

Discovery Learning Tools in Materials Science: Concept Visualization with Dynamic and Interactive Spreadsheets

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Abstract

Many materials science concepts can be developed into animated, interactive spreadsheets to create engaging discovery learning tools. These Excel spreadsheets do not require programming expertise. Learning how to create and use these didactically useful spreadsheets is simple and new examples can be quickly created by instructors.

Introduction

Are the bond lengths in a metal or an ionic compound constant? How are bond lengths measured? These are examples of two rather simple questions that students can discover answers for themselves via dynamic and interactive spreadsheets or Excelets (Java-less applet-like). The MatSci Excelets collection [1] of over thirty dynamic and interactive spreadsheets offers instructors in introductory materials science or other courses such as general chemistry or physics, a way to create an engaging pedagogy in the classroom, whether for lecture, laboratory, or out-of-class assignments. The spreadsheets are all computationally-based (using formulae, not programming) and easily modified by instructors just being introduced to the technology and even by students interested in exploratory learning. This collection complements the Spreadsheet Applications for Materials Science, SAMS, by Meier [2]. This paper describes the pedagogical use of some of the MatSci Excelets in the classroom and student feedback.

The Solid State – A Discovery-based Lecture-Discussion

Here are a series of examples that could be presented in lectures, but allow students to discover the answers guided by the instructor posing questions. The first example, shown in Figure 1,

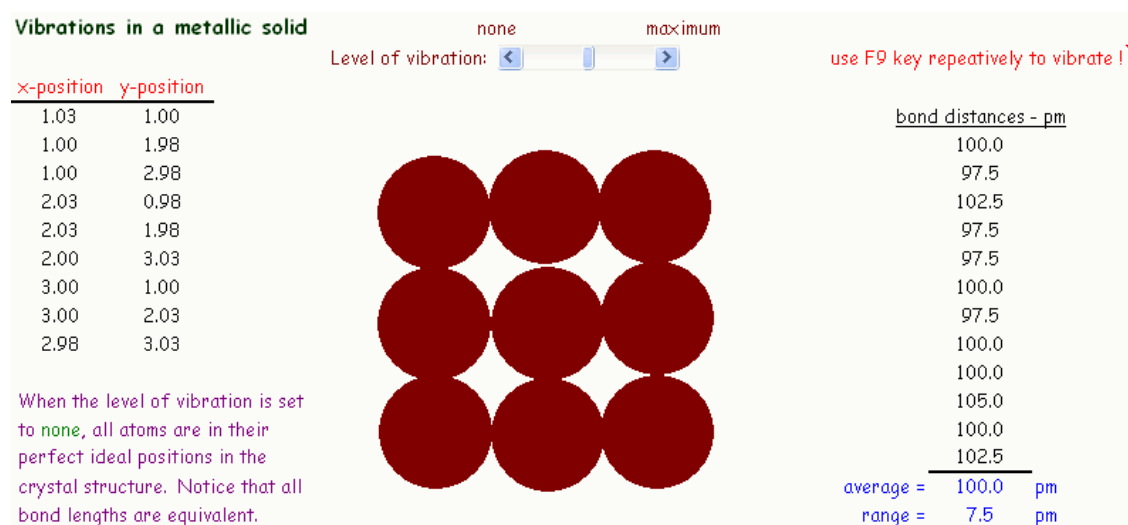


Figure 1. Vibrations in a metallic solid

deals with the question of whether bond lengths in a metal are constant. It starts with all the bond lengths at a distance of 100 pm. Instructors can create vibration at different levels using the scroll bar and hitting the F9 key multiple times, animating the atoms. By increasing the level of vibration, mimicking a temperature increase, the variation in bond lengths increases. This is a simple but nevertheless, a very powerful visualization of a microscopic (atomic) process for novice learners.

Thermal expansion is another important concept in materials. This seemingly simple macroscopic concept can be confusing for students, but some of these issues can be addressed using Excelets. For example, as shown in Figure 2, what is the difference between an isotropic and anisotropic material? What happens if the temperature increases? Here an instructor increases the temperature to cause thermal expansion and students view how the material behaves. They can then deduce the difference between isotropic and anisotropic expansion, as opposed to an instructor just flat out telling them.

