MAX PLANCK INSTITUTE
FOR SUSTAINABLE MATERIALS

Max Planck Institute for Sustainable Materials

Scientific Report 2022–2024

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Max Planck Institute for Sustainable Materials
Max-Planck-Str. 1
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Germany

Front cover

The Max Planck Institute for Sustainable Materials addresses one of today's most urgent challenges: transforming materials, a leading source of greenhouse gas emissions, into sustainable resources for a circular economy. Our research considers the entire lifecycle of materials - from primary synthesis from ores, through manufacturing and processing, to their use in advanced mobility, infrastructure, energy, and medical applications, and finally to their reuse and recycling.

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Preface

This report presents the activities and achievements of the Max Planck Institute for Sustainable Materials, MPI-SusMat (formerly MPI für Eisenforschung GmbH) between 2019 and 2024, with a focus on the last 3 years.

The institute has currently four departments: Computational Materials Design (Prof. J. Neugebauer), Interface Chemistry and Surface Engineering (Prof. M. Stratmann (retired in 2023), provisional head: Prof. J. Neugebauer), Microstructure Physics and Alloy Design (Prof. D. Raabe) and Structure and Nano-/Micromechanics of Materials (Prof. G. Dehm). The MPI-SusMat hosts an Independent Max Planck Research Group on Nanoanalytics and Interfaces (Prof. C. Scheu). Each department consists of 4-5 research groups. The institute also hosts a number of interdepartmental and partner groups where topics of interdisciplinary and emerging character are jointly pursued. Service groups support the scientific departments. These include the synthesis, processing and testing of materials, chemical analysis, hydrogen laboratories, metallography, mechanical workshop, facilities to design and build scientific equipment, electronic workshop, library, computer network centre, research coordination office, international and onboarding office and administration.

The most eminent recent event was the redesignation of the institute, after a 107-year success story, from MPI for Iron Research (Eisenforschung) into MPI for Sustainable Materials (MPI für Nachhaltige Materialien) in 2024.

Despite its positive state and excellent reputation, the institute saw a need to evolve further, towards new research horizons, as the importance of materials in our civilization is changing rapidly (Box 1). The approximately 18 % share of materials synthesis alone as a driver of climate change shows that materials research must realise that sustainability is an intrinsic property of materials and as such must be included and considered in basic research and engineering implementation. This raises the question of how every individual atom found in materials, whether introduced intentionally during synthesis or acquired during service life, can become part of a circular economy with a holistic perspective, from synthesis to disposal to reuse. The answer requires a complete rethinking and new basic scientific approaches and methods, some of which go far beyond the current state of materials science.

Box 1: Materials stand for:

Pro (EU economic area)

- Leveraging 75 % of all emissions
- Influence on 46 % of production
- 3.5 billion € turnover per day
- ...

Con (global mean values, per year)

- 18 % of all CO_2 emissions
- 20 % of the energy consumption
- In some cases, 2000 times the water consumption per mass extracted
- 40 billion tons of destroyed soil
- Recycling between <1% and 40%
- Exploitation of the Global South
- In part >100% annual growth
- ...

The devastating sustainability balance of materials, as well as their great economic importance, are usually hidden behind products and often difficult to recognize. A circular economy *de facto* does not exist, with recycling rates for some strategic materials below 1 %. Uncontrolled contamination with foreign elements degrades recycled materials compared to primary synthesis, an effect we call "chemical hysteresis". In a few cases the opposite effect is observed, where impurities can even have a beneficial effect such as in certain electrocatalysts or in hydrogen storage materials.

Many of the technologies needed to avoid the huge industrial CO_2 emissions do not even exist today because basic physical and chemical insights and foundations for the development of novel technologies are lacking. Often, the fundamental scientific questions behind them have not even yet been asked or tackled till today or were overlooked so far.

With its adjusted direction, the institute is thus placing one of the most pressing challenges of our times at the core of its research, namely the question of how materials, as the largest single contributors to greenhouse gas emissions, can become more sustainable and form the basis of a circular economy. Our vision encompasses aspects of materials synthesis and design, environmental degradation, as well as materials as key enablers and drivers of low-emission technologies.
The topic is ideally suited for an institute like MPI-SusMat, which has roots, in both fundamental materials science and advanced process technology and manufacturing: Tackling the generational tasks described above requires massive basic research, because the challenges cannot be solved by regulatory, economic, or available technological measures alone (Box 2). The topic of sustainable materials lies between traditional disciplines of materials science, chemistry, physics, engineering, mechanics, also branching out into social and economic sciences.
In basic materials research, this new topic is only emerging – only a few 100s papers are published each year on CO_2 avoidance in material synthesis compared to over 65,000 publications per year on the impact of CO_2 on climate – and is poised to become decisive over the coming decades when 12 billion people on the planet, with growing average gross domestic product, need huge quantities of materials for infrastructure, manufacturing and housing. In the linear economy of past millennia, the challenge was to create products from materials consisting of mixtures of pure elements. In a circular economy, the challenge is to break these down again into their starting materials such that they can be used for

Box 2: Topics for basic research on sustainable materials:
New phenomena and foundations of sustainable synthesis

— Materials in the middle of high-dimensional phase diagrams: Thermodynamics, kinetics, electro- chemistry in multicomponent systems with up to 65 elements.
— Basic science behind CO_2 -free synthesis of materials.
— Recycling ab-initio: understanding and utilizing the effect of up to 65 elements in materials.
— Systems theory of the circular economy.
— Hydrogen-based redox systems.
— Chemistry, structure, mechanics, and lattice defects in redox processes at heterogeneous interfaces.
— Urban mining instead of geo-mining.
— Upcycling instead of downcycling.

