Calculation Of Diffusion Barriers For Helium Atom In

Theoretical Modeling of Epitaxial Graphene Growth on the Ir(111) Surface
Annual Reports on NMR Spectroscopy
Defect and diffusion forum. Pt. A
Applications and Industrialization
Proceedings of the International Symposium
Noncontact Atomic Force Microscopy
Physics and Chemistry of Small Clusters
Silicon Surfaces and Formation of Interfaces
Volume 2
Structural Integrity Assessment
Copper Interconnects, New Contact Metallurgies/structures, and Low-k Interlevel Dielectrics
Growth and Properties of Ultrathin Epitaxial Layers
Magnesium Technology 2012
Proceedings of the NATO Advanced Research Workshop on Collective Diffusion on Surfaces: Correlation Effects and Adatom Interactions Prague, Czech Republic 2–6 October 2000
Design of Amorphous Diffusion Barriers for Cu Metallization
Metals, Metal Atoms, and Clusters
Volume 1 - Current Developments
Frontiers in Physics - Rising Stars Asia
Surface Diffusion
Recent Advances in the Science and Technology of Zeolites and Related Materials
Semiconductors, Dielectrics, and Metals for Nanoelectronics 15: In Memory of Samares Kar
Advances in Energy Research, Vol. 1
From Surface Chemistry to Nano Chemistry
First-principles Multiple-barrier Diffusion Theory. The Case Study of Interstitial Diffusion in CdTe
Applications of Continuous and Steady-State Methods to Root Biology
Performance and Reliability of Ultra-thin Diffusion Barriers for Sub-half Micron MOS Devices Integrated with Copper Metallization
Surface Diffusion
Dynamics at Solid State Surfaces and Interfaces
Multiphase Polymer Systems
Graphene Science Handbook
From Physics-of-Failure to Physics-of-Degradation
Reliability of Organic Compounds in Microelectronics and Optoelectronics
Atomic-Scale Modeling of Nanosystems and Nanostructured Materials
Morphological Organization in Epitaxial Growth and Removal

Diffusion Processes in Advanced Technological Materials
Quantum Simulations of Materials and Biological Systems
Journal of Computational and Theoretical Nanoscience
The Formation and Measurement of Electrical Contacts and Diffusion Barriers to Semiconductors
Surface Properties

MAREN GREER

Theoretical Modeling of Epitaxial Graphene Growth on the Ir(111) Surface The Electrochemical Society
This book presents selected papers from the 6th International Conference on Advances in Energy Research (ICAER 2017), which cover topics ranging from energy optimization, generation, storage and distribution, and emerging technologies, to energy management, policy, and economics. The book is inter-disciplinary in scope and addresses a host of different areas relevant to energy research, making it of interest to scientists, policymakers, students, economists, rural activists, and social scientists alike.
Annual Reports on NMR Spectroscopy Materials Research Forum LLC
For the first time, this book unites the theory, experimental techniques and computational tools used to describe the diffusion of atoms, molecules and nanoparticles across metal surfaces. Starting with an outline of the formalism that describes diffusion on surfaces, the authors guide the reader through the principles of atomic movement, before moving on to diffusion under special circumstances, such as the presence of defects or foreign species. With an initial focus on the behaviour of single entities on a surface, later chapters address the movement of clusters of atoms and the interactions between adatoms. While there is a special emphasis on experimental work, attention is paid to the increasingly valuable contributions theoretical work has made in this field. This book has wide interdisciplinary appeal and is ideal for researchers in solid state physics, chemistry as well as materials science, and engineering.
Defect and diffusion forum. Pt. A Springer
Recent Advances in the Science and Technology of Zeolites and Related Materials
Applications and Industrialization Frontiers Media SA
Design of Amorphous Diffusion Barriers for Cu Metallization
Proceedings of the International Symposium Springer Science & Business Media
In this proceedings volume, the following topics are discussed: systems and design; blanket and first wall technology of fission and fusion reactors; fission and fusion materials; radiation damage analysis; calculation codes; databases.
Noncontact Atomic Force Microscopy Springer Science & Business Media
This book provides an excellent illustration of the interrelationship between progress in scientific methodology and conceptual advances, and its publica tion should contribute to further advances. It is well known that major advances in understanding often follow the development of new methods. The development of the acetylene

reduction assay for nitrogenase activity provides a good example of this interrelationship between theory and methods. Theoretical knowledge led to a search for substrates for nitro genase that could be assayed for more easily than ammonium, the normal product of the enzyme. The discovery of the reduction of acetylene to ethylene by nitrogenase provided the ideal answer to the problem by provid ing a rapid, specific, nondestructive, and inexpensive assay for nitrogenase activity. This assay is now used by almost every laboratory doing research on nitrogen fixation. However, further use and development of the acetylene reduction assay has shown that it can underestimate nitrogenase activity and can even give incorrect relative values under some circumstances. The major problem is that exposure of legume nodules to acetylene can cause a large increase in the resistance to oxygen diffusion into the nodule. This reduced supply of oxygen decreases the rate of nitrogenase activity within a few minutes.

