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Microstructure Sensitive Design for Performance Optimization



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**Jeffrey P. Simmons, Lawrence F.
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Graef**

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Fullwood, 2012-12-31 The accelerating rate at which new materials are appearing and transforming the engineering world only serves to emphasize the vast potential for novel material structure and related performance Microstructure Sensitive Design for Performance Optimization MSDPO embodies a new methodology for systematic design of material microstructure to meet the requirements of design in optimal ways Intended for materials engineers and researchers in industry government and academia as well as upper level undergraduate and graduate students studying material science and engineering MSDPO provides a novel mathematical framework that facilitates a rigorous consideration of the material microstructure as a continuous design variable in the field of engineering design Presents new methods and techniques for analysis and optimum design of materials at the microstructure level Authors methodology introduces spectral approaches not available in previous texts such as the incorporation of crystallographic orientation as a variable in the design of engineered components with targeted elastic properties Numerous illustrations and examples throughout the text help readers grasp the concepts

Computational Materials System Design Dongwon Shin, James Saal, 2017-11-10 This book provides state of the art computational approaches for accelerating materials discovery synthesis and processing using thermodynamics and kinetics The authors deliver an overview of current practical computational tools for materials design in the field They describe ways to integrate thermodynamics and kinetics and how the two can supplement each other Machine Learning in Molecular

Sciences Chen Qu, Hanchao Liu, 2023-10-01 Machine learning and artificial intelligence have propelled research across various molecular science disciplines thanks to the rapid progress in computing hardware algorithms and data accumulation This book presents recent machine learning applications in the broad research field of molecular sciences Written by an international group of renowned experts this edited volume covers both the machine learning methodologies and state of the art machine learning applications in a wide range of topics in molecular sciences from electronic structure theory to nuclear dynamics of small molecules to the design and synthesis of large organic and biological molecules This book is a valuable resource for researchers and students interested in applying machine learning in the research of molecular sciences

Horizons in Materials Nicola Maria Pugno, Valeria Cannillo, Huanyang Chen, Jie-Sheng Chen, Jinn P. Chu, Liming Dai, Douglas Soares Galvao, Vincent G. Harris, Weihua Li, Alessandro Pegoretti, John L. Provis, Guang-Ling Song, Peide Ye, 2022-08-23 The Frontiers in Materials Editorial Office team are delighted to present the Horizons in Materials article collection showcasing high impact authoritative and accessible Review articles covering important topics at the forefront of the materials science and engineering field All contributing authors were nominated by the Chief Editors and Editorial Office in recognition of their prominence and influence in their respective fields The cutting edge work presented in this article collection highlights the diversity of research performed across the entire breadth of the materials science and engineering

field and reflects on the latest advances in theory experiment and methodology with applications to compelling problems This Editorial features the corresponding author s of each paper published within this important collection ordered by section alphabetically highlighting them as the great researchers of the future The Frontiers in Materials Chief Editors and Editorial Office team would like to thank each researcher who contributed their work to this collection We are excited to see each article gain the deserved visibility and traction within the wider community ensuring the collection s truly global impact and success Emily Young Journal Manager

Microstructure modeling and crystal plasticity parameter identification for predicting the cyclic mechanical behavior of polycrystalline metals Kuhn, Jannick, 2023-04-04 Computational homogenization permits to capture the influence of the microstructure on the cyclic mechanical behavior of polycrystalline metals In this work we investigate methods to compute Laguerre tessellations as computational cells of polycrystalline microstructures propose a new method to assign crystallographic orientations to the Laguerre cells and use Bayesian optimization to find suitable parameters for the underlying micromechanical model from macroscopic experiments

Multiscale Structural Topology Optimization Liang Xia, 2016-04-27 Multiscale Structural Topology Optimization discusses the development of a multiscale design framework for topology optimization of multiscale nonlinear structures With the intention to alleviate the heavy computational burden of the design framework the authors present a POD based adaptive surrogate model for the RVE solutions at the microscopic scale and make a step further towards the design of multiscale elastoviscoplastic structures Various optimization methods for structural size shape and topology designs have been developed and widely employed in engineering applications Topology optimization has been recognized as one of the most effective tools for least weight and performance design especially in aeronautics and aerospace engineering This book focuses on the simultaneous design of both macroscopic structure and microscopic materials In this model the material microstructures are optimized in response to the macroscopic solution which results in the nonlinearity of the equilibrium problem of the interface of the two scales The authors include a reduce database model from a set of numerical experiments in the space of effective strain Presents the first attempts towards topology optimization design of nonlinear highly heterogeneous structures Helps with simultaneous design of the topologies of both macroscopic structure and microscopic materials Helps with development of computer codes for the designs of nonlinear structures and of materials with extreme constitutive properties Focuses on the simultaneous design of both macroscopic structure and microscopic materials Includes a reduce database model from a set of numerical experiments in the space of effective strain **Applied**

