Session 1526

Spreadsheet Applications for Materials Science

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Abstract

Spreadsheets have the potential to improve the teaching of the use of computers in solving engineering problems. Ideally, they would be integrated into existing courses, rather than teaching separate courses on spreadsheets. If this is done then homework assignments could be made much richer and their use in the laboratory courses would be invaluable. The author is developing a series of tutorials that address a wide range of materials science topics. The spreadsheet exercises in each tutorial start with simple calculations and progress to project-level calculations such as modeling ionic bonding or processing data from experiments. Spreadsheet skills developed include performing simple and complex calculations, importing and exporting data, graphing data, using the numerical tools, and producing attractive, presentable and reusable spreadsheet applications. With spreadsheets already on practically every home and school personal computer implementation of these tutorials can be done at little or no cost, a definite plus for smaller schools, and they will even allow the student to complete these assignments at home, reducing the need for schools to set up computer laboratories, a plus for high-enrollment courses.

Introduction

When the pocket calculator first appeared in the classroom no one talked about technology in the classroom. In many cases it was reluctantly allowed in and eventually, after it seemed that nearly everyone had one, exams, homework and other assignment changed to accommodate and even take advantage of this new, personal, high technology device. Computers are similar in many respects. They have been on our desktops for over 20 years are have only recently began to become an integral part of our curricula. While many of the recent high-profile implementations center around the Internet, multimedia and other interactive software, spreadsheets, which have been on our desktop computers since the beginning, offer a low cost avenue for developing richer and more engaging assignments, much like the pocket calculator did. Like pocket calculators, they can take the tedium out of the number crunching, allowing the student to concentrate on the problem at hand. The spreadsheet's easy learning curve, versatility and ubiquitousness, make them ideal for introducing the students to the use of computers to solving engineering problems.

This paper describes an effort to develop a series of tutorial sand support materials that can be used in undergraduate materials science courses. It describes the design criteria, the contents of each part of the whole package, three current implementations and plans for trying them out in community college and high school classrooms.

Background

For the past five years the author's courses have included carefully chosen assignments that would be easy to complete using spreadsheets but tedious if using only a calculator. Most students stuck with the techniques they already knew and spent a lot of time punching the keys on their calculator, with little time or energy left to learn the materials science behind the assignment.

In our laboratory experiments spreadsheets have become more essential than simply nice to have. These experiments require preliminary calculations to prepare for an experiment, importing the data, analyzing it, comparing it to calculations, and transferring the results to the students' reports. Some experiments require spreadsheets to collect data in the extended group experiments. Practically every experiment would benefit from the use of spreadsheets, but the students' lack of even a basic understanding of not only spreadsheets but any number-crunching software is a problem we continue to struggle with.

The author has informally poled students for several years on their use of computers in general and their use of spreadsheets in particular. Some seniors have extensive experience with high-end FEM and other specialized, and expensive, process-modeling software packages, while few have done any real programming and still fewer have used spreadsheets. This has began to change somewhat as software such as Mathematica and MathCad are introduced into select courses. But in general, many said that if the software was not actually part of a course, they never used it.

These experiences showed that if we want the students to use spreadsheets in our courses that we cannot expect them to simply pick it up in high school or in their spare time. The goal behind the "Spreadsheet Applications for Materials Science" (SAMS) project is to start getting the students to start using a powerful tool they already have on their computer, without having to teach a separate course on using spreadsheets, and at the same time enhancing the learning of materials science. If successful, we will see students using spreadsheets in the same way that years ago we used pocket calculators, without thinking twice about it, and to do interesting new things.

Why Spreadsheets?

Why, when powerful software such as Mathematica, MathCad, HiQ and other programs are available, should the use of spreadsheets in engineering course be considered? Many of the answers are obvious:

- Spreadsheets are inexpensive and in many cases are already installed on the school's and the student's computers.
- Spreadsheets are widely used. Data, calculations and graphs can be easily shared with others.
- With over 500 functions and powerful macro languages, they are quite capable of performing complex engineering calculations.
- Graphing the data is easy to do within the spreadsheet.
- The data, and the objects (cells, tables, and graphs) can be easily exported or copied to other applications, such as the student's laboratory report.
- Learning to use spreadsheets is relatively easy.

