

Approaches to Computational Materials Science

Juri Filatovs, D. M. Pai, S. N. Yarmolenko and J. Sankar
Center for Advanced Materials and Smart Structures
Department of Mechanical Engineering
North Carolina A&T State University
Greensboro, NC 27411

Abstract

There is an increased application of materials computation in the selection, microstructural analysis, simulation, and testing of materials. This is creating a new mode of approaching, and teaching materials science. There is needed familiarity with statistics, modeling, and simulation, in addition to the usual materials science topics. We have used software for microstructural characterization, selection for design, and virtual testing. This paper describes our experiences in incorporation of such software into the graduate and undergraduate curriculum and our strategies for bringing in and bridging the diverse areas of specialization needed.

Introduction and Motivation

Engineering educators pin much hope and expectation on the use of computers for more efficient and better instruction, through the use of software packages for word processing, presentation, calculation and Web collaboration. Far less common is the exposure of students to the computer-aided contemporary skills required in many industrial settings. In a wide ranging, collective specialty such as materials science, there is need to routinely use a wide range of computational and analytic tools; for experimental data analysis, simulation, characterization, and selection for design. Underlying these topics are the central areas of mathematics and statistics. Meaningful coverage of this range of tasks is a major challenge in terms of integration and incorporation into coursework.

There is an emerging discipline known as computational materials science, involving materials modeling, simulation, virtual testing, and such. We are not concerned with the full computation syllabus, but rather the increased use of materials computation within the usual coursework. We share our experiences in several courses, centered on Materials Science topics, both undergraduate and graduate, and taught to mechanical engineering students.

Issues

Materials Science, like many other disciplines, is evolving a new relationship with the computer. The wide-ranging, eclectic and interdisciplinary nature of the field has found applications in materials selection, microstructural analysis, simulation, and testing. As teachers we must face the actuality that most students have little programming experience, and that the use of computer software severely alters the scope of a course. The introduction and integration of this auxiliary information is problematic.

A second issue that arises is that while universities are in the forefront of many uses for computers, industry is marching to its own developments, using computers intensively for many routine tasks. Many modern-day engineering workspaces in industrial settings have been observed to contain only computers, to the almost-total exclusion of books and paperwork. It is important for students to have some introduction to such a mode of work, which again raises many teaching issues.

Implementation Summary

Materials problems involve many interrelated facts, auxiliary information which must be considered in any situation. To select a material requires knowledge of the thermodynamic and force conditions, the structure of the material (the phases present and their response to the environment), the parameter statistics of the structure, and the nature of the available data. All these must be considered together, and some predictive model formed. We attempt to separate these to some extent and organize our experiences around several conceptual areas.

Materials Selection

The selection of materials is central to engineering, and is encountered in a variety of manufacturing, mechanics, and design courses. The software¹ we use is both a general materials database and a compilation of materials concepts; its use conveys much information and is a powerful teaching tool. For conceptual design and preliminary selection, it shows typical properties and functional attributes such as temperature variation, and includes various performance indices, such as the strength to density ratio, which allow multiple optimizations. For final selection, there are extensive databases covering all the major classes of materials, their fabrication processes, and property ranges for various conditions.

Process Selection

Two levels of process selection are done by our students. First, identification of the appropriate manufacturing process for a given material and part configuration is aided by the use of a process module in the CES-4 software referred to above. Second, design of process parameters for applications such as heat treatment of iron and aluminum alloys, frequently collaterally with materials selection is done with the use of thermochemical databases²⁻³, which contain phase diagrams in addition to various physical and thermodynamic properties. Phase diagrams are a standard tool for understanding materials processes, and the ease of calling up a particular phase diagram, and obtaining compositions and temperatures using the cursor, is an important factor in encouraging their use. They need to be easily copied, printed, and annotated for particular conditions.

Microstructural Characterization

Microstructural characterization is our leading case for integrating a large number of specialties. It is an area which has increased its role from largely metallurgical applications to a broad range of materials. Its range of topics includes spatial statistics, structural geometry, the property-structural link, and the foundation topics of mathematics and statistics. We have taught several graduate courses on this topic, which is the evolved equivalent of the former “quantitative metallurgy”, covering microstructures in the optical and scanning electron ranges. We stress the

need for an interpretative strategy in microstructural examination, the understanding of the operative mechanisms that might be contributing to properties in a particular material. We use one of the standard commercial packages⁴, that has a large array of image processing and analysis features, along with good statistical support. We have used this for both undergraduate teaching and research, and have not been able to find a suitable, non-commercial, equivalent.

