A Window on the Solid State

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Abstract

A Window on the Solid State helps students understand and instructors present the structural features of solids. Parts I and II were published previously by *JCE Software* (*1*) and Macintosh versions of Parts I and II are also available (*2*). Parts I and II have been updated to include improvements in art and minor changes in logic. Parts III and IV expand the collection to include the structures of simple ionic solids using the visual effects available in an interactive computer medium. The package provides a tour of the structures commonly used to introduce features of the solid state.

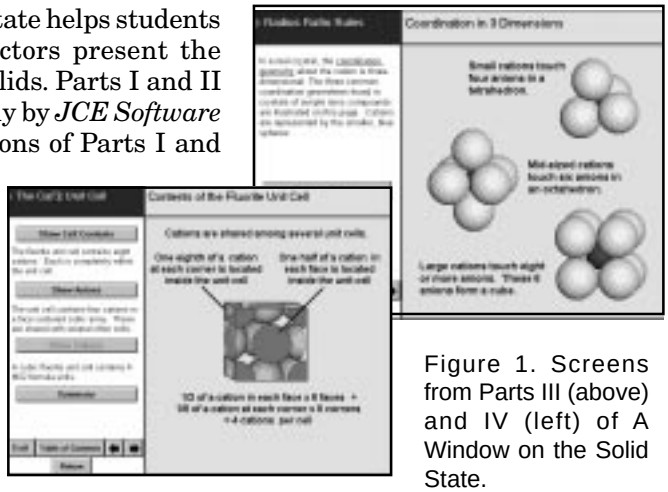

Figure 1. Screens from Parts III (above) and IV (left) of A Window on the Solid State.

Part I: Structures of Metals introduces the four basic structural types found in metals: the hexagonal closest-packed structure, the cubic closest-packed structure, the body-centered cubic structure, and the simple cubic structure. These structures are introduced as stacks of close-packed planes of metal atoms in the hexagonal and cubic closest-packed structures, and stacks of less efficiently packed planes in the other two structures. In addition, Part I also introduces Laves's principle, coordination number, stacking of planes, efficiency of packing, and how to draw the structures using two-dimensional representations. The pseudo-animation used is particularly effective in distinguishing between hexagonal close packing and cubic close packing.

Part II: Unit Cells of Metals addresses the use of a unit cell to describe a two-dimensional structure, then extends the concept to describing the structures of metals using the four basic unit cells of the metals: the simple cubic, body-centered cubic, face-centered cubic, and hexagonal cells. The relationships between the radii of metal atoms in the cubic structures and the cell dimensions are developed. Students are also introduced to counting the number of atoms in a unit cell. Pseudo-animation is particularly effective in illustrating the fractions of atoms that lie in the various unit cells.

Part III: Structures of Ionic Solids describes simple ionic structures in terms of the packing of positive ions in holes in arrays of negative ions. In the course of the presentation, the features common to the packing of ions in binary ionic solids are described. Animation is used to introduce the radius ratio rule (smaller ions "rattle" in larger holes and larger ions do not fit into smaller holes). Tetrahedral and octahedral holes are highlighted in closest-packed arrays of anions. Then the coordinating anions are isolated and rotated to show their geometry.

Cubic holes appear in simple cubic arrays of anions. Finally, the CsCl, CaF_2, NaCl, TiO_2, and cubic ZnS structures are built layer by layer using animation to show alternating layers of anions and cations along with discussion of the type and fraction of holes occupied.

Part IV: Unit Cells of Ionic Solids discusses the unit cells of five common ionic structures: the CsCl, CaF_2, NaCl, TiO_2, and cubic ZnS structures. A pseudo-animation is particularly effective in illustrating the relation of the unit cell to the extended structures described in Part III. The locations of ions of each cell are illustrated with space-filling and ball-and-stick models. When appropriate, the relationship of alternate unit cells is described. Coordination numbers of cations and anions are highlighted and students are shown how to determine the numbers of ions in a unit cell. Pseudo-animation is particularly effective in illustrating the fractions of atoms that lie in the various unit cells. The relationships between the ionic radii and cell dimensions are developed.

All four parts of A Window on the Solid State can be used by students in individual or group tutorial settings. Students can work through the material at their own pace. Each part requires students to identify or predict structural features and includes pop-up boxes that confirm or correct choices. Hotwords are used to link ideas and provide definitions. Parts I and II also have versions optimized for classroom presentation.

Instructor Notes

An understanding of the extended structures of solids is as fundamental to understanding the behavior of matter as is an understanding of the structures of molecules. The bulk of the substances that we interact with every day are solids with extended structures. For example, metals have played a role in human society since the beginning of recorded history. Ionic compounds are found in rocks, minerals, and the solids of which our bodies and buildings are composed. Electronic devices depend on the properties of solids with extended structures.

The presentation of the structural features of solids with extended structures challenges even the experienced instructor. There is no simple way to introduce these concepts. Models are clumsy, and two-dimensional drawings take time to produce and do not always get the job done. One technique that has proved effective involves the use of lap-dissolve slides with a mix of photographs of extended models, photographs of unit cell models, and graphics (*3*). Unfortunately, these slides are not generally available and are not easy to distribute or use. A Window on the Solid State provides similar information but in a format that is easy to use and has been tailored to both lecture and tutorial presentations.

Two versions of Parts I and II are provided. A student tutorial is provided so that a student can work through the material at her/his own pace. This version requires students to identify or predict structural features and includes pop-up boxes that confirm or correct choices. Hot words are used to link ideas and provide definitions. A version designed to be used in lecture demonstration contains all graphics and summary statements from the tutorial program. Parts III and IV are supplied in single versions equally suited for use as student tutorials or lecture demonstrations.

A Window on the Solid State is intended to supplement an introductory presentation, either at the general chemistry level or at the first introduction of the structures of metals at the undergraduate level. These programs emphasize the qualitative and geometric aspects of the structures presented. Although no numerical calculations are requested in these programs, students will be well prepared to tackle quantitative exercises by the information presented.

The Student Assignment section of this manual contains example questions that students should be able to answer by using the programs. Several of the questions make use of graphics taken directly from the programs. You can design similar questions. First copy the screen by pressing the **print screen** key. Then paste the graphic into a word processor. You can edit the pictures by pasting into any graphics (drawing/painting) application.

Acknowledgments

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Citations

1. Robinson, W. R. A Window on the Solid State. *J. Chem. Educ. Software* **1994,** *2D No. 2*.

2. Robinson, W. R.; Sari, C. P. A Window on the Solid State for Macintosh. *J. Chem. Educ. Software* **1994,** *6C No. 2*.

3. Bodner, G. M.; Greenbowe, T.; Robinson, W. R. *J. Chem. Educ.* **1980**, *75*, 555.