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Special Issue Preface

Innovations in materials design

Steven R. LeClair[a,*], Shuichi Iwata[b], Pierre Villars[c]

[a]*U.S. Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, OH, USA*
[b]*Research into Artifacts Center for Engineering, The University of Tokyo, Tokyo, Japan*
[c]*MPDS Materials Phases Data Systems, CH-6354 Vitznau, Switzerland*

A, if not the, principal driver for all prescriptive scientific and engineering endeavors is the 'mapping' of materials information,

i.e., the mapping of structure, to properties, processing and use conditions.

From Mendelev and the 'Periodic Table', to present day electronic databases, the impetus to organize vast amounts of continually evolving information associated with materials remains a challenge. Advances toward organizing materials data has ironically created yet another challenge, and that is the capability to dynamically view these mappings. The inadequacy of processing resources, specifically availability and affordability, is due to the computational intractability of the various methods currently in use. As a consequence, these methods offer little toward complementing the evermore time-consuming and expensive empirical approaches in generating new materials data. There is no escaping this intractability problem, as it is driven by an increasingly competitive (time-to-market) environment, and a near 'atomic-scale' precision in terms of the quality demanded of materials and products in the international marketplace.

1. The problem

At our disposal is an arsenal of computational methods, ranging from *ab initio* to *constitutive* and even *qualitative* models of materials and materials behavior. Because of the vast amounts of information to be considered, there is an apparent need to couple empirical and analytical approaches. The impetus to establish better methods is being popularized, if not by a growing 'web-based society', then by an emerging community of physicists, chemists, and materials researchers across the globe who are collectively driven by the opportunities for 'innovations in materials design'.

Materials, and therein materials design, has evolved over two millennia from the macro-monolithic and composite materials toward the 'atomic-scale' control of lattices, surfaces and interfaces, sometimes referred to as 'crystal engineering', the intricacies and difficulties of which are most notably manifested in the materials processing associated with their manufacture. In the search for more computationally tractable methods, innovation in materials design will need to 'build bridges' between the nano and macro scale views, and in particular, augment fundamental theory to accelerate:

1. large scale first principle calculations, e.g., density functional theory as applied to multi-element property calculations,
2. global optimization of 'n' dimensional problems applied to materials design,
3. large scale molecular dynamics applied to property prediction, e.g., defects as they relate to microstructure and related properties,
4. atomic-level (10^{-13} seconds) structure evolution during material processing.

2. Special issue content and organization

2.1. Semi-empirical and search-based methods

Given the computational challenge to do either material or process design, search-based methods offer an expeditious approach to providing a researcher 'analogs' for both insight and perspective. To begin our special issue is a paper entitled:

THE LINUS PAULING FILE (LPF), A BASIC DATABASE FOR ALLOYS, INTERMETALLICS AND INORGANICS AND ITS APPLICATION FOR

*Corresponding author.

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MATERIALS DESIGN
P. Villars, N. Onodera and S. Iwata

The purpose of this paper is to orient the reader both with regard to the significance of the problem but as well the potential benefit of coupling empirical and analytic methods via relations discovered within and between classes of materials.

A number of search-based methods to classify data, e.g., statistical regression, neural network clustering and function approximation, rough sets, pyramidal nets, et al. provide a means of discovering patterns which effectively serve to establish structure, property, processing and/or use mappings via relations. The following papers not only illustrate the application of these methods to materials design, but also problems involved in their use relative to limitations and difficulties.

