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Nota di contenuto	Title Page; Copyright Page; Contents; List of Contributors; Foreword; Preface; Chapter 1 An Introduction to Corrosion Mechanisms and Models; 1.1 INTRODUCTION; 1.2 MECHANISMS IN CORROSION SCIENCE; 1.2.1 Thermodynamics and Pourbaix Diagrams; 1.2.2 Electrode Kinetics; 1.2.3 Metal Dissolution; 1.2.4 Hydrogen Evolution and Oxygen Reduction; 1.2.5 The Mixed Potential Model for Corrosion; 1.2.6 Selective Dissolution of Alloys; 1.2.7 Passivity of Metals and Alloys; 1.2.8 Inhibition of Corrosion; 1.2.9 Environmentally Assisted Cracking and Embrittlement; 1.2.10 Crystallographic Pitting; 1.2.11 Summary of Corrosion Mechanisms; 1.3 MOLECULAR MODELING; 1.3.1 Electronic Structure Methods; 1.3.2 Interatomic Potentials (Force Fields); 1.3.3 Energy Minimization; 1.3.4 Transition State Theory; 1.3.5 Molecular Dynamics; 1.3.6 Monte Carlo Simulation; 1.4 BRIDGING THE REALITY GAP; 1.4.1 First-Principles Thermodynamics; 1.4.2 Solvation Models; 1.4.3 Control of Electrode Potential and the Presence of Electric Fields; 1.4.4 Materials Defects and Inhomogeneities; 1.5 MOLECULAR MODELING AND CORROSION; REFERENCES Chapter 2 Molecular Modeling of Structure and Reactivity at the Metal/Environment Interface; 2.1 INTRODUCTION; 2.2 STRUCTURE AND REACTIVITY OF WATER OVER METAL SURFACES; 2.3 MOLECULAR MODELING OF CHEMISORBED PHASES UNDER COMPETING ADSORPTION

CONDITIONS; 2.4 COADSORPTION OF IONS AT THE INTERFACE AND PROMOTION OF HYDROGEN UPTAKE; 2.5 DISSOLUTION OF METAL ATOMS; 2.6 SUMMARY AND PERSPECTIVES; REFERENCES; Chapter 3 Processes at Metal-Solution Interfaces: Modeling and Simulation; 3.1 INTRODUCTION; 3.2 SURFACE MOBILITY; 3.3 KMC: DETAILS IN THE MODEL AND SIMULATION TECHNIQUE; 3.3.1 The Model; 3.3.2 Energy Calculations for Silver; 3.3.3 Dipole Moments; 3.3.4 Effect of the Electric Field on the Diffusion Rates; 3.3.5 Energy Calculations for Gold; 3.4 ISLAND DYNAMICS ON CHARGED SILVER ELECTRODES; 3.4.1 Mesoscopic Theory of Step Fluctuations; 3.4.2 Step Fluctuations; 3.4.3 Analysis of the Minimum Curvature of Island Shapes; 3.4.4 Simulations of Islands; 3.5 OSTWALD RIPENING; 3.5.1 Ag/Ag(100): Field and Temperature Effect; 3.6 THE EFFECT OF ADSORBED Cl ATOMS ON THE MOBILITY OF ADATOMS ON Au(100); 3.7 SOME CONCLUSIONS ON SURFACE MOBILITY; 3.8 THEORY OF ELECTROCHEMICAL CHARGE TRANSFER REACTION; 3.8.1 A Model Hamiltonian for Electron and Ion Transfer Reactions at Metal Electrodes; 3.8.2 Principles of Electrocatalysis; 3.8.3 Hydrogen Electrocatalysis; 3.8.4 Heyrovsky Reaction; 3.8.5 Hydrogen at Nanostructured Electrodes; 3.8.6 Comparison With Experimental Data; 3.9 CONCLUSIONS AND OUTLOOK; ACKNOWLEDGMENTS; REFERENCES; Chapter 4 Atomistic Monte-Carlo Simulations of Dissolution; 4.1 INTRODUCTION; 4.1.1 Dissolution and Dealloying; 4.1.2 A First Description of Dissolution; 4.1.3 Evolution of Dissolution and Selective Dissolution Mechanisms

Sommario/riassunto

Presents opportunities for making significant improvements in preventing harmful effects that can be caused by corrosion. Describes concepts of molecular modeling in the context of materials corrosion. Includes recent examples of applications of molecular modeling to corrosion phenomena throughout the text. Details how molecular modeling can give insights into the multitude of interconnected and complex processes that comprise the corrosion of metals. Covered applications include diffusion and electron transfer at metal/electrolyte interfaces, Monte Carlo simulations of corrosion, corrosion in h