Physics and Chemistry of Small Clusters

The Electrochemical Society

The incorporation of Cu interconnects into the manufacturing of integrated circuits has accompanied several modifications to the fabrication process and the associated material systems. The new fabrication process involves the development of dual damascene process, while the new materials systems include development of diffusion barrier materials. The latter imposes a critical challenge as Cu is a fast diffuser in Si and the adjacent dielectric layers, and results in device deterioration and failure. Technology development has been driven mainly by continuous feature size scaling, thus the developed barrier will be required to perform satisfactorily at the continuously reduced thicknesses. The conventional barriers used for Cu interconnects are TaNx based films which require the deposition of an additional Cu seed layer prior to filling of the interconnects by electrochemical deposition. In the face of reducing feature size and barrier thickness, there has been great interest in developing diffusion barriers that are amenable to direct electrodeposition of Cu without the need for a seed layer. However, there is a need for a suitable guide for selecting material systems suitable for diffusion barrier applications. In this thesis, a systematic approach is adopted to select an amorphous, low resistivity diffusion barrier material with the possibility of direct electrodeposition of Cu. After comprehensive consideration of possible alloys, the Ta-Rh system is selected as the candidate barrier. Thermodynamic calculations are performed to select the most stable amorphous composition in the system. The predictions made based on the thermodynamic calculation are verified by detailed structural characterizations. The performance of the selected TaRhx alloy as a diffusion barrier is evaluated by metallurgical and electrical characterizations. The metallurgical characterizations are performed by in-situ and ex-situ heating experiments on Si/diffusion barrier/Cu stacks. The common issues associated with in-situ transmission electron microscopy heating of Cu metallization stacks are identified and addressed. The electrical characterizations are performed by monitoring the capacitance-voltage characteristics of metal oxide semiconductor capacitors after bias temperature stress testing. For comparison, TaNx barriers are deposited

and tested as diffusion barriers using a similar methodology. The reliability of the developed barrier system is compared with the current industry solution, i.e. TaNx.

Silicon Surfaces and Formation of Interfaces Academic Press

Recent advances in experimental techniques now enable researchers to produce in a laboratory clusters of atoms of desired composition from any of the elements of the periodic table. This has created a new area of research into novel materials since clusters cannot be regarded either as a "large" molecule or as a fragment of the bulk. Both experimental and theoretical studies are revealing unusual properties that are not ob served in solid state environments. The structures of micro-clusters are found to be significantly distorted from the most symmetric arrangement, some even exhibiting pentagonal symmetry commonly found in icosahedric structures. The unusual stability of certain clusters, now described as "magic number species", shows striking similarities with the nuclear shell structure. The relative stabilities of clusters depend not only on the composition of the clusters but also on their charged states. The studies on spontaneous fragmentation of mUltiply charged clusters, commonly referred to as Coulomb explosion, illustrate the role of electronic bonding mechanisms on stability of clusters. The effect of foreign atoms on geometry and stability of clusters and the interaction of gas atoms with clusters are showing promise for an indepth understanding of chemisorption and catalysis. The magnetic and optical properties are dependent not only on cluster size but also on its geometry. These findings have the potential for aiding industry in the area of micro-electronics and catalysis.

Volume 2 Springer Science & Business Media

The Magnesium Technology Symposium, which takes place every year at the TMS Annual Meeting & Exhibition, is one of the largest yearly gatherings of magnesium specialists in the world. Papers are presented in all aspects of the field, ranging from primary production to applications to recycling. Moreover, papers explore everything from basic research findings to industrialization. Magnesium Technology 2011 covers a broad spectrum of current topics, including alloys and their properties; cast products and processing; wrought products and processing; forming, joining, and machining; corrosion and surface finishing; ecology; and structural applications. In addition, you'll find coverage of new and emerging applications in such areas as biomedicine and hydrogen storage.