COMPUTATIONAL MATERIALS DESIGN USING ARTIFICIAL INTELLIGENCE METHODS
N.N. Kiselyova, V.P. Gladun and N.D. Vashenko

ROUGH SETS APPLIED TO THE DISCOVERY OF NEW MATERIALS
A.G. Jackson, Z. Pawlak, and S.R. LeClair

MATERIALS DISCOVERY VIA TOPOLOGICALLY-CORRECT DISPLAY OF REDUCED-DIMENSION DATA
Y.H. Pao, Z. Meng. S.R. LeClair and B. Igelnik

MATERIAL STRUCTURE-PROPERTY PREDICTION USING ORTHOGONAL FUNCTIONAL BASIS NEURAL NETWORK
C.L.P. Chen, Y. Cao and S.R. LeClair

UNIFICATION OF NEURAL AND STATISTICAL METHODS AS APPLIED TO MATERIALS STRUCTURE-PROPERTY MAPPING
B.R. Bakshi

PREDICTING ULTRA-HARD BINARY COMPOUNDS VIA CASCADED AUTO- AND HETERO-ASSOCIATIVE NEURAL NETWORKS
S.L. Thaler

2.2. Analytic methods

Whether your view of ‘molecular modeling’ is from a ‘materials’ or a ‘process’ design perspective, with the advent of thin-films, the modeling of materials under growth conditions is forcing the integration of materials and process design. The below listed papers address this very issue, and not only illustrate the coupling of analytical and empirical methods, but begin to suggest new directions for innovation. This coupling is affected by applying fundamental analytical functions such as:

– ab initio density functional molecular model with the local spin density approximation,
– explicit kinetic energy functions by combining the implicit Poisson equation with the Thomas-Fermi energy functional,
– Tersoff’s interatomic potential function and molecular dynamic simulations,
– Buckingham’s interionic potential function and molecular dynamic simulations,

to different model ideas (plasma kinetics models, a simplified charge transfer model, multiscale models and cellular automata modeling). The objective is to simulate the materials behavior on an atomistic scale by linking the selected materials properties with the growth conditions, such as:

– calculation of reactivity in gas-phase chemical reactions in a plasma,
– calculation of the directions of charge transfer,
– calculation of intrinsic properties as a function of pressure, and
– correlate simulations with atomic level experiments.

While such modeling ideas, captured in the below papers, are presented within the context of a restricted and small application range, they clearly illustrate new directions and potential breakthroughs in the use and coupling of computational methods.

A PLASMA KINETICS MODEL: ANALYSIS OF WALL LOSS REACTIONS IN DRY ETCHING OF SILICON DIOXIDE
Kazutami Tago, Hideyuki Kazumi, and Kinya Kobayashi

A SIMPLIFIED CHARGE TRANSFER MODEL: CALCULATIONS USING AN EXPLICIT KINETIC ENERGY FUNCTIONAL
H. Odaka, S. Ohnishi, and S. Iwata

TOWARD MULTISCALE MODELING: THE ROLE OF ATOMISTIC SIMULATIONS IN THE ANALYSIS OF SI AND SIC UNDER HYDROSTATIC COMPRESSION
Kazuki Mizushima, Meijie Tang, and Sidney Yip

TOWARDS CELLULAR AUTOMATA: THE ROLE OF ATOMISTIC SIMULATION IN DETERMINING MATERIAL STRUCTURES
Robin W. Grimes

3. To conclude

The purpose of this special issue is to present various methods that attempt to enable a ‘‘Mapping of Materials Structure to its Properties, Processing and Use Condi-

tions''. Furthermore, our mission is to stimulate the reader to consider yet other ideas and/or methods which will accelerate research – such that we transform our objectives from 'dream' to 'reality'. The widespread application of the below listed methods:

– semi-empirical-based methods to classify materials data, e.g. atomic environment approach
– search-based methods to classify materials data, e.g. statistical regression, neural network clustering, rough sets, pyramidal nets, and
– fundamental function-based methods to describe materials dependences, e.g. ab initio density functionals, explicit kinetic energy functions, Tersoffs interatomic potential function, and Buckingham's interionic potential function,

will also enable the development of extensive materials knowledge bases. It is clear that, regardless of the method(s) used, the generation and availability of these knowledge bases is prerequisite and critically important to materials science. Therefore, the need for an international 'information-knowledge' system is strongly evident, not only as a source of information, but as a workbench providing interoperability to all materials databases and methods.