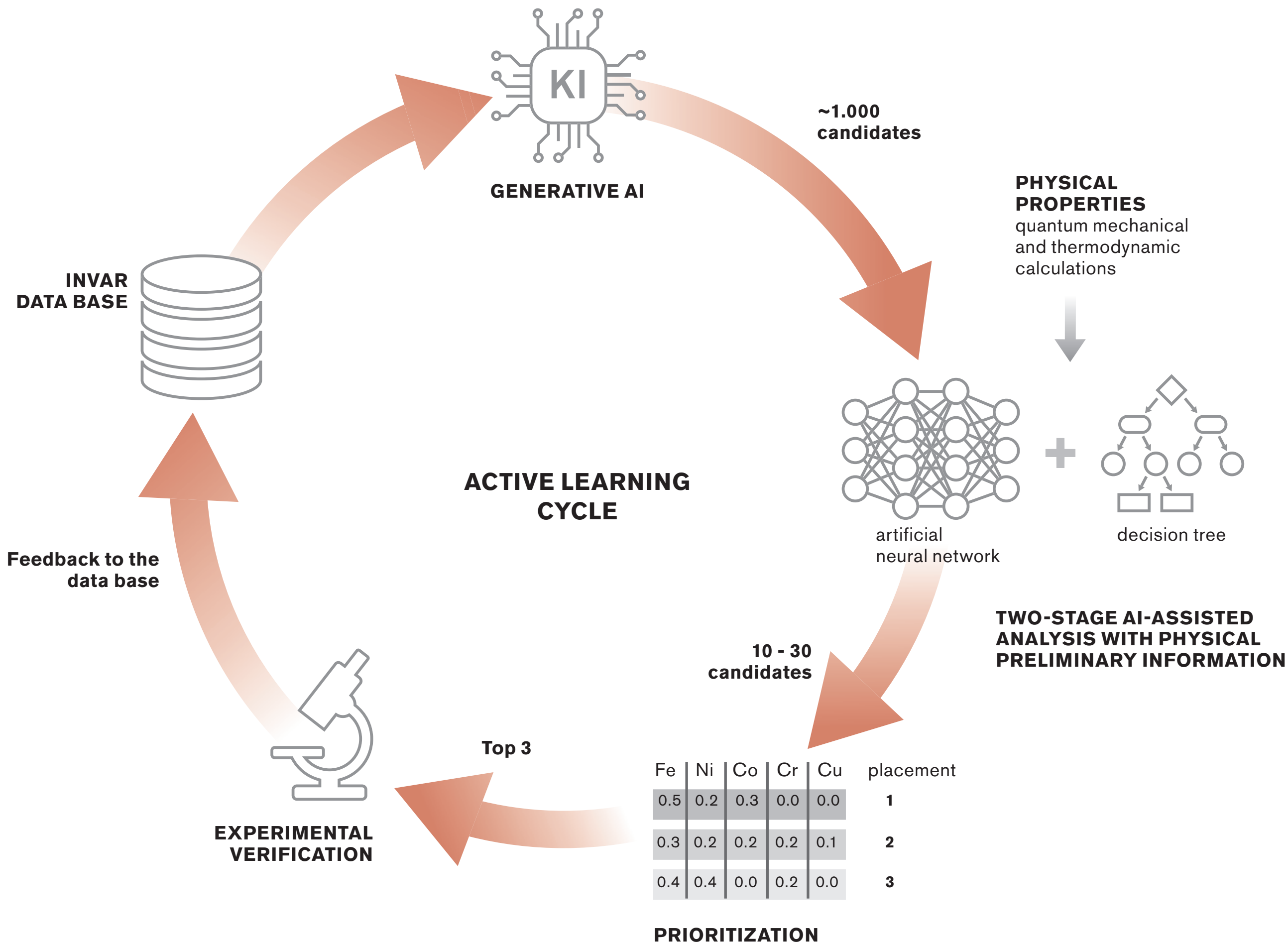
A team at the Max Planck Institute for Sustainable Materials is combining machine learning with database information, physical calculations, and experiments to develop new alloys.

Using AI, the group has developed Invar alloys and soft magnets, among other innovations. They also use language models for scientific research.

Machine-learning methods often rely on a concept known as "neural networks." These networks are first trained to recognize specific patterns. They are called neural networks because, like neurons in the brain, they analyze information across multiple layers. However, a simple neural network is not sufficient for materials research.

To address this challenge, Dierk Raabe and his colleagues have developed a cocktail of AI methods. This approach enables the team to identify promising new alloys in an iterative process – for example, for Invar steels. The process starts with an instruction such as: "Find an Invar alloy for temperature range x that is cheaper than conventional options." In the first step, an AI system generates roughly a thousand potential new Invar alloys from the thousands of alloy datasets stored in data bases. Next, additional AI models, including artificial neural networks, narrow the options down to 20 or 30 candidates. These candidates are further evaluated through physical calculations, such as those based on density functional theory. "The internal structure and properties of materials depend on various quantum mechanical factors, such as the energies between atoms or magnetism," explains Jörg Neugebauer. "The calculations take all these parameters into account and can test whether the alloys proposed in the first step actually exhibit the required properties."

