Interfaces In Materials Atomic Structure Thermodynamics And Kinetics Of Solid Vapor Solid Liquid

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Interfaces In Materials Atomic Structure
Energy-efficient spintronic devices are closer to being realized thanks to a new mechanism predicted by RIKEN physicists for converting between electrical current vortices and a spin current.

2D materials and interfaces can convert spin current into a vortex of charge current
The new tool is based on atomic force microscopy ... two different sections of a material. Those interfaces are key to understanding a material's structure and properties. Images of similar ...

A scattering-type scanning nearfield optical microscope probes materials at the nanoscale
The new tool is based on atomic force microscopy (AFM), in which ... or the interfaces between two different sections of a material. Those interfaces are key to understanding a material’s structure ...

Custom-made MIT tool probes materials at the nanoscale
(b) Heterogeneous interface of BAs-GaN examined by transmission electron microscopy with atomic resolution. Insets, crystal structure of BAs (bottom ... To keep computer processors cool, materials ...

Cooling high power electronics - boron arsenide spreads heat better than diamond
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‘Slidetronics’ makes its debut
An introduction to the properties of engineering materials that emphasizes the correlation between atomic and microscopic structure and the macroscopic ... The course examines the interfaces between ...

Materials Science and Engineering
Material could be used in future quantum computing applications. An international team of physicists led by the University of Minnesota has discovered that a unique superconducting metal is more ...

Researchers Uncover Unique Properties of a Promising New Superconductor for Quantum Computing
remedy this limitation by showing that an intrinsically centrosymmetric vdW material, h-BN, can be engineered on the atomic scale to become ferroelectric. A bulk h-BN crystal has a layered structure .

Two-dimensional ferroelectricity by design
It is well known how the properties of solids arise from their symmetry, whether this is defined within the bulk interior, or by the presence of a surface or interface ... materials design to control ...

Mesoscale Materials Laboratory
We observe changes from the micrometer to the atomic level ... energy storage materials, or biominerals (2–4). Here, functionality is often defined by local heterogeneities in structure and/or ...

Sparse ab initio x-ray transmission spectrotomography for nanoscopic compositional analysis of functional materials
2 Department of Physical Chemistry, School of Chemistry, The Raymond and Beverly Sackler Faculty of Exact Sciences and The Sackler Center for Computational Molecular and Materials ... map of the ...

Interfacial ferroelectricity by van der Waals sliding
These distinct properties at interfaces and surfaces of materials often play ... on the direction of oscillation of the light field relative to the atomic arrangement in the material. "We take ...

Tailored Laser Fields Reveal Properties of Transparent Crystals
Friction and wear of materials accounts for enormous losses in performance ... and mechanical behavior in a class of transition metal nitrides deposited using plasma-enhanced atomic layer deposition.

GOALI: Ultra-Low Wear Plasma Enhanced Atomic Layer Deposited Nitride Thin Films: Exploring Processing, Structure, Properties and Mechanisms
Low-power information processing could be possible using a new method for converting between spin and charge currents enter the cellular nucleus.

Two-dimensional materials and interfaces can convert spin current into a vortex of charge current
These distinct properties at interfaces and surfaces of materials ... oscillation of the light field relative to the atomic arrangement in the material. "We take advantage of this dependence ...

An Instructor's Manual presenting detailed solutions to all the problems in the book is available from the Wiley editorial department.

Many of the most important properties of materials in high-technology applications are strongly influenced or even controlled by the presence of solid interfaces. In this work, leading international authorities review the broad range of subjects in this field focusing on the atomic level properties of solid interfaces.

The behaviour of many materials critically depends on processes at interfaces and surfaces. This volume presents up-to-date reviews on atomic structure and properties of interfaces.

While much progress has been made in the microscopic characterization of bulk materials, understanding the behavior, at the atomic scale, of complex materials interfaces remains a challenging problem in condensed matter physics and materials science. Development of predictive theory and modeling for interfacial systems is not only important to aid experimental interpretations but is also crucial to accelerate materials design efforts for a broad range of technological applications from the semiconductor industry to the development of new sources of energy. This dissertation presents a computational framework that combines first-principles molecular dynamics simulations for the determination of interfacial atomic structures, and advanced electronic structure methods for the description of electronic properties to understand, predict and design materials interfaces. In particular, the research presented in this thesis was carried out in two parallel directions: 1. Predictions of the interfacial atomic structure of complex materials interfaces using first-principles molecular dynamics, and validation of the predictions by relating structural models to experiments, e.g., data from X-ray, infrared spectra and sum-frequency generation spectroscopy experiments.In particular, I investigated structural and dynamical properties of the ice Ih surface and of the Al2O3/water interface. While the study of the ice surface is the first step towards the understanding of complex semiconductor/water interfaces, the Al2O3/water interface represents a suitable prototype interface for extensive comparisons between theory and experiments. 2. Development of advanced first-principles techniques to study electronic states at interfaces and application of these techniques to gain insights on the relationship between between local interface structure and electronic properties. I devised a new technique to study excited states and photoemission spectra based on many-body perturbation theory, within the so-called GW approximation, which improves both the computational efficiency and accuracy of existing methodologies, and that can be employed to study realistic systems. In addition, in the thesis I employed the new GW technique to investigate a variety of systems including molecules, nanostructures, semiconducting interfaces, liquid water and simple aqueous solutions. These studies are crucial to build a fundamental understanding of the electronic structure of semiconductor/liquid water interfaces and of, e.g., water with dissolved ions under different pH conditions, interfaced with a photoelectrode. Information provided by these two parallel research directions helped establish a structure-electronic properties-chemical reactivity paradigm, that is general and applicable to a large class of materials. An example presented in the thesis is that of functionalized Si surfaces interfaced with liquid water, in which I studied the effect of surface functionalization on the alignment between Si band edges and water redox potentials, and I suggested a possible approach to engineer and design semiconductor surfaces for photoelectrochemical water splitting.