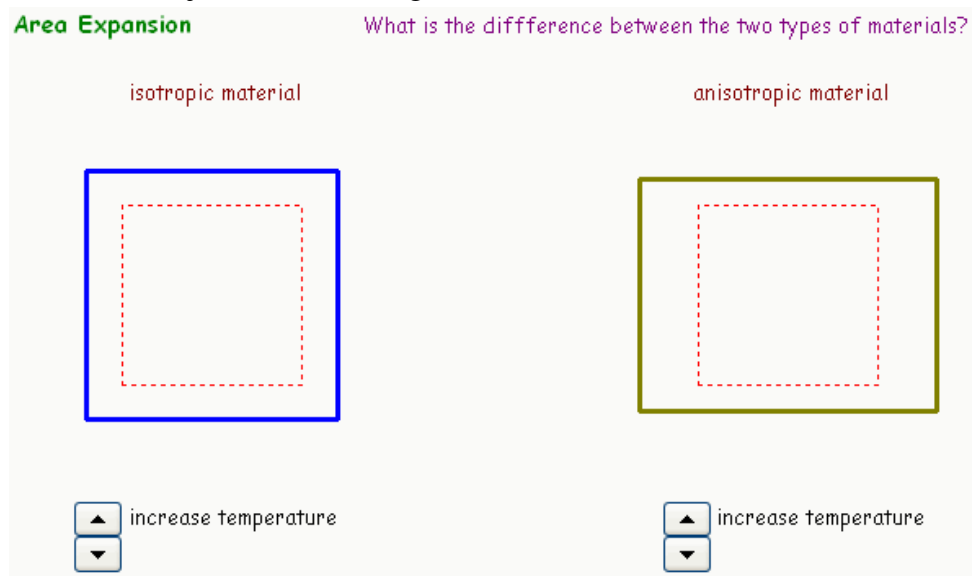


Figure 2. Part of Thermal Expansion Excelet

Now consider crystal structures. How does the radius of the metal influence the packing in a simple cubic lattice? How is the radius related to the lattice parameter? Here (Figure 3) via an animated two-dimensional graphic and the use of a scroll bar in Excel, these two questions can be addressed easily in a visual fashion. Then in the same spreadsheet the more complicated face-centered and body-centered lattices and on another spreadsheet hexagonal close packing can be explored. The use of two-dimensional graphics alongside three-dimensional ones gives the novice learner a better chance to develop an understanding. The lattice parameter obtained from x-ray measurements can easily be related and can be explored using the X-rays and the Crystalline State of Matter Excelet (Bragg's Law) too. All of this is accomplished by a mode of questioning that drives student discovery.

After examining metals, exploring the alkali halides, all ionic compounds with sodium chloride structures, allows ionic radii, lattice energy, and the Born-Haber cycle to be covered. The variation of ionic radius can be examined and related to the face-centered cubic crystal

