PREFACE

This report documents the scientific activities and achievements of researchers at the Max-Planck-Institut für Eisenforschung GmbH (MPIE) between 2013 and 2015. Moreover, we present some long-term methodological developments in the fields of computational materials science, advanced microstructure characterization, electrochemistry and synthesis.

The mission of the MPIE lies in understanding and designing complex nanostructured materials under real environmental conditions down to the atomic and electronic scales. More specific, the Institute conducts basic research on structural and functional materials, specifically steels and related alloys, considering their complex chemical-physical synthesis, characterization and properties, as well as their use in systemic components and under harsh environmental conditions.

Projects are conducted highly interdisciplinary, in an atmosphere of permanent mutual stimulation among experimentalists and theoreticians as well as among the different departments. The methodological interplay reaches from macroscopic and combinatorial synthesis up to thermomechanical processing of novel alloy classes through the observation of individual atoms by high resolution electron microscopy and atomic probe tomography, closely flanked by corresponding through-process and atomistic simulations.

The MPIE laboratories and simulation groups cover the entire synthesis, processing, microstructure and property chain, i.e. the materials development and understanding include and control the entire history of every specimen. Due to our interdisciplinary research approach we defined a number of core topical areas:

- Development of new structural materials
- Analysis of microstructure-related material properties
- Analysis and enhancement of the stability of surfaces and interfaces
- Development of scale-bridging simulation of materials
- Enhancement of energy materials

Through its focus on advanced complex materials the MPIE occupies a key role in enabling progress in a number of fields such as

- Mobility (e.g., ductile magnesium sheet alloys, high strength steels and soft magnets for light weight hybrid vehicles)
- Energy (e.g., hydrogen-tolerant structural alloys, efficiency of thermal power conversion through better high temperature alloys, semiconducting materials for photovoltaics and photo-electrochemistry, fuel cell components)
- Infrastructure (e.g., steels for large infrastructures such as wind turbines and chemical plants)
- Health (e.g., development of elastically soft titanium hip implants)
- Safety (e.g., nanostructured bainitic steels for gas pipelines).

We conduct projects with strong rooting in knowledge-oriented and pre-competitive basic research on the one hand and include aspects associated with the application and commercial relevance of the materials, processes and methods on the other hand. With its system-oriented research agenda and its institutional co-sponsoring by industry, the Institute constitutes a unique example of public-private partnership both, for the Max Planck Society and for the European industry.

Strengthening of the Institute's scientific profile is achieved by strategic collaborations with several academic partners, namely, R. Kirchheim (materials physics and atom scale characterization; University of Göttingen) who is external scientific member of the Max Planck Society, J. Schneider (combinatorial and thin film materials design; RWTH Aachen University) who is Fellow of the Max Planck Society, and G. Eggeler (high temperature alloys and energy-related materials; Ruhr-Universität Bochum) who is external group leader at the MPIE. With these colleagues a number of very close joint projects are pursued (e.g. exploring the limits of strength in Fe−C systems; hydrogen-propelled materials and systems; defectant theory; creep of superalloys; self-reporting and damage tolerant materials; atomic scale analysis of interfaces in superalloys and hard coatings).

The Institute hosts currently about 300 people, the majority being scientists. As 180 employees are funded by the basic budget provided by the shareholders of the Institute, around 120 additional scientists work at the MPIE supported by extramural sources such as the ERC, DFG, RFCS, AvH, DAAD, BMBF, BMWi and CRC to name but a few essential funding agencies.

An increasing number of co-operations with strategically selected industrial partners has provided further extramural momentum to the dynamic growth of the MPIE during the past three years. Besides the well established links to the steel industry and related companies in the domains of alloy design (bulk and surface), advanced characterization, surface functionalization, and computational materials science, new industrial co-operations were established in a number of novel fields: These new project directions are particularly valuable for the Institute's further development from a materials-oriented laboratory towards a system-driven institute developing complex materials in a holistic approach. This approach carries complicated engineering systems and environmental conditions into advanced materials science and manufacturing processes. New areas of growth including strong interactions with industry are in the fields of steels and related materials for automotive hybrid- and electro-mobility, energy conversion and storage, renewable energy, health, hydrogen-based industries, and computational materials science. This contribution of third-party funds and its balance between fundamental and applied science places the MPIE into a singular position within the Max Planck Society.

Further scientific momentum is currently fueled by the requirement for a better understanding of the often complex interactions between electrochemistry and microstructure. Modern materials are both, enabled and limited by the presence of interfaces and surfaces and their reactivity with the environment. This stimulates new experimental and theoretical projects at the MPIE in the fields of atomic scale and in-situ reaction analysis at interfaces regarding electrochemistry, transport, reactions and damage; hydrogen effects; combinatorial surface-electrochemistry; in-situ and multi-probing of interfaces; corrosion protection; interface cohesion and solid-liquid interfaces.

MPIE researchers have achieved several scientific breakthroughs in the past years such as the development of 7 GPa strong pearlitic steels, observation of mechanically induced martensite formation by severe plastic deformation, joint structural and chemical characterization of segregation in nanocrystalline steels and semiconductors at the atomic scale, development of long-term reliable corrosion sensitive self-healing coating systems, derivation of a scaling strategy predicting large-scale properties such as adhesion or cell-cell interactions on the basis of single-molecule measurements, design criteria to control the fracture toughness in metallic glasses, the discovery of linear confined structural and chemical states (complexions) at dislocations, understanding the complex interplay between vibronic and magnetic degrees of freedom in steels, the discovery of novel 2D interfacial phases in complex oxides, linking transport properties in semiconducting phases to growth conditions and defects and understanding degradation mechanisms in energy generating devices. These recent highlights were enabled by a number of long-term methodological projects which led to a variety of novel experimental and simulation tools. Examples are the combinatorial corrosion and catalysis probing cell, the scanning Kelvin probe, correlative atom probe tomography (TEM analysis conducted on the same specimens), the simulation toolbox DAMASK, the wet chemical cell for in-situ reaction analysis in TEM, high precision *ab initio* simulation methods, development of automated computational tools for high-throughput calculations, and development of site specific mechanical testing strategies under environmental conditions.

This report is structured into four parts:

- Part I presents the organization of the Institute including a short section on recent scientific developments, new scientific groups, new scientific laboratories, long-term oriented method development and large network activities.
- 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 short papers which summarize major recent scientific achievements in the topical areas of common interest of the MPIE.
- Part IV summarizes some statistically relevant information about the Institute.

The Directors of the MPIE

Düsseldorf, November 2015