Structural Integrity Assessment Trans Tech Publications Ltd

Explore the Practical Applications and Promising Developments of Graphene The Graphene Science Handbook is a six-volume set that describes graphene’s special structural, electrical, and chemical properties. The book considers how these properties can be used in different applications (including the development of batteries, fuel cells, photovoltaic cells, and supercapacitors based on graphene) and produced on a massive and global scale. Volume One: Fabrication Methods Volume Two: Nanostructure and Atomic Arrangement Volume Three: Electrical and Optical Properties Volume Four: Mechanical and Chemical Properties Volume Five: Size-Dependent Properties Volume Six: Applications and Industrialization This

handbook describes the fabrication methods of graphene; the nanostructure and atomic arrangement of graphene; graphene's electrical and optical properties; the mechanical and chemical properties of graphene; the size effects in graphene, characterization, and applications based on size-affected properties; and the application and industrialization of graphene. Volume six is dedicated to the application and industrialization of graphene and covers: The design of graphene- and biomolecule-based nanosensors and nanodevices The use of graphene-based field-effect-transistor (GFET)-like structures as sensing substrates and DNA aptamers as sensing elements Recent advances in graphene-based DNA sensors The antibacterial properties of graphene-based nanomaterial (NM) The chemical and physical properties of graphene and its current uses The development of sensitive and selective field-effect transistors (FET) biosensors based on graphene The unique properties of ordered graphene (G) Various methods currently employed for the production of graphene nanocomposites The supramolecular chemistry of graphene derivatives, and more

Copper Interconnects, New Contact Metallurgies/structures, and Low-k Interlevel Dielectrics John Wiley & Sons

This edition is published by results of the 2018 International Symposium on Structural Integrity (ISSI2018, Nov. 2-5, 2018, Nanjing, China). The articles cover a variety of topics associated with research in the area of the structural integrity assessment and ensuring, while the fracture mechanics, damage mechanisms and structural strength aspects of engineering materials have been closely focused on. The publication of the proceedings aims to present the current solutions in the field of structural integrity research of materials, components and structures.

Growth and Properties of Ultrathin Epitaxial Layers World Scientific

Although there has been steady progress in understanding aspects of epitaxial growth throughout the last 30 years of modern surface science, work in this area has intensified greatly in the last 5 years. A number of factors have contributed to this expansion. One has been the general trend in surface science to tackle problems of increasing complexity as confidence is gained in the methodology, so for example, the role of oxide/metal interfaces in determining the properties of many practical supported catalysts is now being explored in greater detail. A second factor is the recognition of the potential importance of artificial multilayer materials not only in semiconductor devices but also in metal/metal systems because of their novel magnetic properties. Perhaps even more important than either of these application areas, however, is the newly-discovered power of scanning probe microscopies, and most notably scanning tunneling microscopy (STM), to provide the means to study epitaxial growth phenomena on an atomic scale under a wide range of conditions. These techniques have also contributed to revitalised interest in methods of fabricating and exploiting artificial structures (lateral as well as in layers) on a nanometre scale. This volume, on Growth and Properties of Ultrathin Epitaxial Layers, includes a collection of articles which reflects the present state of activity in this field. The emphasis is on metals and oxides rather than

semiconductors.

Magnesium Technology 2012 Elsevier

Quantum Simulations of Materials and Biological Systems features contributions from leading world experts in the fields of density functional theory (DFT) and its applications to material and biological systems. The recent developments of correlation functionals, implementations of Time-dependent algorithm into DFTB+ method are presented. The applications of DFT method to large materials and biological systems such as understanding of optical and electronic properties of nanoparticles, X-ray structure refinement of proteins, the catalytic process of enzymes and photochemistry of phytochromes are detailed. In addition, the book reviews the recent developments of methods for protein design and engineering, as well as ligand-based drug design. Some insightful information about the 2011 International Symposium on Computational Sciences is also provided. Quantum Simulations of Materials and Biological Systems is aimed at faculties and researchers in the fields of computational physics, chemistry and biology, as well as at the biotech and pharmaceutical industries.

Proceedings of the NATO Advanced Research Workshop on Collective Diffusion on Surfaces: Correlation Effects and Adatom Interactions Prague, Czech Republic 2–6 October 2000 Springer

The interest in the problem of surface diffusion has been steadily growing over the last fifteen years. This is clearly evident from the increase in the number of papers dealing with the problem, the development of new experimental techniques, and the specialized sessions focusing on diffusion in national and international meetings. Part of the driving force behind this increasing activity is our recently acquired ability to observe and possibly control atomic scale phenomena. It is now possible to look selectively at individual atomistic processes and to determine their relative importance during growth and reactions at surfaces. The number of researchers interested in this problem also has been growing steadily which generates the need for a good reference source to farniliarize newcomers to the problem. While the recent emphasis is on the role of diffusion during growth, there is also continuing progress on the more traditional aspects of the problem describing mass transport in an ensemble of particles. Such a description is based on the statistical mechanical analysis of a collection of particles that mutually interact and develop correlations. An average over the multitude of atomistic processes that operate under these conditions is necessary to fully describe the dynamics in the system.