The first and last item above help make the strongest case for spreadsheets. The low cost means that smaller schools and poorer students can afford them, and the easy learning curve means they can be introduced into early engineering and even pre-engineering education. Early introduction of spreadsheets would make learning the more advanced tools easier and would give the student valuable skills they can use in all future course work.

Regarding the suitability of spreadsheets for use in a chemical engineering curriculum, Shacham and Cutlip's[1] evaluated several numerical software packages, including Mathematica, MathCad, MatLab, Maple and Excel. Their conclusion regarding Excel was that it could complete eight of the nine benchmark tests but the ninth, which involved several ordinary differential equations could only be completed using very advanced techniques, including external code written in Visual BASIC. They demonstrated that these software packages were indeed very powerful (in several cases the professional versions were required) and that while Excel is very capable, it is not appropriate for all cases.

Two recent books also promote the idea of using spreadsheets in science and engineering courses. In a book entitled "Spreadsheet Tools for Engineers, Excel 2000 Version" [2] the author focuses on engineering analysis as a systematic process for which spreadsheets can help solve the problem, once the problem has been defined and the solution set up properly. He then shows how Excel can be used to solve many of the classic types of engineering problems, such as fitting equations to data, interpolation, solving single and simultaneous equations, and others.

The idea of developing spreadsheet applications for a particular field of study has been explored in the book "Spreadsheet Applications in Chemistry using Microsoft Excel"[3]. The authors of this book note that scientists these days need to be more multi-functional than ever before and literate in the many uses of the computer (plotting, data analysis, modeling, reports, presentations, communications) and that spreadsheets can play a vital role in these activities. In their introduction they note that some teachers and researchers may need a little help and encouragement getting started using spreadsheets and to achieve this they offered a number of chemistry applications.

There are also many examples in the literature where spreadsheets have been used in specific, often ambitions, lessons. Obviously the concept is not new but in this case the goal is to make spreadsheets an integral part of all courses and the product will be a set of modules that can be used in any materials science program.

Designing Modules for Use in Other People's Courses

Primary challenge facing this effort will be gaining the acceptance of other instructors. They already have well established courses and may reluctant to change them to incorporate my ideas. In addition, they might not be that familiar with spreadsheets, would be concerned that exercises are not appropriate or divert too much of the students' attention and energies from the core subject matter. To address these concerns the SAMS projects will:

- Concentrate on the core subjects that are taught in most materials science programs.
- The materials science content of the modules will be developed sufficiently enough that instructors may want to use them as supplements.
- The basic exercises should be similar to those used in many courses. Many will be straight-forward extensions of these by, for instance, asking the student to repeat the calculation for several cases, generate plots for complicated equations, etc.
- Use only spreadsheet exercises that involve a compelling materials science concept. Do not include spreadsheet exercises that are more about spreadsheets than materials science.
- Use spreadsheet exercises that the students will appreciate. Ideally, the student will come away from the course with a set of useful spreadsheets.
- Build in flexibility. Some instructors may wish to use only small parts of SAMS while a few may want to use complete modules.
- Make the materials appropriate for a wide range of spreadsheet skill levels. Provide support for beginners and yet challenge the more experienced.
- Exploit the versatility of spreadsheets. Include exercises and projects that range from simple plots to multi-step modeling of materials phenomena, or importing data files to using spreadsheets to allow students to post and compile data from group experiments.
- Develop exercises that can be used for routine homework assignments, for term projects, and for laboratory experiments.

Format of the Applications and Tools

With the above design criteria in mind, the following three-component approach has been adopted.

