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Laboratory Experiment

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Using Latex Balls and Acrylic Resin Plates To Investigate the Stacking Arrangement and Packing Efficiency of Metal Crystals

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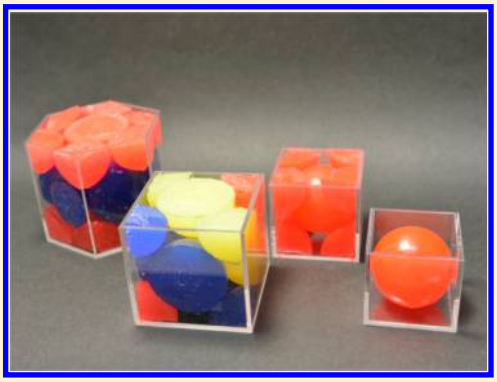
Supporting Information

ABSTRACT: A high-school third-year or undergraduate first-semester general chemistry laboratory experiment introducing simple-cubic, face-centered cubic, body-centered cubic, and hexagonal closest packing unit cells is presented. Latex balls and acrylic resin plates are employed to make each atomic arrangement. The volume of the vacant space in each cell is measured by weighing water poured into the unit cell model, and the packing efficiency of each unit is obtained from the volume of vacant space. The observed values are compared with the theoretical calculations. Students can easily understand experimentally and theoretically that the packing efficiency of the face-centered cubic is the same as that of the hexagonal closest packing and significantly greater than that of the body-centered cubic. Moreover, they can understand the number of the neighboring atoms for any atom (coordination number) in each cell.



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It is well-known that most metallic elements crystallize in face-centered cubic, hexagonal closest packing, or body-centered cubic lattices at room temperature (see Table 1, Supporting Information).[1] The reason such lattice structures are favorable is explained by the packing efficiency of the structures. It seems interesting for students to examine the packing efficiencies of various types of lattice structures experimentally and theoretically. The crystal lattice models in classroom demonstrations have been proposed.[2−10] Commercial display models are also available through companies such as Carolina Biological Supply Company and Indigo Instruments in the United States and Maruzen Company and Kenis Co. Ltd. in Japan.[11] Although these models are very convenient to show the crystalline lattice in the classroom, it is difficult to understand the concepts of the unit cell, atomic arrangement, and coordination number of atoms using the space-filling-type models; on the other hand, the concepts of closest packing and packing efficiency in the lattice structures are hard to understand using the ball-and-stick type models.

A new laboratory experiment is presented that emphasizes not only the packing arrangement and the packing efficiency, but also the number of atoms and the coordination number of simple cubic, face-centered cubic, body-centered cubic, and hexagonal closest-packing lattices using latex balls and acrylic resin plates. A merit to using the latex ball and transparent acrylic plate is that it is easy to understand how many balls and which portion of the balls are included in a unit cell because students cut the balls to add them to the transparent unit cell box. The latex spherical balls of various colors and sizes known as "Super Balls" are very cheap and easily cut with a knife, as shown in Figure 1.

Figure 1. A latex ball is cut with a knife. It is necessary to draw a circle on the surface of the ball before cutting.

The 36 mm balls are easier for handling than those of other sizes. The transparent acrylic resin plates with a thickness of 2 mm are stuck together with an adhesive to make the unit cells. It is necessary for the acrylic resin unit cell to hold water. The structures in the unit cells of simple cubic, face-centered cubic, body-centered cubic, and the hexagonal closest packing are made using the colored balls. Each unit cell structure is made with the parts of balls and is inserted in the acrylic resin unit cell. The number of balls and the packing arrangement in a unit cell can be easily understood because the unit cell wall is transparent. Water is poured into each unit cell, and the vacant space in the void of the balls is calculated from the volume of water added to the void. The packing efficiency of each lattice is easily obtained from the ratio of the volume of water in the void to the whole volume of the unit cell. Then the experimental value is compared with the corresponding one obtained by the

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theoretical calculation. Students can easily understand the packing arrangement, the number of atoms in a unit cell, and the packing efficiency after the experiment.

