



Special Issue Reprint

First-Principles Approaches to Metals, Alloys, and Metallic Compounds

www.mdpi.com/books/reprint/873

Edited by Richard Dronskowski

ISBN 978-3-03897-358-4 (Softback) ISBN 978-3-03897-359-1 (PDF)

Current fundamental electronic-structure theory allows for the accurate prediction and characterization of elemental metals adopting any allotropic structure, intermetallic compounds, and other metal-rich phases. From an engineering perspective, there is a need for structural materials that are suitable for mechanical and civil engineering as well as energy production and conversion. While different microstructural features influence the macroscopic behaviour, quantum-mechanical simulation may enormously accelerate and guide the entire development process since atomistic modelling allows for the generation of structural models and the calculation of enthalpies and other free energies as a function of pressure and temperature. Among other things, this volume covers high-manganese steels, some of which have come to light within Collaborative Research Centre 761 ("Steel ab initio"). In particular, it deals with short-range ordering from experiment and theory, also highlighting carbide-like precipitates, and it bridges the gap between atomistic and continuum levels, in particular for hydrogen embrittlement. Molecular dynamics simulates crack propagation, and first-principles theory helps in growing better intermetallic thin films and predicts structural and elastic properties. Eventually, multiscale modelling of hydrogen transport is provided, and the chemical reasons for H-trapping κ -carbides are highlighted. First-principles theory has acquired a powerful role in the fundamental and applied research of metals, alloys, and metallic compounds.



Order Your Print Copy You can order print copies at www.mdpi.com/books/reprint/873



MDPINBOOKS Publishing Open Access Books & Series

MDPI Books offers quality open access book publishing to promote the exchange of ideas and knowledge in a globalized world. MDPI Books encompasses all the benefits of open access – high availability and visibility, as well as wide and rapid dissemination. With MDPI Books, you can complement the digital version of your work with a high quality printed counterpart.



Open Access

Your scholarly work is accessible worldwide without any restrictions. All authors retain the copyright for their work distributed under the terms of the Creative Commons Attribution License.



Author Focus

Authors and editors profit from MDPI's over two decades of experience in open access publishing, our customized personal support throughout the entire publication process, and competitive processing charges as well as unique contributor discounts on book purchases.



High Quality & Rapid Publication

MDPI ensures a thorough review for all published items and provides a fast publication procedure. State-of-the-art research and time-sensitive topics are released with a minimum amount of delay.



ᆔ

High Visibility

Due to our global network and well-known channel partners, we ensure maximum visibility and broad dissemination. Title information of books is sent to international indexing databases and archives, such as the Directory of Open Access Books (DOAB), and the Verzeichnis Lieferbarer Bücher (VLB).

Print on Demand and Multiple Formats

MDPI Books are available for purchase and to read online at any time. Our print-on-demand service offers a sustainable, cost-effective and fast way to publish MDPI Books printed versions.

MDPI AG Grosspeteranlage 5 4052 Basel Switzerland Tel: +41 61 683 77 34 www.mdpi.com/books books@mdpi.com