Micromechanics of Complex Microstructures Majid Baniassadi, Mostafa Baghani, Yves Rémond, 2023-03-02 Applied Micromechanics of Complex Microstructures explains the fundamental concepts of continuum modeling of various complicated microstructures covering nanocomposites multiphase composites biomaterials biological materials and more The authors outline the calculation of effective mechanical and thermal properties allowing readers to understand the step by

step modeling and homogenization of complicated microstructures and the book also features a chapter on microstructure hull and material design Modeling of complex samples with nonlinear properties such as neural tissue bone microstructure and liver tissue is also explained and analyzed Explains the core concepts of continuum modeling of different complex microstructures including nanocomposites multiphase composites biomaterials and biological materials Provides detailed calculations of effective mechanical and thermal properties allowing the audience to understand the modeling and homogenization of complex microstructures Covers several methods for designing the microstructure of heterogeneous materials

Integrated Design of Multiscale, Multifunctional Materials and Products David L. McDowell, Jitesh Panchal, Hae-Jin Choi, Carolyn Seepersad, Janet Allen, Farrokh Mistree, 2009-09-30 Integrated Design of Multiscale Multifunctional Materials and Products is the first of its type to consider not only design of materials but concurrent design of materials and products In other words materials are not just selected on the basis of properties but the composition and or microstructure is designed to satisfy specific ranged sets of performance requirements This book presents the motivation for pursuing concurrent design of materials and products thoroughly discussing the details of multiscale modeling and multilevel robust design and provides details of the design methods strategies along with selected examples of designing material attributes for specified system performance It is intended as a monograph to serve as a foundational reference for instructors of courses at the senior and introductory graduate level in departments of materials science and engineering mechanical engineering aerospace engineering and civil engineering who are interested in next generation systems based design of materials First of its kind to consider not only design of materials but concurrent design of materials and products Treatment of uncertainty via robust design of materials Integrates the materials by design approach of Olson Ques Tek LLC with the materials selection approach of Ashby Granta Distinguishes the processes of concurrent design of materials and products as an overall systems design problem from the field of multiscale modeling Systematic mathematical algorithms and methods are introduced for robust design of materials rather than ad hoc heuristics it is oriented towards a true systems approach to design of materials and products

Hierarchical Materials Informatics Surya R. Kalidindi, 2015-08-06 Custom design manufacture and deployment of new high performance materials for advanced technologies is critically dependent on the availability of invertible high fidelity structure property processing SPP linkages Establishing these linkages presents a major challenge because of the need to cover unimaginably large dimensional spaces Hierarchical Materials Informatics addresses objective computationally efficient mining of large ensembles of experimental and modeling datasets to extract this core materials knowledge Furthermore it aims to organize and present this high value knowledge in highly accessible forms to end users engaged in product design and design for manufacturing efforts As such this emerging field has a pivotal role in realizing the goals outlined in current strategic national initiatives such as the Materials Genome Initiative MGI and the Advanced Manufacturing Partnership AMP This book presents the foundational elements of this new discipline as it relates to

the design development and deployment of hierarchical materials critical to advanced technologies Addresses a critical gap in new materials research and development by presenting a rigorous statistical framework for the quantification of microstructure Contains several case studies illustrating the use of modern data analytic tools on microstructure datasets both experimental and modeling