Simple Cubic Lattice: How is the Lattice Parameter related to Metal Radius

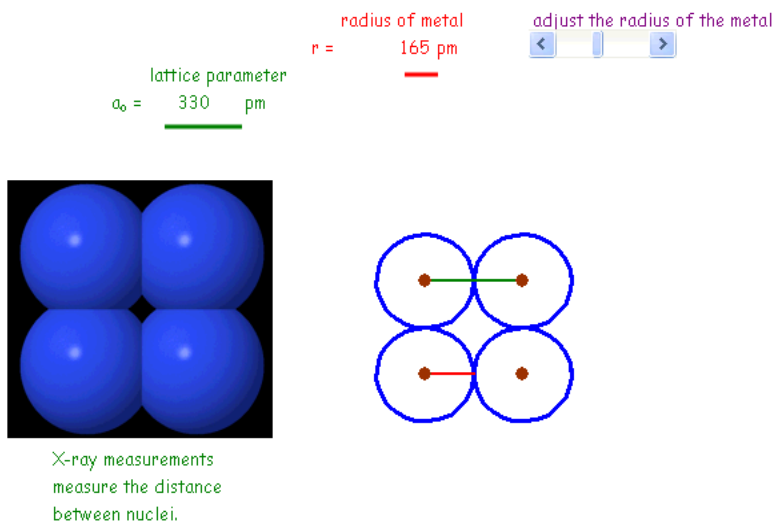


Figure 3. Simple Cubic Lattice

structure. Now the trends of the lattice parameter (a typical crystallographic measurement) as a function of anion size can be explored graphically (Figure 4) using the spreadsheet to handle a small database and allowing student control (check boxes on the right of the screenshot) of the data on the graph. Students can discover how the ionic radii influence the trends as both cation and anion sizes vary. More of the database aspects can be found in Exploring the Periodic Table: Metal-Nonmetal Comparison.

Exploring the Lattice Parameters of the Alkali Halides

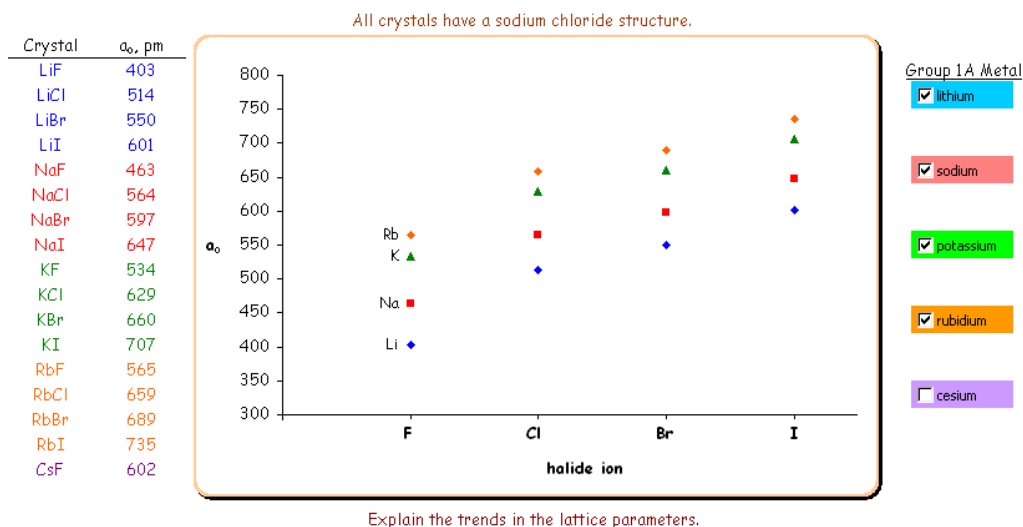


Figure 4. Exploring the Lattice Parameters

The Bonding in Sodium Chloride Crystals Excellet demonstrates the use of graphing the calculation of the attractive and repulsive energies for sodium chloride (Figure 5). Using a tracer line to find the minimum energy on the net energy curve, which is the sum of the attractive and

repulsive energies, students can discover the radius (sum of cation and anion) that minimizes energy. This is an excellent example of camouflaging the mathematics (essentially the Lennard-Jones potential calculation) to introduce the concept and then the instructor can decide how far to bring in the mathematics.