EXPERIMENTAL PROCEDURE

Preliminary Experiment of Simple Cubic Lattice

Spherical balls and acrylic resin plates were purchased from SankeiGom Co. Ltd. and Sakura-Jushi Co. Ltd., respectively.[12] For the preliminary experiment, a simple cubic lattice structure in Figure 2, panel a was made. All the balls (atoms) are aligned

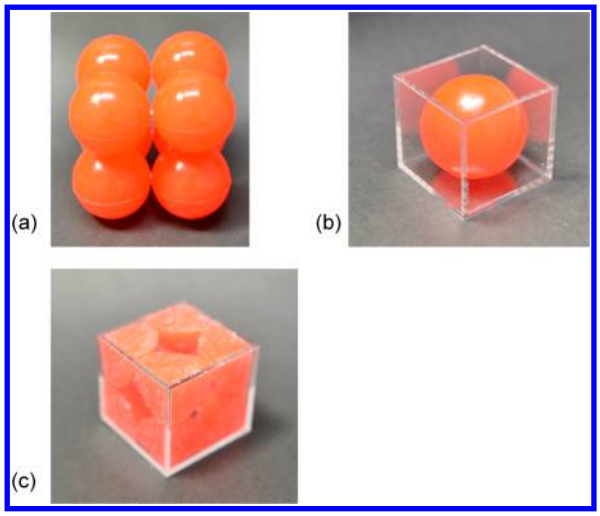

Figure 2. (a) Simple cubic lattice structure and its unit cell (b) with a ball in the cell and (c) with the origin at the center of the ball.

linearly along the three rectangular axes. An open-topped cubic box with an inside length of 36 mm is made, and a ball is inserted in the box as shown in Figure 2, panel b. Because the origin of the unit cell is usually taken at a center of atom, it is necessary to slide the origin of the box at the center of a ball, which is shown in Figure 2, panel c. This means that all eight corners of the box are occupied by one-eighth of a ball.

To estimate the volume of the vacant space in the cell, the weights of the box are measured at the following four conditions: the vacant box, M_1; the box full of water, M_2; the box with a ball, M_3; and the box with a ball and full of water, M_4. Assuming the density of water is 1.0 g cm^{-3}, the packing efficiency, PE, is obtained as follows:

$$PE\ (\%) = 100\left(1 - \frac{M_4 - M_3}{M_2 - M_1}\right) \quad (1)$$

To examine whether the packing efficiency is changed when the origin of the unit cell is shifted in the lattice structure, the weights of M_3 and M_4 of the model in Figure 2, panel c are measured. It is made clear that the M_3 and M_4 values in Figure 2, panel c are the same as the corresponding ones in Figure 2, panel b. Instructions on how to make the models in Figure 2 and the models shown in the following sections are explained in detail in the Supporting Information.

Stacking Models of Two Closest Packings

A hexagonally packed layer as shown in Figure 3, panel a. There are two types of voids between the three balls, A and B, if a three-fold rotation axis passing through a central ball is considered. To make the hexagonal closest packing (hcp), the second layer with blue balls is placed on the first layer, with

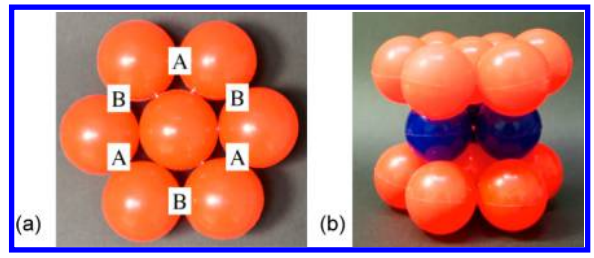

Figure 3. (a) A hexagonally packed layer and (b) three layers are piled to form hexagonal closest packing.

each ball of the second layer situated on the hollow space, A, of the first layer. Then, the third layer is piled up on the second layer in the same way as that of the second layer, so that each ball of the third layer is directly above a ball in the first layer, as shown in Figure 3, panel b.

