1. Record Nr. UNINA9910765769103321

Titolo	First-principles approaches to metals, alloys, and metallic compounds / / edited by Richard Dronskowski
Pubbl/distr/stampa	Basel, Switzerland : , : MDPI, , [2018] ©2018
ISBN	3-03897-359-9
Descrizione fisica	1 online resource (180 pages) : illustrations
Disciplina	620.16
Soggetti	Intermetallic compounds
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references.
Nota di contenuto	About the Special Issue Editor vii -- Richard Dronskowski First-Principles Approaches to Metals, Alloys, and Metallic Compounds Reprinted from: Metals 2018, 8, 705, doi:10.3390/met8090705 . 1 -- Tobias A. Timmerscheidt, Poulumi Dey, Dimitri Bogdanovski, Jorg ¨ von Appen, Tilmann Hickel, Jorg ¨ Neugebauer and Richard Dronskowski The Role of -Carbides as Hydrogen Traps in High-Mn Steels Reprinted from: Metals 2017, 7, 264, doi:10.3390/met7070264 . 4 -- Hideaki Sawada, Shunsuke Taniguchi, Kazuto Kawakami and Taisuke Ozaki Transition of the Interface between Iron and Carbide Precipitate From Coherent to Semi-Coherent Reprinted from: Metals 2017, 7, 277, doi: 10.3390/met7070277 . 19 -- Xianfeng Li, Cunjuan Xia, Mingliang Wang, Yi Wu and Dong Chen First-Principles Investigation of Structural, Electronic and Elastic Properties of HfX (X = Os, Ir and Pt) Compounds Reprinted from: Metals 2017, 7, 317, doi:10.3390/met7080317 . 32 -- Yanqiu Zhang and Shuyong Jiang Molecular Dynamics Simulation of Crack Propagation in Nanoscale Polycrystal Nickel Based on Different Strain Rates Reprinted from: Metals 2017, 7, 432, doi:10.3390 /met7100432 . 47 -- Simon Sevsek and Wolfgang Bleck Ab Initio-Based Modelling of the Yield Strength in High-Manganese Steels Reprinted from: Metals 2018, 8, 34, doi:10.3390/met8010034 58 -- Wenwen Song, Dimitri Bogdanovski, Ahmet Bahadir Yildiz, Judith E. Houston, Richard Dronskowski and Wolfgang Bleck On the Mn-C Short-Range Ordering in a High-Strength High-Ductility Steel: Small Angle

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Sommario/riassunto

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 -carbides are highlighted. First-principles theory has acquired a powerful role in the fundamental and applied research of metals, alloys, and metallic compounds.