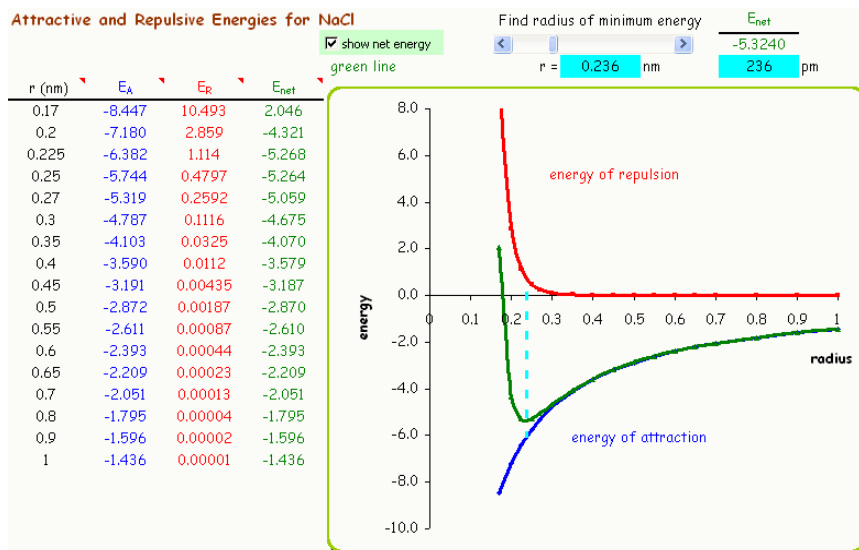


Figure 5. Bonding in sodium chloride structure

Out-of-class Projects

Many of the MatSci Excelets contain assessment questions using data that expand on concepts covered in the particular Excelet as seen in Figure 6. Here we get students to use the spreadsheet to handle, graph, and analyze data plus construct a mathematical model in many cases. This is a very important skill for scientists.

Hexagonal Close Packing for Elements

Element	X-ray Measurements, pm				Radius of element, pm	
	a_c	c_c	c_c/a_c	% error	r from a_c	r from c_c
Be	228.6	358.4				
Cd	297.89	561.69				
Co	250.7	407				
Dy	359.04	564.77				
Er	355.89	558.76				
Gd	363.61	578.28				
Hf	319.47	505.13				
Ho	357.74	561.6				
Lu	350.32	555.11				
Mg	320.95	521.07				
Os	273.54	431.93				
Re	276	445.8				
Ru	270.59	428.18				
Sc	330.91	527.35				
Tc	273.5	438.8				
Tb	360.11	569.38				
Tl	345.67	552.5				
Tm	353.76	555.48				
Ti	295.12	468.45				
Y	364.75	573.08				
Zn	266.5	494.7				
Zr	323.13	514.79				

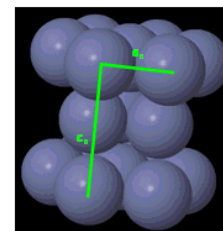
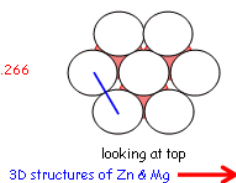
Data from Cullity (1978), *Elements of X-ray Diffraction*, 2nd ed., Addison-Wesley Publ.

For HCP:

$c_c/a_c = 1.633$ for perfect spheres

$r = a_c/2$

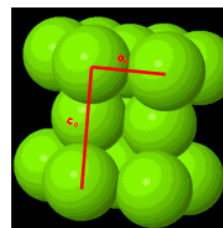
$r = c_c/3.266$



Zn HCP

TASK:

1. Plot a graph of c_c as a function of a_c . What should the slope of the line represent? Can you explain the difference.
2. Calculate the c_c/a_c in the column.
3. Examine the % error compared to the perfect spheres value. (This will calculate when the ratio is done.)
4. Calculate the radius of the element using the formulas given above.



Mg HCP

Sinex 2009

Figure 6. Assessment Questions

At present, there are 32 spreadsheets in the collection. The ones that involve crystal structures also have associated web pages with Chime structures (interactive 3D structures). Many of the topics such as Brinell hardness, the Avrami equation, and three-point load test for fracturing ceramics are covered in typical sophomore level textbooks for materials science such as Callister [3]. All of the MatSci Excelets are freely available for download at http://academic.pgcc.edu/~ssinex/excelets/matsci_excelets.htm.

Student Feedback

The interactive nature of Excelets was favored because it allowed students to play and experiment (18%), discover on their own (18%), think (7%) or all three of these (56%). In general, the visual aspects were appreciated and students felt it enhanced their understanding of concepts. Table 1 below summarizes four questions from a survey of 28 students in general chemistry in spring 2009.