This handbook brings together, under a single cover, all aspects of the chemistry, physics, and engineering of surfaces and interfaces of materials currently studied in academic and industrial research. It covers different experimental and theoretical aspects of surfaces and interfaces, their physical properties, and spectroscopic techniques that have been applied to a wide class of inorganic, organic, polymer, and biological materials. The diversified technological areas of surface science reflect the explosion of scientific information on surfaces and interfaces of materials and their spectroscopic characterization. The large volume of experimental data on chemistry, physics, and engineering aspects of materials surfaces and interfaces remains scattered in so many different periodicals, therefore this handbook compilation is needed. The information presented in this multivolume reference draws on two decades of pioneering research on the surfaces and interfaces of materials to offer a complete perspective on the topic. These five volumes-Surface and Interface Phenomena; Surface Characterization and Properties; Nanostructures, Micelles, and Colloids; Thin Films and Layers; Biointerfaces and Applications-provide multidisciplinary review chapters and summarize the current status of the field covering important scientific and technological developments made over past decades in surfaces and interfaces of materials and spectroscopic techniques with contributions from internationally recognized experts from all over the world. Fully cross-referenced, this book has clear, precise, and wide appeal as an essential reference source long due for the scientific community. The complete reference on the topic of surfaces and interfaces of materials The information presented in this multivolume reference draws on two decades of pioneering research Provides multidisciplinary review chapters and summarizes the current status of the field Covers important scientific and technological developments made over past decades in surfaces and interfaces of materials and spectroscopic techniques Contributions from internationally recognized experts from all over the world

Ceramic Materials: Science and Engineering is an up-to-date treatment of ceramic science, engineering, and applications in a single, integrated text. Building on a foundation of crystal structures, phase equilibria, defects and the mechanical properties of ceramic materials, students are shown how these materials are processed for a broad diversity of applications in today's society. Concepts such as how and why ions move, how ceramics interact with light and magnetic fields, and how they respond to temperature changes are discussed in the context of their applications. References to the art and history of ceramics are included throughout the text. The text concludes with discussions of ceramics in biology and medicine, ceramics as gemstones and the role of ceramics in the interplay between industry and the environment. Extensively illustrated, the text also includes questions for the student and recommendations for additional reading. KEY FEATURES: Combines the treatment of bioceramics, furnaces, glass, optics, pores, gemstones, and point defects in a single text Provides abundant examples and illustrations relating theory to practical applications Suitable for advanced undergraduate and graduate teaching and as a reference for researchers in materials science Written by established and successful teachers and authors with experience in both research and industry

A crucial first step in understanding the effect that internal interfaces have on the properties of materials is the ability to determine the atomic structure at the interface. As interfaces can contain atomic disorder, dislocations, segregated impurities and interphases, sensitivity to all of these features is essential for complete experimental characterization. By combining Z-contrast imaging and electron energy loss spectroscopy (EELS) in a dedicated scanning transmission electron microscope (STEM), the ability to probe the structure, bonding and composition at interfaces with the necessary atomic resolution has been obtained. Experimental conditions can be controlled to provide, simultaneously, both incoherent imaging and spectroscopy. This enables interface structures observed in the image to be interpreted intuitively and the bonding in a specified atomic column to be probed directly by EELS. The bonding and structure information can then be correlated using bond-valence sum analysis to produce structural models. This technique is demonstrated for 25[degrees], 36[degrees] and 67[degrees] symmetric and 45[degrees] and 25[degrees] asymmetric[001] tilt grain boundaries in SrTiO[sub 3] The structures of both types of boundary were found to contain partially occupied columns in the boundary plane. From these experimental results, a series of structural units were identified which could be combined, using continuity of gain boundary structure principles, to construct all[001] tilt boundaries in SrTiO[sub 3]. Using these models, the ability of this technique to address the issues of vacancies and dopant segregation at grain boundaries in electroceramics is discussed.

Keywords: STEM, defects, characterization, simulation, Al2O3, Ge, HfO2, GaAs, Si, high k dielectric, dislocation, Z-contrast, EELS.