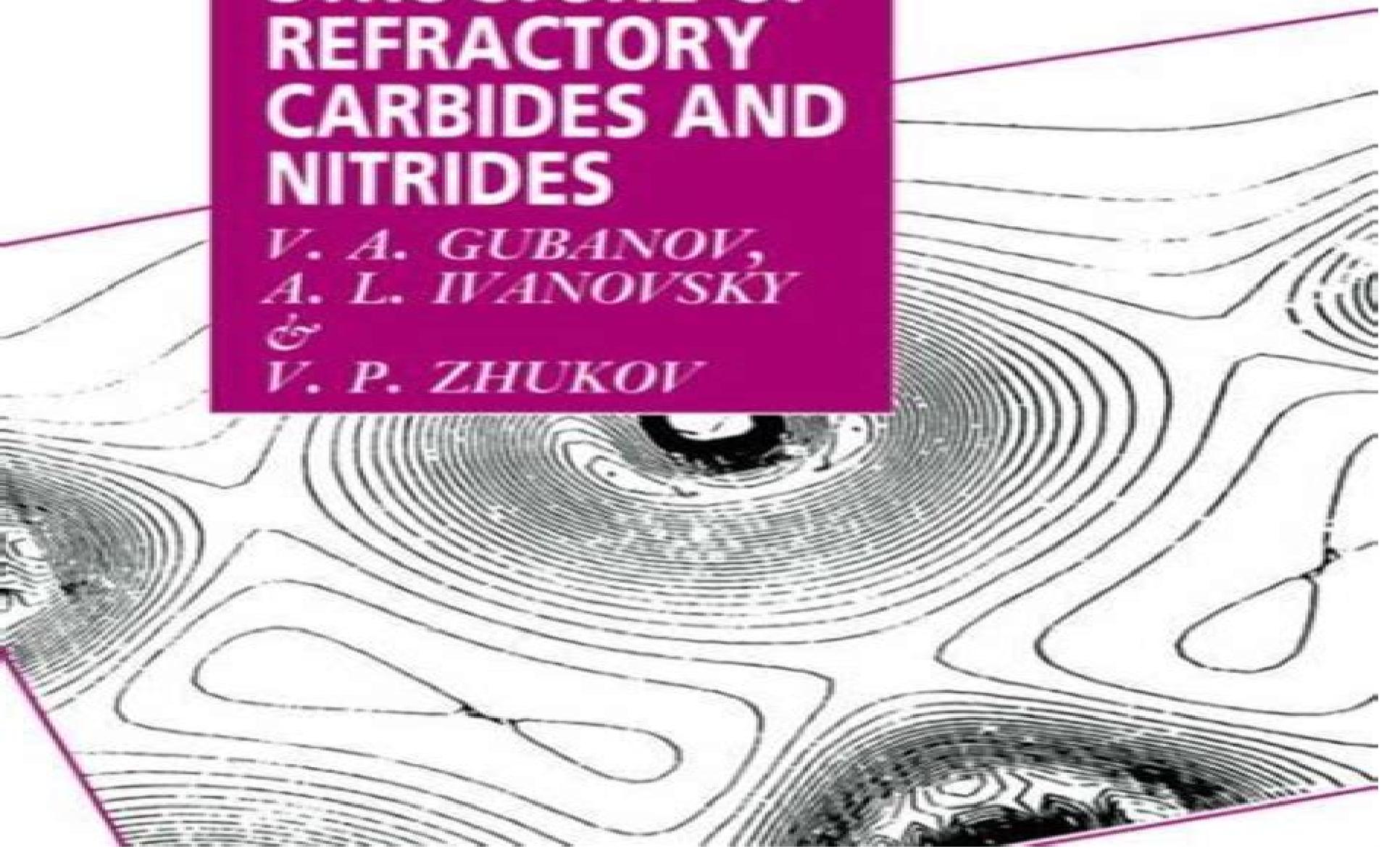


# ELECTRONIC STRUCTURE OF REFRACTORY CARBIDES AND NITRIDES

*V. A. GUBANOV,  
A. L. IVANOVSKY  
&  
V. P. ZHUKOV*



# Electronic Structure Of Refractory Carbides And Nitrides

**D.E. Ellis**



## **Electronic Structure Of Refractory Carbides And Nitrides:**

Electronic Structure of Refractory Carbides and Nitrides V. A. Gubanov, A. L. Ivanovsky, V. P. Zhukov, 1994-02-03 This book presents a systematic description of the electronic and physico chemical properties of transition metal carbides and nitrides The discussion is devoted to the theoretical modeling of refractory carbides and nitrides and alloys based on them and the authors uniquely make use of computational methods to calculate their spectroscopic electric magnetic superconducting thermodynamical and mechanical properties

