INVESTIGATION 2
Notes for the Instructor

PURPOSE

To have students begin to understand that the behavior of the wire that they observed in Investigation 1 can ultimately be explained in terms of the transformations that occur between two subtly different structures (phases) of the NiTi alloy from which the wires were made. To have students build or view a number of structures and elucidate unit cells within them. To relate unit cell characteristics to properties like density.

METHOD

Since an understanding of the features of the shape-memory metal cycle is dependent upon the relationship between the structures of the high- and low-temperature phases of this material, it is suggested that these structures be discussed at an early stage of this unit. This may be accomplished in one of two ways: 1) make an overhead transparency of the figure below; or 2) better yet, have some or all students build models of both the austenite (high temperature) and martensite (low temperature) structures using the Solid State Model Kit* that the entire class may view.

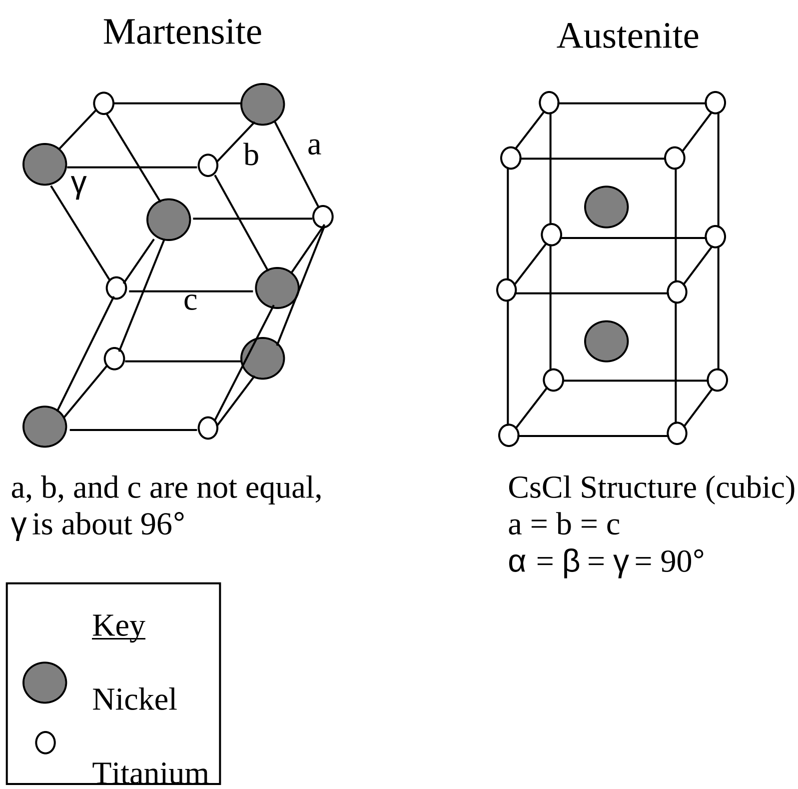
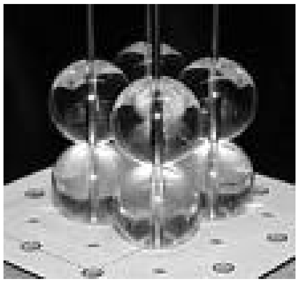


Figure 1. Unit cell of NiTi in the martensite and austenite phases.

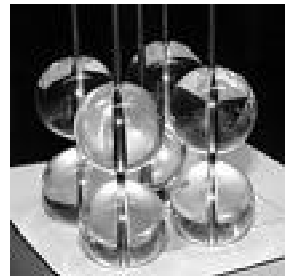
*Available from the Institute for Chemical Education (ICE), University of Wisconsin-Madison Department of Chemistry, 1101 University Avenue, WI 53706-1396, Phone: 608/262-3033, 800/991-5534, Fax: 608/265-8094, ICE@chem.wisc.edu, http://ice.chem.wisc.edu/. Less complicated models may also be assembled from styrofoam spheres (or oranges) appropriately cut.

Crystalline materials like NiTi have a patterned arrangement of atoms that extend in all directions to the surfaces of the sample. A useful way of describing this pattern is to consider a three-dimensional cube, which, when reproduced and moved along each of its edges by a length equal to that of the edge, generates the entire structure of atoms in the crystal. Such a cube is called a unit cell and it provides a template for the atoms and the empty spaces between the atoms in the structure.*



Simple Cubic

Face Centered Cubic



Body Centered Cubic

Figure 2. Examples of unit cell structures.