Spreadsheet Reference Guide

The reference guide covers the functions and features of spreadsheets that will be employed in the materials science applications. These modules will be essentially condensed versions of the type of printed manual that software developers once included with their software, but designed for the engineering student and instructor. Major topics covered in the reference guides are:

1. Introduction
2. Overview
3. A Tour of the Desktop
4. Writing Formulas
5. Working with Functions
6. Numeric Tools
7. Importing Data
8. Working with Charts and Graphs
9. Printing
10. Working with Form Controls
11. Writing Macros

Spreadsheet Skills Tutorials

These tutorials cover selected spreadsheet skills, procedures and practices that are required when using the materials science applications. These "how to" modules teach spreadsheet programming skills by reviewing the essentials of each topic, offering practical advice, and then using interesting non-engineering exercises to illustrate the lessons. While most of these tutorials cover topics such as entering and formatting numbers, creating tables, and using advanced numerical tools, one tutorial describes how to lay out a new spreadsheet application so that it can be easily debugged and be useful to and readable by other persons. All exercises include detailed instructions on how to complete them, even which menu items to use and buttons to press. These tutorials can be used to help teach basic spreadsheet skills or as a student's companion in case they run into problems with the applications. Major topics covered are:

1. Introduction
2. Exploring the Spreadsheet's Desktop
3. Creating a New Spreadsheet
4. Entering Data
5. Entering Formulas
6. Using Functions
7. Working with Tables and Arrays
8. Importing and Exporting Data
9. Charts and Graphs
10. Using Advanced Numerical Tools
11. Adding Form Controls to Your Project
12. Copying and Pasting to and from Other Applications
13. Final Notes

Materials Science Applications

The materials science applications are a series of modules covering selected materials science topics. Each application module starts with fairly basic materials concepts and simple spreadsheet skills. The first exercise is usually accompanied by a screen shot of the spreadsheet to help the student get started using spreadsheets. As the materials science topic is developed further the exercises become more sophisticated and while they focus on only the immediate topic they draw from the skills and results from the earlier exercises. At the end of the module there are a number of project-scale exercises that bring all previous concepts together by asking the student to analyze data or to develop a fuller model of the topic. The following list of exercises and projects, used in the x-ray radiography module, illustrates this approach.

Spreadsheet Exercises in the X-ray Radiography Module

1. Enter and plot the mass absorption coefficients of selected elements.
2. Calculate and plot the mass absorption coefficients of selected alloys and compounds. (This exercise requires the mass absorption coefficients of the elements.)
3. Calculate and plot the transmitted beam intensity for various thicknesses for various alloys and compounds. (This exercise requires the results from the previous exercise.)
4. Calculate and plot the film density for several materials and for a range of exposures and different films. (This exercise requires the results from the previous exercise.)
5. Estimate the image sharpness characteristics for a specific arrangement of object, source and film.

Spreadsheet Projects in the X-ray Radiography Module

1. Confirm the z and λ-dependence of the mass absorption coefficient. (This exercise involves regression analysis and effective ways of comparing measured and calculated results.)
2. Estimate the mass absorption coefficients of several alloys from knowledge of the thickness of the samples and the density of the exposed film. The data are provided but this can be implemented as a laboratory experiment.
3. Calculate and plot the relative intensity of the transmitted beam for a cylindrical sample.
4. Calculate and plot a slice of a digitized radiographic image of cylindrical steel bar in a copper pipe.
5. Create a spreadsheet that will help one select the proper film, exposure time, and source-to-object and object-to-film distances for any thickness of any material.

In addition to the above reference guides and tutorials, 4-page reference cards have been developed for Quattro Pro and Excel. These will remind the students how to enter data and numbers, create a chart, import data, use common math and engineering functions, etc.

All tutorials and exercises are being developed in Quattro Pro, the author's preferred spreadsheet, and then translated to Excel, practically everyone else's preference. Obviously Excel is the dominate spreadsheet on the market, but a quick Internet search will show that Quattro Pro is also used at many schools.

Format of a Typical Spreadsheet Application

An important aspect of teaching students how to use spreadsheets to solve engineering problems is teaching them how to set out their solution in a logical and readable manner. The format for the spreadsheet exercises, analogous to laboratory report formats, is derived from good programming style and from the type of reports often found in ASTM standards. The sections of the spreadsheet are:

Header	Identify the author, creation and revision date, and file name and a brief description of what the spreadsheet does.
Constants	Physical constants and conversion factors
Parameters	Input section, parameters used with all equations
Body	The main body of the spreadsheet, consisting of the columns and tables of numbers and calculations, output from advanced numerical tools, etc.
Results	Presentation and summary of the essential results, comparison to reference data, etc.