Design of Amorphous Diffusion Barriers for Cu Metallization CRC Press

The book covers a variety of applications of modern atomic-scale modeling of materials in the area of nanoscience and nanostructured systems. By highlighting the most recent achievements obtained within a single institute, at the forefront of material science studies, the authors are able to provide a thorough description of properties at the nanoscale. The areas covered are structural determination, electronic excitation behaviors, clusters on surface morphology, spintronics and disordered materials. For each application, the basics of methodology are provided, allowing for a sound presentation of approaches such as density functional theory (of ground and excited states),

electronic transport and molecular dynamics in its classical and first-principles forms. The book is a timely collection of theoretical nanoscience contributions fully in line with current experimental advances.

Metals, Metal Atoms, and Clusters Linköping University Electronic Press

The study of surfaces has experienced dramatic growth over the past decade. Now, the editors of the internationally celebrated series Advances in Chemical Physics have brought together in this self-contained, special topic volume contributions from leading researchers in the field treating some of the most crucial aspects of the experimental and theoretical study of surfaces. This work delves into such core issues as: * Kinetics and dynamics of hydrogen adsorption on silicon surfaces. * Potential energy surfaces of transition-metal-catalyzed chemical reactions. * High-resolution helium atom scattering as a proof of surface vibrations. * Ordering and phase transitions in adsorbed monolayers of diatomic molecules. * The influence of dimensionality on static and dynamic properties of a system. * New applications to fields as varied as catalysts and the passage of molecules through membranes. This valuable resource provides important insights into the current state of knowledge about surface properties. Prigogine and Rice's latest work will stimulate the imagination and motivate the exploration of other aspects of this fascinating subject.

Volume 1 - Current Developments Springer Science & Business Media

This two-volume work covers ultrafast structural and electronic dynamics of elementary processes at solid surfaces and interfaces, presenting the current status of photoinduced processes. Providing valuable introductory information for newcomers to this booming field of research, it investigates concepts and experiments, femtosecond and attosecond time-resolved methods, as well as frequency domain techniques. The whole is rounded off by a look at future developments.

Frontiers in Physics - Rising Stars Asia Elsevier

Crystal growth far from thermodynamic equilibrium is nothing but homoepitaxy - thin film growth on a crystalline substrate of the same material. Because of the absence of misfit effects, homoepitaxy is an ideal playground to study growth kinetics in its pure form. Despite its conceptual simplicity, homoepitaxy gives rise to a wide range of patterns. This book explains the formation of such patterns in terms of elementary atomic processes, using the well-studied Pt/Pt(111) system as a reference point and a large number of Scanning Tunneling Microscopy images for visualization. Topics include surface diffusion, nucleation theory, island shapes, mound formation and coarsening, and layer-by-layer growth. A separate chapter is dedicated to describing the main experimental and theoretical methods.

Surface Diffusion Academic Press

Silicon, the basic material for a multibillion-dollar industry, is the most widely researched and applied semiconductor, and its surfaces are the most thoroughly studied of all semiconductor surfaces. Silicon Surfaces and Formation of Interfaces may be used as an introduction to graduate-level physics and chemical physics. Moreover, it gives a specialized and comprehensive description of the most common faces of silicon crystals as well as their interaction with adsorbates and

overlayers. This knowledge is presented in a systematic and easy-to-follow way. Discussion of each system is preceded by a brief overview which categorizes the features and physical mechanisms before the details are presented. The literature is easily available, and the references am numerous and organized in tables, allowing a search without the need to browse through the text. Though this volume focuses on a scientific understanding of physics on the atomistic and mesoscopic levels, it also highlights existing and potential links between basic research in surface science and applications in the silicon industry. It will be valuable to anyone writing a paper, thesis, or proposal in the field of silicon surfaces.

Recent Advances in the Science and Technology of Zeolites and Related Materials World Scientific

Annual Reports on NMR Spectroscopy provides a thorough and in-depth accounting of progress in nuclear magnetic resonance (NMR) spectroscopy and its many applications. Nuclear magnetic resonance (NMR) is an analytical tool used by chemists and physicists to study the structure and dynamics of molecules. In recent years, no other technique has gained as much significance as NMR spectroscopy. It is used in all branches of science in which precise structural determination is required, and in which the nature of interactions and reactions in solution is being studied. This book has established itself as a premier means for both specialists and non-specialists who are looking to become familiar with new techniques and applications pertaining to NMR spectroscopy. Serves as the premier resource for learning the new techniques and applications of NMR spectroscopy Provides a key reference for chemists and physicists using NMR spectroscopy to study the structure and dynamics of molecules Covers all aspects of molecular science, including MRI (Magnetic Resonance Imaging)