Table 1. Student Feedback

Which do you prefer:	
static graphs in textbook	7% (2)
dynamic graphs in Excel	89% (25)
both	4% (1)
Using Excelets does not require that you be familiar with Excel.	
most definitely	25% (7)
I think so	36% (10)
just barely	32% (9)
not at all	7% (2)
don't know	
Excelets offer a more visual experience with graphs instead of using just the mathematical equations.	
most definitely	75% (21)
I think so	14% (4)
just barely	14% (4)
not at all	
don't know	
Excelets make it easier to grasp or learn a concept.	
most definitely	43% (12)
I think so	54% (15)
just barely	4% (1)
not at all	
don't know	

Students were asked to rank how Excelets were used in the class. The results are listed in order from most (1 of 5) to least (5 of 5) favorable: group activity done in class (1.8) > lecture using Excelet (1.9) > group activity done out of class (3.2) > individual project (3.3) > lecture with no Excelet (4.0). This reflects how the students wanted the instructor to use the Excelets.

Constructing Interactive Excel Spreadsheets or Excelets

The wherewithal for producing Excelets can be found at the Developer's Guide to Excelets [4], which includes a tutorial, illustrated instructions, and many more examples. We strongly encourage others to take the interactive features tour to see what can be done in Excel. The forms toolbar provides a variety of features (spinners, scroll bars, checkboxes, etc.) that are

easy to use, and when combined with logical functions, lookup tables, conditional formatting, and a number of simple tricks provides a wealth of interactivity and dynamic display. The use of the forms toolbar allows Excelets to function on both PC and Mac platforms. All of this is done using computations (a.k.a. - formulas and available functions) in the cells. The use of comment boxes adds explanation, hints, and answers for students as well. One should always look under the graphs, as many of the tricks, such as turning lines on graphs on and off or tracer points are explained there. The support materials for mathematical modeling are also given. This includes modeling and simulations with cookies, introduction to linear regression, goodness of fit for linear models, interpolation and extrapolation, and non-linear models as well.

Many of the Excelets will be completely functional in Open Office Calc, which is open source (free) software available at <http://www.openoffice.org>. Calc functions very much like Excel. One may have to clean up the files for cosmetic reasons. Check boxes will become colorless and the words true and false which are under them need to be hidden (turn the font white). If option buttons are in the Excelet, they have a slightly different syntax in Calc and the formula must be amended in Calc for the spreadsheet to function.

Some Final Thoughts

Excelets provide a “click-and-think” mode of learning for students in a large variety of topics in introductory materials science and general chemistry using an off-the-shelf software package. Even in a lecture environment, the “chalk-and-talk” mode can be minimized by using Excelets. Classical lectures can evolve into a more discussion-based format with students discovering concepts through predict-test-analyze (the “what if” scenarios) using technology as well. Student engagement via out-of-class projects or follow-up activities in the laboratory is increased considerably. Excelets also provide another great way to add interactivity to instruction in online classes.

Excelets address the visual (various types of graphs, use of conditional formatting) and kinesthetic (interactive features) learning styles. With the mode of questioning, they drive students toward deeper learning using an engaging pedagogy.

This work is supported by the Howard/Hopkins/PGCC Partnership for Research and Education in Materials (PREM), funded by NSF Grant No. DMR-0611595.

References

1. The MatSci Excelets collection is freely available for download at http://academic.pgcc.edu/~ssinex/excelets/matsci_excelets.htm (accessed January 2010).
2. Meier, M.L. (2003) Spreadsheet Applications for Materials Science, Proceedings of the 2003 American Society for Engineering education Annual Conference. Collection of spreadsheets available at <http://www.kstreetstudio.com/sams/index.htm> (accessed January 2010).
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4. Sinex, S.A. (2009) Developer's Guide to Excelets: Dynamic and Interactive Visualization with "Javaless" Applets or Interactive Excel Spreadsheets, <http://academic.pgcc.edu/~ssinex/excelets> (accessed January 2010).