Current Implementations

Three modules are currently being used in materials science courses. The largest course, with an enrollment of 112, is a sophomore-level introductory materials science course. Portions of several spreadsheet modules are being used in the laboratory component of the course. The spreadsheet exercises include:

- A simple assignment designed to introduce the students to spreadsheets and ionic bonding.
- A full laboratory session devoted to modeling ionic bonding in NaCl-type compounds and deriving properties such as elastic moduli, density and melting point.
- Creating bar charts to compare the tensile properties and hardnesses of several alloys.
- Importing time-temperature data and plotting the cooling curves produced in a Bi-Sn equilibrium phase diagram experiment.
- Compiling data from a group experiment dealing with the heat treatment of brass. The data will also be plotted to show the trends in hardness, strength and other properties as a function of annealing temperature.

These exercises are designed to teach several basic spreadsheet skills, how to compile and manage data, to enhance their understanding of the subject, and to write better reports. The students will also be taught how to cut and past charts and tables from their spreadsheet to their wordprocessor.

The other two courses are upper division lecture and laboratory courses on the structure of engineering materials. In the lecture course, students will be using the application module dealing with x-ray radiography. The instructor, Jim Shackelford, will use this module as a supplement to the course's text and will use several of the spreadsheet exercises as homework assignments.

The third course is the laboratory companion to the above course and focuses on x-ray diffraction (crystal structure) and optical microscopy/metallography (microstructure) but includes demonstrations of x-ray radiography and electron microscopy. Portions of the x-ray diffraction module will be used in this course. The students will use spreadsheets in their diffraction experiments to:

- Calculate the peak positions for any unit cell, any plane, and any x-ray source and for the source's $k_{\alpha1}$, $k_{\alpha2}$, k_{β} characteristic radiation as well as for W-L_{α}. This "diffraction calculator" will be useful in other assignments.
- Calculate the "5 fingers" region of the diffraction pattern of quartz. The Cauchy profile will be used, and the calculated peaks will be compared to the measured peaks.
- Calculate and plot the x-ray intensity ratio I/I_{pure} (I=intensity of the mixture, I_{pure}=intensity for the pure phase) for any phase mixture using the matrix-flushing method. Data collected during the experiment will be added to this graph.
- Analyze results from crystallite size measurements performed on nano-crystalline anatase (TiO_2) or aluminum oxide. Results form both the Scherrer and Warren-Averbach methods are employed and are combined to obtain a single log-normal size distribution.
- Calculate the peak positions for a piezoelectric material for different field strengths. Use a Windows-style slider control to change the voltage. Compare the calculations to the measured diffraction profile.

These exercises will help the students understand many aspects of x-ray diffraction and will produce data and figures that they will use in their reports. They will also be used to help prepare for the experiments.

Assessment

Assessment tools that will help measure the effectiveness of our initial implementations have been developed. The principal tool is a survey, taken at the beginning and end of the quarter, that will help answer questions on the students' initial and final:

- Experience and level of expertise with spreadsheets
- Experience and level of expertise with other software
- Experience and level of expertise with computers in general
- Experience in and ability to use spreadsheets to solve engineering problems
- Degree to which the spreadsheet assignments enhanced the learning of materials science
- How much extra effort did solving engineering problems using spreadsheets involve
- Likelihood that the students will use spreadsheets in future courses

At the time of this writing the final surveys are not in.

The other assessment tool will be evaluation of the student's class work. As part of the normal grading of students' work instructors and teaching assistants will note each student's ability to complete the spreadsheet part of the assignment as well as the quality of the work.

High School and Community College Trials

Two high school science instructors are collaborating on this project. Portions of several applications modules will be repackaged for high school science courses so that the students will get a chance to learn a little materials science and spreadsheet programming. The class that uses the radiography module will be able to send their samples to the author to have radiographs taken. Students who use the x-ray diffraction module will be given data from our diffractometer and may be able to operate our diffractometer remotely, via the Internet, as part of an outreach program that features our instrumentation.