**Electric Refractory Materials** Yukinobu Kumashiro, 2000-08-24 An exploration of electric refractory materials this book covers developments of blue light emitting diodes using GaN based nitrides for laser and high temperature and frequency devices Electric Refractory Materials introduces growth and evaluation standards of films and bulk crystals with consideration of band structure surface electronic structure and lattice vibrations It also covers heat capacity and thermal conductivity irradiation properties and selective surfaces Focusing on diamond material the book examines its synthesis and characterization as well as its electrical optical and conductive properties The book also discusses the use of silicon carbide boron compounds and other material used in electronic and light emitting devices

**Density Functional Theory of Molecules, Clusters, and Solids** D.E. Ellis, 2012-12-06 Rapid advances are taking place in the application of density functional theory DFT to describe complex electronic structures to accurately treat large systems and to predict physical and chemical properties Both theoretical content and computational methodology are developing at a pace which offers researchers new opportunities in areas such as quantum chemistry cluster science and solid state physics This volume contains ten contributions by leading scientists in the field and provides an authoritative overview of the most important developments The book focuses on the following themes determining adequate approximations for the many body problem of electronic correlations how to transform these approximations into computational algorithms applications to discover and predict properties of electronic systems and developing the theory For researchers in surface chemistry catalysis ceramics and inorganic chemistry

Groups IV, V, and VI Transition Metals and Compounds T. F. Connolly, 2012-12-06 responsibility To Betty Edwards and Emily Copenhaver my thanks for what must have seemed endless typing retyping and correcting of these bibliographies over a span of years Availability of Documents U S Government contractor reports usually identified by an alpha numeric report number can be purchased from National Technical Information Service U S Department of Commerce Springfield Virginia 22151 and often on request from the issuing installation USAEC reports are also available from International Atomic Energy Agency Kaerntnerring A 1010 Vienna Austria National Lending Library Boston Spa England Monographs and reports of the National Bureau of Standards are for sale by Superintendent of Documents U S Government Printing Office Washington D C 20402 Theses listed as Dissertation Abstracts number are available in North or South America from University Microfilms Dissertation Copies P O Box 1764 Ann Arbor Michigan 48106 and elsewhere from University Microfilms Ltd St John s Road

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**Proceedings of the 1st International Conference on Materials and Thermophysical Properties**

Sarita Kumari, Amanpal Singh, Balram Tripathi, Mahesh Baboo, 2025-07-01 This book highlights the latest research advancements and developments in the fields of materials science and thermophysical properties It includes peer reviewed articles from the 1st International Conference on Materials and Thermophysical Properties ICMTF 2024 held at the University of Rajasthan Jaipur India from November 21 to 23 The proceedings cover a wide range of topics including polymeric materials multifunctional materials materials for energy and biological applications glass and ceramic materials and thermophysical properties With contributions from leading scientists researchers and industry professionals this book serves as a valuable resource for academicians and practitioners alike fostering knowledge exchange and collaboration in these critical areas of research The topics and subtopics of the edited book may be arranged in the following manner Section I Polymeric Materials Section II Multifunctional Materials Section III Materials for Biological Applications Section IV Materials for Energy Applications Section V Glass and Ceramic Materials Section VI Materials for Nuclear Applications

**Ultra-High Temperature Materials II** Igor L. Shabalyn, 2019-04-24 This exhaustive work in three volumes and over 1300 pages provides a thorough treatment of ultra high temperature materials with melting points over 2500 C The first volume focuses on Carbon and Refractory Metals whilst the second and third are dedicated solely to Refractory compounds and the third to Refractory Alloys and Composites respectively Topics included are physical crystallographic thermodynamic thermo physical electrical optical physico mechanical nuclear and chemical solid state diffusion interaction with chemical elements and compounds interaction with gases vapours and aqueous solutions properties of the individual physico chemical phases of carbon graphite graphene refractory metals W Re Os Ta Mo Nb Ir and compounds oxides nitrides carbides borides silicides with melting points in this range It will be of interest to researchers engineers postgraduate graduate and undergraduate students alike The reader is provided with the full qualitative and quantitative assessment for the materials which could be applied in various engineering devices and environmental conditions at ultra high temperatures on the basis of the latest updates in the field of physics chemistry materials science and engineering