The principal software we have used is briefly summarized below. We favor commercial software, because we have found the expectations in industry are difficult to simulate with do-it-yourself versions.

CES4

Cambridge Engineering Selector¹ is based, to a large extent, on the approach of Ashby⁵, Esawi and Ashby⁶, and Ashby and Cebon⁷. The use of performance indices is particularly stressed. Additional modules are available for MIL-specification data, suitable for commercial design, giving the usual design minimum and test averages. Case studies based on this software have been employed in junior level introductory manufacturing process classes, where students first underwent the materials selection process based on the design requirements and then selected manufacturing processes in concordance with the work material and the designer specified dimensional and surface finish tolerances and cost restrictions. Based on student feedback forms, these modules enabled students to develop expertise in initial screening (go/no go) of processes and the development of quantitative norms (indices) for the systematic ranking and identification of optimal processes from a universe of hundreds of processes.

Image Pro

Image-Pro⁴ is a commercial digital image processing software with a large number of functionalities suitable for materials research, development, and routine characterization, along with an array of statistical and graphics modules.

MAPP and TAPP

Thermochemical and Physical Properties – TAPP², is a database of general properties; physical, structural, elastic, thermal expansion, conductivity, diffusivity, etc, of pure materials and compounds. Of particular interest to us are the binary and ternary phase diagrams. MAPP³ is a database of properties for engineering materials, developed by the vendor in collaboration with ASM International as an interface to the latter's Mat.DB databases.

Other Software

In addition to the above software with direct materials relevance, we also use Matlab⁸ and LabView⁹ in our department for general computation and mathematical modeling. We have also used specialized software such as OOF¹⁰, which can assign materials properties to real or simulated images enabling the calculation of macroscopic properties.

Case Study

As a more specific example we sketch a case study of a course titled “Materials Characterization by Digital Microscopy,” taught to graduate students¹¹. This is a software-based

course, centered on Image-Pro, and is the evolved equivalent of “Quantitative” Metallography, the examination of microstructures in the optical and scanning microscope ranges. The software has a large number of functionalities tailored for materials research and is rich in subject matter possibilities.

The formal lectures focused on the core topics of statistics, spatial geometry, and the property-structure link. Individual projects, based on the students’ thesis or research topics, were the basis for more specialized topics. The materials involved were primarily composites (carbon/polymer, carbon/carbon, ceramic/ceramic) or monolithic ceramics. A project on carbon/carbon materials is sketched below:

Carbon-carbon composites (Figure 1) are an exceptional class of high-temperature materials that have low density and very high temperature capability. The purpose of the project was to study the microstructures of a carbon/carbon composite during its different processing stages towards carbonization. The primary focus is on the composite while it is post-cured, capturing cross-section images to analyze fiber volume fraction, which is an important parameter affecting the composite’s mechanical properties. The fiber density (number/area) in tow and unit cell, fiber radial distribution and average fiber diameter etc. are examined, comparing voids and cracks’ change after different manufacturing steps.