The author will be teaching an introductory materials science course at a local community college next year. The ionic bonding module and portions of other modules will be used in this course.

Conclusions

SAMS is a work in progress that is in its first year in the classroom. The students, teaching assistants, the author and another instructor are using the modules and are already providing valuable feedback. Formal assessment tools will be able to provide additional information as to the educational value of this effort. High school and community college trials are planned for next year.

The spreadsheets tutorials, reference cards and several materials science applications modules have been completed while the spreadsheets reference guide and a number of other applications modules are in development.

Samples of the assignments, modules, reference cards and other materials will be available on the web at www.matsci.ucdavis.edu/meier/SAMS.

Acknowledgments

The author would like to acknowledge the support of the National Science Foundation's Course, Curriculum and Laboratory Improvement program (Division of Undergraduate Education) for supporting this work through grant number 0127591.

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Biographical Information

Michael L. Meier received his B.S. in Materials Engineering from North Carolina State University in 1979 and his M.S. (1986) and Ph.D. (1991) in Materials Science and Engineering from the University of California, Davis. After a two-year post-doctoral research at the Universität Erlangen-Nürnberg in Erlangen, Germany he returned to UC Davis where he is now the director of Materials Science Central Facilities, a materials characterization facility, and is very active in developing the laboratory teaching program.

Appendix: Summary of Selected Spreadsheet Applications Modules

This appendix contains brief descriptions of the applications modules that are currently nearing completion. Each module consists of descriptions of the materials phenomenon along with spreadsheet exercises and projects.

Ionic Bonding

This tutorial incorporates the concepts of crystal structure, coordination number, lattice energy, equilibrium atomic spacing as well as the properties that are directly related to the nature of the ionic bond – elastic constants, density, melting point and theoretical strength. The tutorial starts with simple calculations of atomic spacing, followed by minimum lattice energy (bar graphs are used to illustrate the results) and eventually a spreadsheet project that puts it all together.

Introduction to Crystallography

This tutorial starts with a number of simple calculations that deal with the sizes and numbers of individual atoms. Next comes a series of exercises that start with the concept of coordination numbers and end with the essentials of crystal systems and Bravias lattices. Using the most generalized versions of the equations, the student will build a useful spreadsheet that calculates the volume of any unit cell, any d-spacing, angle or distance between atoms, etc. In the more advanced exercises matrix versions of these calculations will be performed. In another project the student will be able to input the lattice parameters, atoms positions and types of atoms for any structure and will calculate the atomic packing factor, density and other properties. The final project will show the student how to calculate an image of any unit cell – scaled, rotated and projected onto the 2D plane of a computer's monitor or printout. This 3-matrix spreadsheet employs a simple macro and, optionally, form controls that make the spreadsheet fun to use.

X-ray Powder Diffraction

This tutorial starts with simple calculations dealing with the operating characteristics of the x-ray tube. Next are a series of exercises involving Bragg's law that provide the student with a handy tool that can be used in other exercises. This is followed by calculations of the structure factor and the intensity of the diffracted beam. This topic leads into an exploration of the use of x-ray diffraction for quantitative analysis. The final exercises and projects include calculating the "5 fingers" region of the diffraction pattern for quartz and comparing these to data that is imported and plotted in the same graph, calculating the peak shifts due to biasing of a piezoelectric material and comparing the calculations to experimental data, and similar treatments of peak broadening due to crystallite size and peak shifts due to residual stress. The final exercise involves estimating the systematic errors in a diffractometer and using it to determine which adjustments are needed to improve the alignment of the instrument.

X-ray Radiography

This tutorial consists of a series of spreadsheet exercises that start with simple calculations involving the mass absorption coefficients followed immediately by straight-forward applications of Beer's law. Following these are discussions of and exercises that demonstrate the concepts of image sharpness, film characteristics and exposure parameters. Finally there are a number of project-level exercises such as determining the mass absorption coefficient from radiographs, verifying the z^3 and λ^3 dependence of the mass absorption coefficient and calculating a digitized radiographic image.