Of the up to 30 candidates that remain, those predicted by the models to have the lowest thermal expansion coefficients are produced and tested in the lab. The results are fed back into the alloy database, completing the cycle and allowing it to start again. Because the system learns from its own analysis, Jörg Neugebauer and Dierk Raabe refer to it as active learning. Using this method, their team has developed two new Invar alloys for hydro-



GRAPHIC: GCO, FROM ZIYUAN RAO ET AL., MACHINE LEARNING-ENABLED HIGH-ENTROPY ALLOY DISCOVERY. SCIENCE 378, 78–85 (2022).

In an active learning cycle looking for new Invar materials: Based on alloy properties stored in data bases, a generative AI model first proposes potential new compositions. From approximately 1,000 suggestions, additional AI models, including artificial neural networks, narrow the options down to no more than 30 candidates. They also consider the results of physical calculations. The top three candidates with the lowest thermal expansion coefficients are experimentally tested and added to the database.

gen and natural gas tanks that change their volume even less during temperature fluctuations than conventional alloys do. Dierk Raabe explains why developing such materials is so challenging: the finished material has to fulfill a wide range of requirements. An aluminum alloy for an electric vehicle, for example, must be strong and rigid – while also being corrosion resistant and recyclable. In addition, the material must be easy to work with, such as for casting, welding, or shaping, and each individual process should become more energy efficient.

However, there's yet another challenge. For several years now, alloys have been incorporating far more chemical elements than they did in the past. Charles Édouard Guillaume needed only iron and nickel for the first Invar steel. Modern alloys, such as those used in aircraft turbines, sometimes contain more than ten different chemical elements. Specialists often refer to these as high-entropy alloys. These have the advantage of combining multiple, sometimes even contradictory, properties in a single material. Several years ago, high-entropy steels were developed at the Max Planck Institute in Düsseldorf. These are extremely strong but deform easily under heavy loads – making them the ideal material for a car's crumple zone. In an accident, these steels can deform by up to 35 percent, absorbing the energy of the impact.

