

IC-MPPE
Integrated Computational
Materials Process and Product
Engineering.

Programme: FFG Produktion der Zukunft

Programme Line: COMET- K2 Zentrum

Project: PREHY, 10/2022-12/2025, single-firm



Hydrogen tanks and vehicles, Image: AI generated by MCL

NEW MATERIAL: HIGHER STRENGTH AND BETTER HYDROGEN RESISTANCE

DIGITAL MATERIALS DEVELOPMENT COMBINES ATOMISTIC SIMULATIONS, MACHINE LEARNING, AND AI, REDUCING DEVELOPMENT TIME AND MATERIAL COSTS.

The transition to CO₂-neutral energy requires hydrogen as an energy storage medium. For its safe use, materials must exhibit both high strength and ductility, even at very low temperatures down to 20 K (−253.15°C). However, long-term operation often leads to hydrogen embrittlement, the susceptibility to which increases with higher strength.

In this project, a digitally supported alloy development approach was used, combining density functional theory, thermodynamics, machine learning, and AI to systematically evaluate design principles such as stacking fault energy, lattice mismatch, and hydrogen trapping. This enabled the identification of two promising new materials - an austenitic steel and a nickel-based alloy - for more

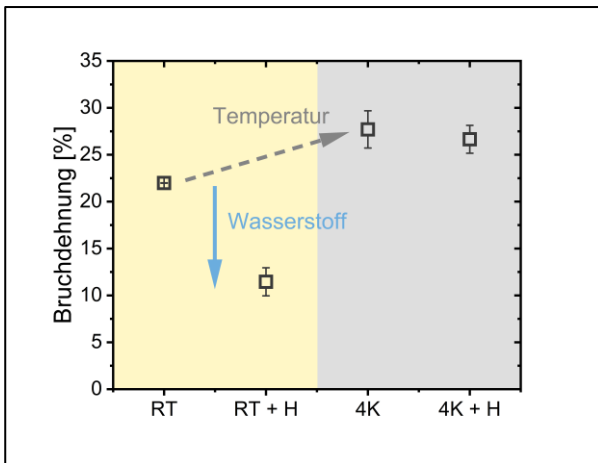
hydrogen-resistant precipitation-hardened alloys. The fully digital workflow replaces costly trial-and-error experiments and significantly shortens development time.

As part of the project, in collaboration with voestalpine BÖHLER Edelstahl GmbH & Co KG and Montanuniversität Leoben, two new materials—an austenitic steel and a nickel-based alloy with higher strength and improved hydrogen resistance—were successfully developed and patented. Experimental tests at 4 K and room temperature confirm their high resistance to hydrogen embrittlement.

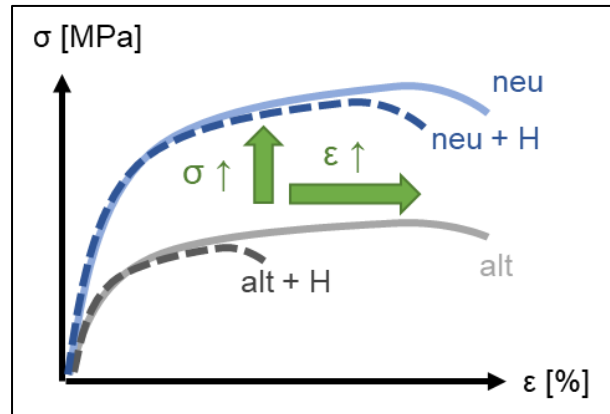
SUCCESS STORY

Impacts and Effects

The newly developed materials increase reliability and safety in hydrogen systems, enable lighter and more compact components, and thereby reduce weight, costs, and raw material consumption compared to conventional materials, making a substantial contribution to the energy transition. At the same time, the developed digital approach demonstrates how data-driven materials research can sustainably combine innovation and economic efficiency.



Effect of hydrogen and the reduction in temperature from room temperature (RT) to 4 K (-269°C) on the elongation at fracture of an austenitic steel, copyright MCL



Increase in strength and ductility of the old and new material illustrated in a schematic stress-strain diagram, copyright MCL

The patented materials are intended for pilot applications in hydrogen tanks and cryogenic systems. Through faster development cycles and reduced material costs, the digital materials design method improves the long-term competitiveness of European hydrogen technologies and supports strategic independence from critical raw materials.

Project Coordination (Story)

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