For the face-centered cubic (fcc) structure, the packing mode of the first and second layers is the same as that of the hcp structure. The yellow third layer is placed on top, such that each ball of the third layer is not situated directly above a ball in the first layer but on the hollow B of the first layer, then a fourth layer is piled up just above the balls in the first layer, as shown in Figure 4, panel a. To understand that the packing

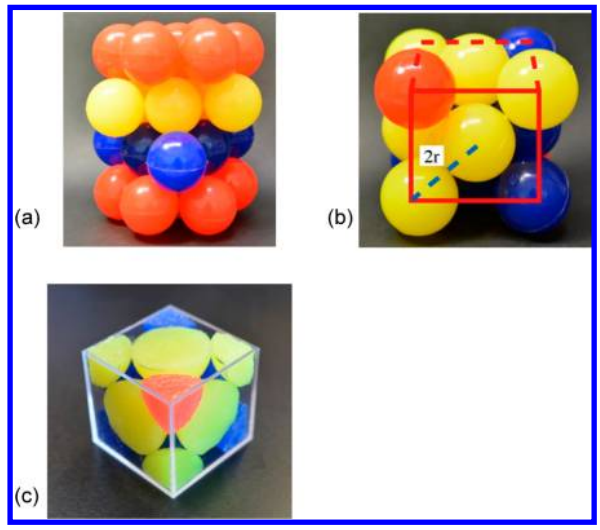

Figure 4. The (a) piled-up fourth layers, (b) fcc cubic lattice structure, and (c) a unit cell.

makes a cubic lattice, the 14 balls, which are composed of one (orange) from the first layer, six (blue) from the second layer, six (yellow) from the third layer, and one (orange) from the fourth layer, are picked up from the layered structure in Figure 4, panel a, as shown in Figure 4, panel b. The cubic cell is drawn with red lines. It is easy to understand that the eight balls at the corners (two orange, three yellow, and three blue balls) and six balls at the center of the six faces (three yellow and three blue balls) make a unit cell of the face-centered cubic lattice.

Face-Centered Cubic Closest Packing

Considering the packing mode of the fcc structure shown in Figure 4, panel b, the unit cell length can be easily deduced to $\sqrt{2} \times 2r$, where r is the radius of a ball. There is an eighth ball at each cubic corner and a hemisphere ball at each face center in the fcc structure. This means that there are four balls in the unit cell because there is a total of one ball at the eight corners and a total of three balls at the centers of six faces. A cubic box

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with the edge length of $\sqrt{2} \times 2r$ was made with acrylic resin plates. The parts of the balls were inserted in the box as shown in Figure 4, panel c. The packing efficiency (PE) of the fcc cell is estimated in the same way as that of the simple cubic cell.

Hexagonal Closest Packing

The packing mode of the hexagonal closest packing (hcp) structure is shown in Figure 3, panel b. Although the unit cell should be taken as a minimum repeating unit, that is, a rhombus unit cell (red color), as shown in Figure 5, panel a, it

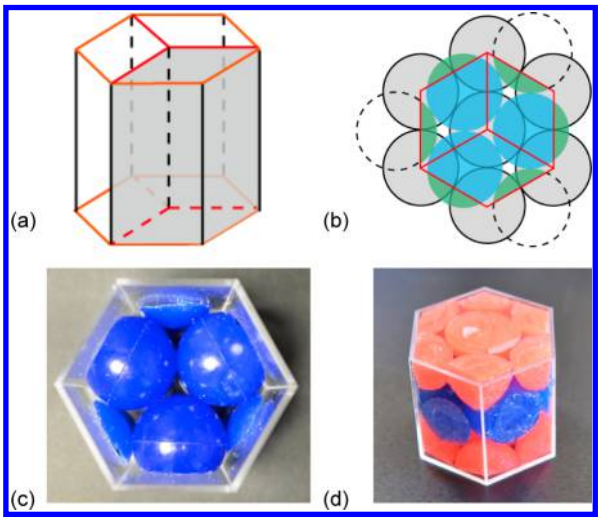

Figure 5. (a) The rhombus unit cell and hexagonal unit, (b) projection of the hcp structure viewed along the hexagonal axis, (c) packing mode of the second layer in the hexagonal unit, and (d) the hcp structure in a hexagonal unit.