Methods

— Synthesis ab-initio: atomistic description of dynamic phenomena in sustained synthesis, under extreme conditions and in multicomponent systems.
— AI for "sparse data" problems, multicomponent systems, and efficient processes.
— High-throughput methods in theory, synthesis, and characterization to understand the impact of contaminants on materials and to develop chemically tolerant materials.
— Precision and in-operando analytics in electrochemistry and for hydrogen detection.
— Multi-probe characterization, in which contaminated materials are chemically and structurally analysed down to the electronic level at the same sample location.
— In-situ and in-operando characterization of highly dynamic diffusion, transformation, and redox processes down to the atomic and electronic level.
...

Sustainable materials under harsh environmental conditions

— Material property control through defect engineering and nanostructuring instead of complex chemical composition.
— Sustainable magnet and energy materials without critical elements.
— Electrochemistry and nanomechanics of materials longevity.
— “Cross-over” and multifunctional materials that are tolerant to contamination.
— Role of lattice defects as sinks for impurities in materials.
— Self-healing, durable, corrosion-resistant and hydrogen-resistant materials.
— Metals as renewable fuels and baseload-capable metal-air batteries.
— Materials from highly contaminated raw materials ("Science of Dirty Materials").
— ...

new syntheses with the smallest possible chemical hysteresis and to design materials that can tolerate massive and time-variable impurities or even to exploit them to reach a net positive effect.
Materials have conventionally been designed along the edges of phase diagrams with only a few chemical components, as in engineering alloys, semiconductors, and ceramics, where one element or oxide usually dominates. In a circular economy, about 2/3 of the secondary materials, which have to find their way back into the cycle in the future, are mixed beforehand in products and processes in such a way that they can contain 10–65 elements (e.g. computers and cellphones). In addition, there are hardly any chemically pure ores available, but minute amounts (some <1.5 %) are now extracted from complex minerals for many important elements (e.g. Ni, Co, Cu), sometimes resulting in up to 50 times more CO_2 emission relative to the mass of the element extracted. Material design and synthesis must therefore be reinvented based on these highly intermixed many-component materials arising from the circular economy and from complex and chemically "poor" raw materials, based on the kinetic, thermodynamic and microstructural principles of a high-dimensional chemical space with up to 10^{65} possible elemental combinations. This poses new challenges for the development of experimental and theoretical methods, which can only be addressed by a deep synergistic understanding of quantum mechanics, nonequilibrium thermodynamics and kinetics, and microstructure jointly applied to material design, synthesis, property testing, and recycling. This must be done with consideration of minimizing chemical hysteresis losses with constant contamination, accumulation, and transformation of materials in a circular economy. There is as yet no systematic basic research on any of these challenges, although many fundamental new questions are emerging (Box 2). The leverage of such basic research would be enormous (Box 1).

All departments of the institute are already working intensively in the field of sustainable materials and have been advancing it together for several years with high synergy (e.g. IMPRS Sustainable Metallurgy; ERC Advanced Grant on Green Steel; various Nature and Science articles).
Beyond these new research topics, the MPI-SusMat’s mission remains largely unchanged with regards to its previous basic materials research fields, namely, to understand and design novel materials for structural and functional applications down to atomic and electronic scales, fully including the impact of real environments. Using latest analysis methods and theory, many of them developed in-house, we start to resolve and quantify material complexity in terms of its rich nano-cosmos, manifested by hierarchical and entangled atomic-scale structural and electro-chemical building units and defects. Accessing this complexity at a fundamental level is highly challenging and requires the constant development of experimental and theoretical techniques as most of the constituting nano-features are buried in the

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bulk, change over time (4D materials), and experience entanglements with correlations that range from a few atomic distances to micrometres. The structural complexity of advanced materials requires also huge efforts in probing how such materials respond to external or internal chemical, physical, bio-medical, and mechanical stimuli. The portfolio of research topics and their relation to the new and previous research priorities is shown in Fig. 1.

Fig. 1: *Topics along the new and established research priorities of MPI-SusMat.*

The institute also participates in several large network programs, amongst others 7 Collaborative Research Centres funded by the German Research Foundation and hosts 5 grants by the European Research Council (ERC) (Gault, Bitzek, Dehm, Ramachandramoorthy, Raabe) in the reporting period (in total 8 ERC Grantees since 2012). The institute won in 2017, 2020 and 2023 highest positions in the Ranking of the Humboldt Foundation among all non-university research organizations in Germany (rank 1 in engineering, rank 3 over all sciences) with 52 won scholarships and awards between 2019 and 2024 and hosted two scouts for the Alexander von Humboldt Foundation.
Over the past 3 years, around 30 members gained professorships from prestigious universities around the globe, underlining the institute’s ambition to propel careers. The MPI-SusMat heads the International Max Planck Research School - IMPRS SurMat and the successor school IMPRS SusMet, and has hosted 1 Max-Planck – Fraunhofer joint research initiatives during the reporting period.

The institute evolved not only scientifically. Work and life at the institute also opened: The MPI-SusMat has a Team Green, which is committed to create a sustainable and ecological working environment. The health management assessed that the overall working conditions are above average and so is also the overall working satisfaction.

This report is divided into four parts:
– *Part I* contains information on recent scientific developments, new scientific groups, large network activities, new scientific laboratories, and on the work and life at MPI-SusMat.
– *Parts II* and *III* cover the research activities of the institute. Part II provides a description of the scientific activities in the departments and Part III contains selected highlights, which summarize major recent scientific achievements in several topical areas of common interest.
– *Part IV* summarizes statistically relevant information about the institute.

The Directors of MPI-SusMat

Düsseldorf, November 2024

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