Architecting Robust Co-Design of Materials, Products, and Manufacturing Processes Anand Balu Nellippallil, Janet K. Allen, B. P. Gautham, Amarendra K. Singh, Farrokh Mistree, 2020-06-13 This book explores systems based co design introducing a Decision Based Co Design DBCD approach for the co design of materials products and processes In recent years there have been significant advances in modeling and simulation of material behavior from the smallest atomic scale to the macro scale However the uncertainties associated with these approaches and models across different scales need to be addressed to enable decision making resulting in designs that are robust that is relatively insensitive to uncertainties An approach that facilitates co design is needed across material product design and manufacturing processes This book describes a cloud based platform to support decisions in the design of engineered systems CB PDSIDES which feature an architecture that promotes co design through the servitization of decision making knowledge capture and use templates that allow previous solutions to be reused Placing the platform in the cloud aids mass collaboration and open innovation A valuable reference resource reference on all areas related to the design of materials products and processes the book appeals to material scientists design engineers and all those involved in the emerging interdisciplinary field of integrated computational materials engineering ICME

Statistical Methods for Materials Science Jeffrey P. Simmons, Lawrence F. Drummy, Charles A. Bouman, Marc De Graef, 2019-02-13 Data analytics has become an integral part of materials science This book provides the practical tools and fundamentals needed for researchers in materials science to understand how to analyze large datasets using statistical methods especially inverse methods applied to microstructure characterization It contains valuable guidance on essential topics such as denoising and data modeling Additionally the analysis and applications section addresses compressed sensing methods stochastic models extreme estimation and approaches to pattern detection

Information Science for Materials Discovery and Design Turab Lookman, Francis J. Alexander, Krishna Rajan, 2015-12-12 This book deals with an information driven approach to plan materials discovery and design iterative learning The authors present contrasting but complementary approaches such as those based on high throughput calculations combinatorial experiments or data driven discovery together with machine learning methods Similarly statistical methods successfully applied in other fields such as biosciences are presented The content spans from materials science to information science to reflect the cross disciplinary nature of the field A perspective is presented that offers a paradigm codesign loop for materials design to involve iteratively learning from experiments and calculations to develop materials with optimum properties Such a loop requires the elements of incorporating domain materials knowledge a database of descriptors the genes a surrogate or statistical model developed to predict a given

property with uncertainties performing adaptive experimental design to guide the next experiment or calculation and aspects of high throughput calculations as well as experiments The book is about manufacturing with the aim to halving the time to discover and design new materials Accelerating discovery relies on using large databases computation and mathematics in the material sciences in a manner similar to the way used to in the Human Genome Initiative Novel approaches are therefore called to explore the enormous phase space presented by complex materials and processes To achieve the desired performance gains a predictive capability is needed to guide experiments and computations in the most fruitful directions by reducing not successful trials Despite advances in computation and experimental techniques generating vast arrays of data without a clear way of linkage to models the full value of data driven discovery cannot be realized Hence along with experimental theoretical and computational materials science we need to add a fourth leg to our toolkit to make the Materials Genome a reality the science of Materials Informatics

Handbook On Big Data And Machine Learning In The Physical Sciences (In 2 Volumes) ,2020-03-10 This compendium provides a comprehensive collection of the emergent applications of big data machine learning and artificial intelligence technologies to present day physical sciences ranging from materials theory and imaging to predictive synthesis and automated research This area of research is among the most rapidly developing in the last several years in areas spanning materials science chemistry and condensed matter physics Written by world renowned researchers the compilation of two authoritative volumes provides a distinct summary of the modern advances in instrument driven data generation and analytics establishing the links between the big data and predictive theories and outlining the emerging field of data and physics driven predictive and autonomous systems

Materials Science and Engineering Surya R. Kalidindi,2013-07-10 Accelerated design and development of new advanced materials with improved performance characteristics and their successful insertion in engineering practice are largely hindered by the lack of a rigorous mathematical framework for the robust generation of microstructure informatics relevant to the specific application In this chapter we describe a set of novel data driven computationally efficient protocols that are capable of accelerating significantly the process of building the necessary microstructure informatics for a targeted application Specific applications in establishing processing structure property linkages are discussed as representative examples of how data science can potentially transform the current practices in the materials design and development arena

Homogenization and materials design of mechanical properties of textured materials based on zeroth-, first- and second-order bounds of linear behavior Lobos Fernández, Mauricio,2018-07-09 This work approaches the fields of homogenization and of materials design for the linear and nonlinear mechanical properties with prescribed properties profile The set of achievable properties is bounded by the zeroth order bounds which are material specific the first order bounds containing volume fractions of the phases and the second order Hashin Shtrikman bounds with eigenfields in terms of tensorial texture coefficients for arbitrarily anisotropic textured materials