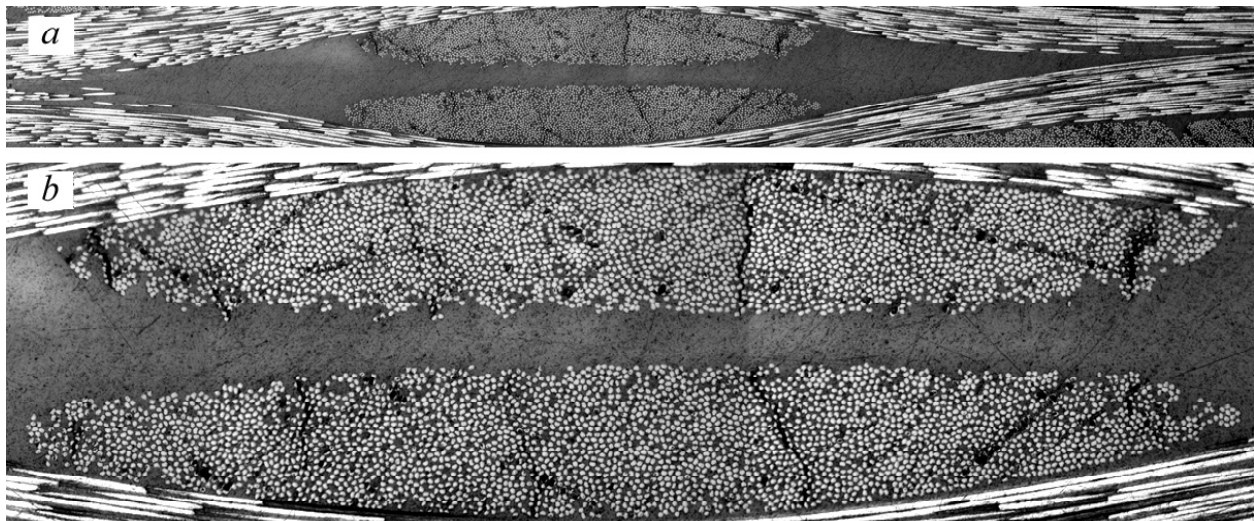


Figure 1. Carbon/carbon composite tow analysis¹¹: a) unit cell with 2 tows (combined from 6 images at magnification 100X); b) tows (200X): fiber volume fraction in unit cell = 22.38%; fiber density in unit cell = 0.00923 μm^{-2} ; fiber density in upper tow = 0.0179 μm^{-2} ; fiber density in lower tow = 0.0178 μm^{-2} ; ratio for fiber density in tows/unit cell = 1.93; average number of fibers in one tow = $(2991+3010)/2 = 3001$ (3K expected).

Summary Observations and Strategies

The ever increasing link of materials science with computers is raising expectations in the use and development of materials. Universities appear to be lagging industry in the everyday use of software for this. The above attempts are founded on our observations of industrial practice, although the implementation is specialized to our teaching environment. We have summarized

some of our experiences and approaches, and some points we feel need stressing.

It is tempting, and easier, to use student-friendly software; this may give a false impression of the scope and depth of current industrial practice. Conversely, industrial software tends to be daunting, and the ease of analysis of many situations and obtaining of various parameters and statistics make it necessary to understand the limitations of applicability of such software. In teaching, there is a balance between the amount of fundamentality of principles, and the extent of software involvement. Both careful selection of software and major accommodation of topics are important for maintaining this balance

The computer related aspects of programming, specific software use, and such are treated as laboratory-type activities, largely outside of the classroom lectures. An early lesson we have learned is that the translation of problems into the framework of computer-aided format is not trivial for students. Our general approach is a mix of traditional analysis and computer-aided methods, we largely allow students to choose the ratio of these. It gives scope for apportioning computer expertise, allowing choosing of the level of computer involvement with which a student is comfortable. It takes considerable time to learn a particular software application, and there is individual variation in this skill. We have found project based assignments, allowing for customizing to individual skills and levels of experience, the best approach within most of our courses, which are upper-undergraduate to PhD level.

We believe our approach has been reasonably successful. Evaluated in terms of downstream results, we have noticed an increased use of microstructural information and analysis in thesis and research work, and a better appreciation of microstructural issues in subsequent courses.

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Biographies

G. JURI FILATOVS is a Professor of Mechanical Engineering at NC A&T State University. He received his Ph.D. from the University of Missouri-Rolla. He has worked for McDonnell Aircraft and the US Bureau of Mines. His research is in the area of materials and their properties. He teaches materials science and the capstone design courses in mechanical engineering.

DEV DAS M. PAI is Associate Professor of Mechanical Engineering at NC A&T State University. He received his M.S. and Ph.D. from Arizona State University. He teaches manufacturing processes and machine design. A registered Professional Engineer in North Carolina, he serves on the Professional Licensure Committees of the NCEES and SME and is active in the Manufacturing Division of ASEE and the Materials Division of ASME.

SERGEY N. YARMOLENKO is a Senior Research Scientist of the NSF-CREST Center for Advanced Materials and Smart Structures at NC A&T State University. He received his Ph.D. from Institute of Organic Chemistry, Ukrainian Academy of Sciences. He conducts research and teaches courses related to advanced materials.

JAG SANKAR is a Professor of Mechanical Engineering at NC A&T State University and Director/PI of the NSF-CREST Center for Advanced Materials and Smart Structures at NC A&T State University. He received his Ph.D. from Lehigh University. He conducts research and teaches courses related to advanced materials.