*See Appendix A for a more detailed discussion of unit cells.

Of course, not all crystals are in the form of cubes, which are a special kind of parallelepiped having exclusively 90^o angles and equal edge lengths, but this approach will allow students to better understand what unit cells are and some of their features. Make sure that students understand the concept of coordination numbers from Part 1 of the Investigation. **Size does not make a difference if all the spheres are the same size. If the spheres are of different sizes, as the size of the central sphere increases so can the coordination number. In the austenite and martensite stuctures the nearest neighbors would be spheres of the other color.** Cereal boxes or matchboxes may be used to show other kinds of non-cubic 3-D unit cells.

MATERIALS

Either overheads of Figures 1 and 2 above or several Solid-State Model Kits from ICE.

PROCEDURE

PART 1: General Considerations.

Determine how many larger spheres you can pack around a marked sphere in the same plane. It may be easier to hold the spheres in the palm of your hand while doing this. If all the spheres are the same size does the coordination number depend on size? What if the central sphere is smaller? Larger ? Check your predictions. **Note: Students may find a chart helpful in organizing the data for this part.**

PART 2: This part of the investigation requires that teams work together, using the Solid State Model Kits or following alternate procedures outlined by your instructor. Each team will build one of the following structures. All teams will then compare and contrast their structures and together answer questions.

Team A: Following the instructions in the kit, assemble the Simple Cubic Structure.
Team B: Following the instructions in the kit, assemble the Body Centered Cubic Structure.
Team C: Following the instructions in the kit, assemble the CsCl Structure with the Cl atoms at the corners.

Team D: Following the instructions in the kit, assemble the CsCl Structure with the Cs atoms at the corners.
Team E: Following the instructions in the kit, assemble the Austenite Structure.
Team F: Following the instructions in the kit, assemble the Martensite Structure.

ANSWERS TO FOLLOW-UP QUESTIONS

1. For each structure complete the table below, indicating HOW MANY SPHERES LIEWITH THEIR CENTERS AT THE ________________OF THE UNIT CELL.

Structure	Corners	Edges	Faces	Inside
A	**8**	**0**	**0**	**0**
B	**8**	**0**	**0**	**1**
C	**8**	**0**	**0**	**1**
D	**8**	**0**	**0**	**1**
E	**8**	**0**	**6**	**0**
F	**8**	**0**	**6**	**0**

2. With how many other unit cells are the spheres at the ___________of the cell shared?

a) corners___**7**___cells b) edges___**3**___cells c) faces___**1**___cells

3. What fraction of each sphere lying with their center at the ____is part of that cell?

a) corner __**1/8**__ b) edge __**1/4**__ c) face __**1/2**__

4. For each structure complete the table below, indicating HOW MANY TOTAL SPHERES OCCUPY EACH SITE.

Structure	Corners	Edges	Faces	Inside	Total in Cell
A	**1**	**0**	**0**	**0**	**1**
B	**1**	**0**	**0**	**1**	**2**
C	**1**	**0**	**0**	**1**	**2**
D	**1**	**0**	**0**	**1**	**2**
E	**1**	**0**	**3**	**0**	**4**
F	**1**	**0**	**1**	**2**	**4**

5. Compare the models of austenite and martensite.

a) What packing arrangement is used in the austenite structure?

Simple cubic with respect to a given atom.

b) How is the austenite structure altered to yield the martensite structure?

It is distorted; some 90° angles are lost.

c) Compare the number of spheres per unit cell for each structure. How does the density of martensite compare to that of austenite?

Based on the number of atoms per cell; densities are the same. Packing efficiency, however, makes the martensite marginally denser.

d) From what you have learned about these structures, which do you think would be the more flexible low-temperature phase of the wire in Investigation 1? Explain.

The explanations to date have been over-simplified. Students will have a difficult time adequately answering this question and a class discussion would be appropriate in trying to explain this answer. Ultimately, the answer lies in the fact that during the transformation from austenite to martensite there are 24 different ways this may be carried out. This leads to 24 different "variants" within the martensite phase and the ability to re-orient these variants leads to mechanical flexibility. See Appendix B for examples of variants.