**Kirk-Othmer Concise Encyclopedia of Chemical Technology, 2 Volume Set** Kirk-Othmer, 2007-07-16 This is an easily accessible two volume encyclopedia summarizing all the articles in the main volumes Kirk Othmer Encyclopedia of Chemical Technology Fifth Edition organized alphabetically Written by prominent scholars from industry academia and research institutions the Encyclopedia presents a wide scope of articles on chemical substances properties manufacturing and uses on industrial

processes unit operations in chemical engineering and on fundamentals and scientific subjects related to the field

Nuclear Science Abstracts, 1976      *Ultra-High Temperature Ceramics* William G. Fahrenholtz, Eric J. Wuchina, William E. Lee, Yanchun Zhou, 2014-10-10 The first comprehensive book to focus on ultra high temperature ceramic materials in more than 20 years Ultra High Temperature Ceramics are a family of compounds that display an unusual combination of properties including extremely high melting temperatures 3000 C high hardness and good chemical stability and strength at high temperatures Typical UHTC materials are the carbides nitrides and borides of transition metals but the Group IV compounds Ti Zr Hf plus TaC are generally considered to be the main focus of research due to the superior melting temperatures and stable high melting temperature oxide that forms in situ Rather than focusing on the latest scientific results Ultra High Temperature Ceramics Materials for Extreme Environment Applications broadly and critically combines the historical aspects and the state of the art on the processing densification properties and performance of boride and carbide ceramics In reviewing the historic studies and recent progress in the field Ultra High Temperature Ceramics Materials for Extreme Environment Applications provides Original reviews of research conducted in the 1960s and 70s Content on electronic structure synthesis powder processing densification property measurement and characterization of boride and carbide ceramics Emphasis on materials for hypersonic aerospace applications such as wing leading edges and propulsion components for vehicles traveling faster than Mach 5 Information on materials used in the extreme environments associated with high speed cutting tools and nuclear power generation Contributions are based on presentations by leading research groups at the conference Ultra High Temperature Ceramics Materials for Extreme Environment Applications II held May 13 19 2012 in Hernstein Austria Bringing together disparate researchers from academia government and industry in a singular forum the meeting cultivated didactic discussions and efforts between bench researchers designers and engineers in assaying results in a broader context and moving the technology forward toward near and long term use This book is useful for furnace manufacturers aerospace manufacturers that may be pursuing hypersonic technology researchers studying any aspect of boride and carbide ceramics and practitioners of high temperature structural ceramics      **Review**, 1983

**Ultra-High Temperature Materials III** Igor L. Shabalyn, 2020-07-07 This exhaustive work in several volumes and over 2500 pages provides a thorough treatment of ultra high temperature materials with melting points around or over 2500 C The first volume focuses on carbon graphene graphite and refractory metals W Re Os Ta Mo Nb and Ir whilst the second and third are dedicated to refractory transition metal 4 5 groups carbides Topics included are physical structural thermal electro magnetic optical mechanical nuclear and chemical more than 3000 binary ternary and multi component systems including those used for materials design data on solid state diffusion wettability interaction with various elements and compounds in solid and liquid states gases and chemicals in aqueous solutions properties of these materials It will be of interest to researchers engineers postgraduate graduate and undergraduate students alike The readers users are provided with the full

qualitative and quantitative assessment which is based on the latest updates in the field of fundamental physics and chemistry nanotechnology materials science design and engineering

The Cold Spray Materials Deposition Process, 2007-09-21 The cold spray process produces dense low oxide coatings which can be used in such diverse applications as corrosion control and metals repair It has emerged as an important alternative to thermal spray coating techniques in certain areas This pioneering book reviews both the fundamentals of the process and how it can best be applied in practice The first part of the book discusses the development of the process together with its advantages and disadvantages in comparison with thermal spray coating techniques Part two reviews key process parameters such as powders nozzle design particle temperature and velocity and particle substrate interaction It also describes portable and stationary cold spray systems The final part of the book discusses how the cold spray process can be applied in such areas as improved wear corrosion protection electromagnetic interference shielding and repair of damaged components The cold spray materials deposition process is a standard reference on this important process and its industrial applications Examines the fundamentals of the cold spraying process Assesses how the technique can best be applied in practice Describes portable and stationary cold spray systems

