PREFACE

This report documents the scientific activities and achievements of the Max-Planck-Institut für Eisenforschung GmbH (MPIE) focussing on the years 2016 to 2018. For evaluation purposes, some main trends are described over the past 6 years. Also, selected long-term methodological and large collaborative projects are presented.

Our mission is to understand and design nanostructured materials down to atomic and electronic scales. In this spirit, we conduct basic research on structural and functional materials, mostly metallic alloys, embracing synthesis and processing, characterization and properties, as well as their response in engineering components exposed to harsh environmental conditions.

We work interdisciplinary, with intense mutual stimulation among experimentalists and theoreticians as well as among different groups and departments. Fields of particularly intense interaction are:

- Stability of Surfaces and Interfaces
- Microstructure-related Materials Properties
- Development of Advanced Materials
- Scale-bridging Simulation and Materials Informatics

Along these topics we enable progress in key fields of highest relevance for manufacturing and society:

- Mobility (e.g., ductile magnesium, steels and magnets for light weight hybrid vehicles)
- Energy (e.g., hydrogen-tolerant structural alloys, catalysis materials, high temperature alloys, semiconducting materials for photovoltaics and photo-electrochemistry, fuel cell components)
- Infrastructure (e.g., steels for infrastructures, such as wind turbines and chemical plants)
- Medicine (e.g., biomedical tribology, compliant implant alloys)
- Safety (e.g., high toughness alloys, cryogenic alloys, coatings and thin film materials, hydrogen tolerant materials).

Our projects rest on pre-competitive fundamental research, yet, we also consider applications and system challenges. With this agenda and our institutional co-sponsoring by industry, the MPIE is a unique example of more than 100 years public private partnership both for the Max Planck Society and for the European industry. We took this last year's anniversary also as an opportunity to celebrate with a scientific colloquium, a public outreach program and a scientific project about the history of the Institute. We pursue strategic collaborations with several academic partners, namely, R. Kirchheim (materials physics; University of Göttingen) who is an external scientific member of the Max Planck Society, J. Schneider (combinatorial and self-reporting materials; RWTH Aachen University) who is a fellow of the Max Planck Society and with G. Eggeler (high temperature alloys; Ruhr-Universität Bochum) who is an external group leader at the MPIE. These and other collaborations have helped to intensify our scientific network with participation in large projects funded by Deutsche Forschungsgemeinschaft, e.g., the collaborative research centers SFB 761 (TWIP steels), TR 103 (novel superalloys), TR 188 (damage controlled forming), and SFB 1232 (combinatorial alloys design).

Out of the 372 people working at the MPIE the majority (266) are scientists. 130 scientists are funded from the basic budget and about 136 additional scientists are supported by external sources, such as the European Research Council (ERC), German Research Foundation (DFG), Alexander von Humboldt Foundation (AvH), Research Fund for Coal and Steel (RFCS), German Academic Exchange Service (DAAD), Bundesministerium für Bildung und Forschung (BMBF), the Max Planck Graduate School IMPRS-SurMat, Chinese Scholarship Council (CSC), and Bundesministerium für Wirtschaft und Energie (BMWi) to name but a few.

Numerous strategically selected industry partners provide further momentum to the dynamic growth of the MPIE. Besides well-established links to the steel industry regarding medium manganese steels, advanced characterization, surface functionalization, and computational materials science, several new collaborations were established also in non-ferrous materials research fields. Examples are additive manufacturing

and design of aerospace alloys, through process and texture simulation in the aluminium industry, fuel cell and hydrogen-systems related materials for the automotive industry, superalloys for airplane turbines and hydrogen tolerant Nickel alloys. This mixture of third-party funds from fundamental and applied science places the MPIE into a singular position within the Max Planck Society.

The MPIE researchers have achieved several scientific breakthroughs in the past years, e.g., on the interplay of lattice defects and local composition, machine learning and quantitative simulation in materials science, nanostructured steels and high entropy alloys, self-healing coating systems, structure-chemistry imaging of catalyst nanoparticles, ductile Magnesium alloys, and new methods on joint atomic scale imaging of structure and chemistry.

These breakthroughs were enabled by several long-term methodological projects which led to the development of novel experimental and simulation tools. Examples are the combinatorial corrosion and catalysis probing cell, the scanning Kelvin probe, the correlative atom probe tomography (APT) - transmission electron microscopy (TEM) analysis conducted on the same specimens, the field ion microscopy time of flight methods, the simulation toolbox DAMASK, the wet chemical cell for *in situ* reaction analysis in TEM, the computational framework *pyiron* that provides automated tools for high-throughput calculations using high precision *ab initio* simulation methods and the site specific mechanical testing strategies under harsh 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, large network activities, and new scientific laboratories.
- *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 several topical areas of common interest at the MPIE.
- *Part IV* summarizes statistically relevant information about the Institute.

The Directors of the MPIE

Düsseldorf, December 2018