Handbook of Software Solutions for ICME

Georg J. Schmitz, Ulrich Prahl, 2016-09-20 As one of the results of an ambitious project this handbook provides a well structured directory of globally available software tools in the area of Integrated Computational Materials Engineering ICME The compilation covers models software tools and numerical methods allowing describing electronic atomistic and mesoscopic phenomena which in their combination determine the microstructure and the properties of materials It reaches out to simulations of component manufacture comprising primary shaping forming joining coating heat treatment and machining processes Models and tools addressing the in service behavior like fatigue corrosion and eventually recycling complete the compilation An introductory overview is provided for each of these different modelling areas highlighting the relevant phenomena and also discussing the current state for the different simulation approaches A must have for researchers application engineers and simulation software providers seeking a holistic overview about the current state of the art in a huge variety of modelling topics This handbook equally serves as a reference manual for academic and commercial software developers and providers for industrial users of simulation software and for decision makers seeking to optimize their production by simulations In view of its sound introductions into the different fields of materials physics materials chemistry materials engineering and materials processing it also serves as a tutorial for students in the emerging discipline of ICME which requires a broad view on things and at least a basic education in adjacent fields

Fundamentals of Uncertainty Quantification for Engineers Yan Wang, Anh.V. Tran, David L. McDowell, 2025-05-30 Fundamentals of Uncertainty Quantification for Engineers Methods and Models provides a comprehensive introduction to uncertainty quantification UQ accompanied by a wide variety of applied examples and implementation details to reinforce the concepts outlined in the book Sections start with an introduction to the history of probability theory and an overview of recent developments of UQ methods in the domains of applied mathematics and data science Major concepts of copula Monte Carlo sampling Markov chain Monte Carlo polynomial regression Gaussian process regression polynomial chaos expansion stochastic collocation Bayesian inference model form uncertainty multi fidelity modeling model validation local and global sensitivity analyses linear and nonlinear dimensionality reduction are included Advanced UQ methods are also introduced including stochastic processes stochastic differential equations random fields fractional stochastic differential equations hidden Markov model linear Gaussian state space model as well as non probabilistic methods such as robust Bayesian analysis Dempster Shafer theory imprecise probability and interval probability The book also includes example applications in multiscale modeling reliability fatigue materials design machine learning and decision making Introduces all major topics of uncertainty quantification with engineering examples and implementation details Features examples from a wide variety of science and engineering disciplines e g fluids structural dynamics materials manufacturing multiscale simulation Discusses sampling methods surrogate modeling stochastic expansion sensitivity analysis dimensionality reduction and more

Artificial Intelligence in Tissue and Organ Regeneration Chandra P. Sharma, Thomas Chandy, Vinoy

Thomas,2023-08-18 Artificial Intelligence in Tissue and Organ Regeneration discusses the role of artificial intelligence as a highly sought after technology in the area of organ and tissue regeneration Certain groups have made significant progress in mass producing mini organs and organoids from stem cells utilizing such techniques As time goes on there will be a need to improve these procedures protocols regulatory guidelines and their clinical implications Integrates existing literature in a highly interdisciplinary area Presents comprehensive current and future perspectives combining artificial intelligence and machine learning with organ and tissue regeneration Provides new and emerging technology that is useful in healthcare and the medical field

Microstructural Characterisation Techniques Gunturi Venkata Sitarama Sastry,2022-09-15 This textbook is aimed at graduate and upper undergraduate students studying materials science and metallurgy It comprehensively covers the topic of microstructural characterization and includes an emphasis on Fourier analysis and Fourier transformation electron diffraction electromagnetic waves and electron waves lens parameters transmission electron microscopy optical microscopy and scanning electron microscopy The author has included pedagogical features such as end of chapter exercises and worked examples with varying degrees of difficulty to augment learning and self testing This book will be a useful guide for upper undergraduate and graduate students along with researchers and professionals working in the field of microstructural characterization

Advanced Metrology X. Jane Jiang,Paul J. Scott,2020-04-08 Advanced Metrology Freeform Surfaces provides the perfect guide for engineering designers and manufacturers interested in exploring the benefits of this technology The inclusion of industrial case studies and examples will help readers to implement these techniques which are being developed across different industries as they offer improvements to the functional performance of products and reduce weight and cost Includes case studies in every chapter to help readers implement the techniques discussed Provides unique advice from industry on hot subjects including surface description and data processing Features links to online content including video code and software

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