Model Systems in Catalysis Robert Rioux, 2009-11-11 This book is an excellent compilation of cutting edge research in heterogeneous catalysis and related disciplines surface science organometallic catalysis and enzymatic catalysis In 23 chapters by noted experts the volume demonstrates varied approaches using model systems and their successes in understanding aspects of heterogeneous catalysis both metal and metal oxide based catalysis in extended single crystal and nanostructured catalytic materials To truly appreciate the astounding advances of modern heterogeneous catalysis let us first consider the subject from a historical perspective Heterogeneous catalysis had its beginnings in England and France with the work of scientists such as Humphrey Davy 1778 1829 Michael Faraday 1791 1867 and Paul Sabatier 1854 1941 Sabatier postulated that surface compounds similar to those familiar in bulk to chemists were the intermediate species leading to catalytic products Sabatier proposed for example that NiH moieties on a Ni surface were able to hydrogenate ethylene whereas NiH was not In the USA Irving Langmuir concluded just the opposite namely that chemisorbed surface species are chemically bound to surfaces and are unlike known molecules These chemisorbed species were the active participants in catalysis The equilibrium between gas phase molecules and adsorbed chemisorbed species yielding an adsorption isotherm produced a monolayer by simple site filling kinetics

**Transition Metal Carbides and Nitrides** Louis Toth, 2014-04-11 Refractory Materials Volume 7 Transition Metal Carbides and Nitrides discusses the developments in transition metal carbide and nitride research This volume is organized into nine chapters that emphasize the mechanical and superconducting properties of these compounds The introductory chapters deal with the general properties preparation techniques characterization crystal chemistry phase relationships and thermodynamics of transition metal carbides and nitrides The following chapter highlights the mechanical properties of these compounds such as elastic and plastic deformation fracture

strengthening mechanisms and hardness The discussion then shifts to specific electrical and magnetic properties including electrical resistivity Hall coefficient and magnetic susceptibility A separate chapter is devoted to carbides and nitrides as superconductors The concluding chapters explore certain theories that explain the mechanisms of band structure and bonding in carbides and nitrides This volume is of great value to research workers in metallurgy ceramics physics chemistry and related fields as well as to advanced students investigating problems concerning high temperature materials or interstitial compounds Revista mexicana de física ,2004 **Handbook of the Chemical Elements** Hermann Sicius,2024-10-28 This reference work describes comprehensively compactly and precisely the history properties production and application of all elements of the periodic table Particular attention is paid to the chemical compounds of the elements which are also presented extensively This book contains 23 chapters each of which includes the elements in the form of subchapters of the eight main groups the first and second as well as the fourth to tenth subgroups the rare earth metals and the third subgroup as well as the actinides Finally there is an outlook on the as yet undiscovered elements of the eighth and ninth periods on alternative more environmentally friendly drives for motor vehicles such as batteries and fuel cells as well as on semiconductor technology i e areas that will continue to see increasing research activity in the future Whenever possible the author has always maintained the order of chalcogenides halides pnictogenides and other compounds when presenting the chemical compounds of the elements The introductory part which illuminates the history of the respective element often contains biographies of well known researchers whose creative periods range from the near past to the Middle Ages You will not only find portraits of chemists but also of nuclear physicists astronomers and medical doctors **Quantum Mechanical Cluster Calculations in Solid State Studies** R. W. Grimes,Charles Richard Arthur Catlow,1992 This review volume takes an indepth look at the current research done in this important area of solid state science Although the emphasis is on modelling the properties of definite materials perfect crystal lattices are also considered in some detail It is noteworthy that the review articles are written by some of the best known experts in the field *Scientific and Technical Aerospace Reports* ,1970 U.S. Government Research & Development Reports ,1967 **Synthesis and Characterization of Group V Metal Carbide and Nitride Catalysts** Heock-Hoi Kwon,1998

## Unveiling the Energy of Verbal Art: An Emotional Sojourn through **Electronic Structure Of Refractory Carbides And Nitrides**

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