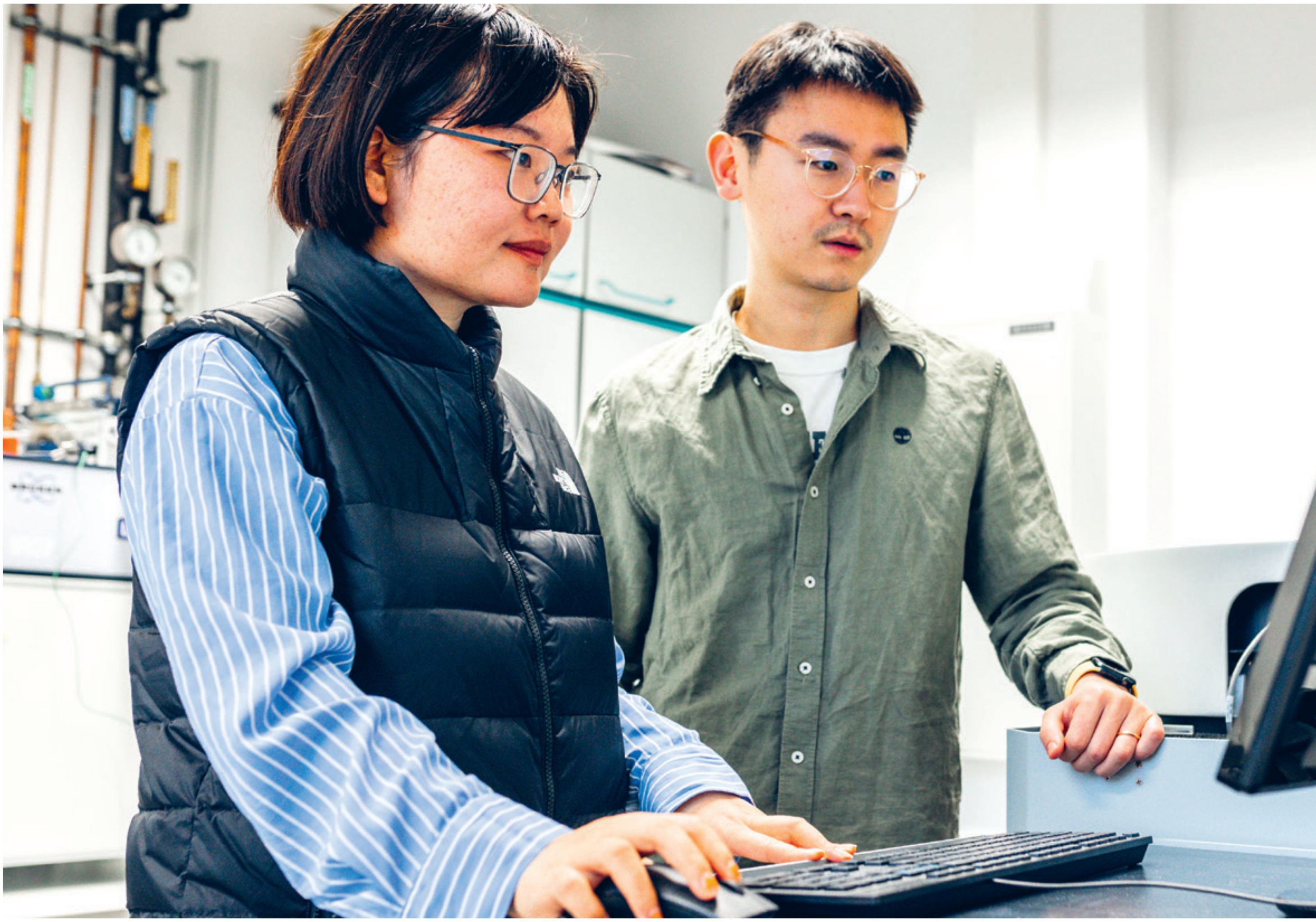


PHOTO: MAX-PLANCK-INSTITUTE FOR SUSTAINABLE MATERIALS GMBH

The challenge in developing high-entropy alloys lies in the exponential increase in possible variations as the number of chemical elements grows. Even when considering only the most commonly used elements for alloys, there are 1050 possible variations. The Düsseldorf institute does have sputtering systems that can produce tens of thousands of alloys in ultra-thin layers within a short time. "But this doesn't allow us to test how a steel, later produced on a 1,000-metric-ton scale, will behave in a finished component," says Jörg Neugebauer. "No one would likely board an aircraft made from materials tested only as nanolayers." Without the help of AI, millions of larger samples would need to be produced to test the properties of high-entropy alloys. This is unfeasible and makes AI indispensable.

Robust magnets for wind turbines

The team at the Max Planck Institute for Sustainable Materials recently achieved a breakthrough, using AI to develop a new high-entropy alloy for soft magnets. These magnets can be magnetized and reversed even using relatively weak magnetic fields. The market for such soft magnets is growing, as they are essential for generators and nearly all electric motors used in wind turbines, hydropower plants, and electric vehicles. Conventional soft magnets are not always robust enough for this purpose, as they can be damaged under heavy mechanical stress or corrode. Until now, there have been few mechanically durable soft magnets, as robustness and soft magnetism typically conflict in existing materials. The new high-entropy alloys – composed of iron, nickel, cobalt, tantalum, and aluminum – combine both

Did the artificial intelligence get it right? Hongyu Chen (left) and Liuliu Han analyze the properties of soft magnetic alloys, for which algorithms predicted high mechanical stability.

qualities: they are mechanically strong, yet maintain their "soft" magnetization. They are also more durable than conventional magnetic materials.

The cocktail of methods for active learning is already proving highly effective for Dierk Raabe, Jörg Neugebauer, and their team. "However, AI isn't yet at the point where it nudges us in a specific direction – along the lines of: "Hey, check out this or that alloy," says Jörg Neugebauer. "We still have to set the direction and feed it with data for finding new alloys, for instance, quantum mechanical data." But artificial intelligence excels at identifying relationships between numerous parameters and recognizing patterns that are too complex for humans to grasp. "Who knows, maybe in the future it'll be enough to define just a few parameters describing the properties of a new alloy – and AI will handle the rest," says Jörg Neugebauer.

Language models facilitate data research

Dierk Raabe and Jörg Neugebauer are now also using an AI technique popularized by ChatGPT – Large Language Models (LLMs). These models are trained on vast amounts of text, learning which letters and word combinations are most likely to appear together. This enables them to generate text. At the Max Planck Institute in Düsseldorf, an LLM is being used to search for corrosion-resistant alloys. The project combines AI-based methods with quantum mechanical knowledge and information from databases. However, the study of corrosion also relies heavily on lab reports and test protocols that describe the corrosion behavior of materials in plain language. The team in Düsseldorf feeds these documents into an LLM to process findings more quickly. "Of course, LLMs initially know nothing about physical relationships," says Dierk Raabe. "They might produce nonsense at first. But they can still be incredibly helpful." They are particularly well suited to handling specific tasks, such as analyzing lab reports. "LLMs compile information, which simplifies our search for alloys. We researchers are increasingly becoming conductors, merely guiding the process."

Some time ago, Dierk Raabe used an LLM to identify the largest scrap trading hubs in the world and the residual materials traded there. With the shift toward a circular economy, the amount of scrap that needs to be recycled is set to increase significantly. This will require the use of a wide variety of scrap types, including mixed and contaminated scrap of lower quality. It would be a remarkable step if AI could show materials researchers how to turn such scrap into high-quality alloys and products. "Even just exploring the global scrap supply was fascinating," says Dierk Raabe. "The software provided this information in half a day," he says. Without AI, it would have been far more time-consuming. "This is all incredibly exciting. I'm very curious to see where AI will take us next."

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GLOSSARY

INVAR ALLOY
A material whose volume remains nearly unchanged during temperature fluctuations.

SOFT MAGNETIC
A material that can be magnetized or demagnetized by a relatively weak magnetic field. Materials like this are used in power generators and electric motors, among other applications.