is better to make a hexagonal unit (orange color) composed of three rhombus unit cells than to prepare a rhombus regular cell because it is easier for students to understand the hexagonal closest packing. The projection of the hcp structure along the hexagonal axis is shown in Figure 5, panel b. There are three rhombus unit cells related by a three-fold axis in a hexagonal unit, which is drawn with orange lines. The gray balls in the first and third layers are completely overlapped, and the blue balls in the second layer are situated on the hollows A of the first layer. The height of the hexagonal cell is $2\sqrt{(8/3)}r$ because three balls of the first layer and a ball of the second layer make a tetrahedron with the edge length of $2r$; the distance between the top and the base plane of the tetrahedron is $\sqrt{(8/3)}r$. It is important to count the number of the balls in the hexagonal unit. From the first and third layers, there are two hemispheres at the centers of the hexagons and 12 parts of a sixth of the ball at the corners. This indicates that three balls are included in the hexagonal unit from the first and third layers. Although small parts of the three balls in the second layer are outside of the hexagonal unit, which is indicated as the green-colored areas in Figure 5, panel b, the same portions of the neighboring balls are included in the unit as shown in Figure 5, panel c. This means a total of six balls are included in the hexagonal unit.

The hexagonal unit of the hcp lattice is obtained as shown in Figure 5, panel d. The PE value of the hcp cell is measured in the same way as that of the simple cubic cell. It is very important to examine that the PE value of the hcp cell is the same as that of fcc within experimental error.

Body-Centered Cubic Packing

Another crystal structure observed in metals is the body-centered cubic (bcc) structure. Each ball (atom) is surrounded by eight balls (atoms) in the arrangement. The unit cell length is $(4/\sqrt{3})r$. An eighth ball is fixed at each cubic corner, and a spherical ball is set in the center of the cube as shown in Figure 6. There are two balls in the unit cell. The PE value is also obtained.

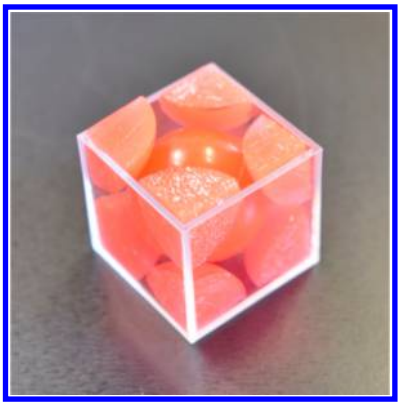

Figure 6. Unit cell structure of the bcc structure.

From the above experiments, students can understand the structures of simple cubic, face-centered cubic, hexagonal closest packing, and body-centered cubic lattices. Moreover, they easily understand how many balls are included in the unit cell of each structure. They can also understand that the PE values of the hcp and fcc structures are the same within experimental error and that the PE of the body-centered cubic is smaller than those of hcp and fcc. Moreover, the PE value of the simple cubic is too small to be observed in usual metal structures.[13]

HAZARDS

Latex balls and acrylic resin plates are commonly used materials in hobby, but caution should be taken by those who are allergic to latex. A knife is usually used to cut the balls.

THEORETICAL CALCULATIONS

To examine the experimental results, the theoretical PE values are calculated by students themselves using the following formula:

$$PE = \frac{\text{total volume of included balls}}{\text{volume of a unit-cell}} \times 100 \quad (2)$$

For the simple cubic structure, the volume of the box is $8r^3$ because the edge length of the cubic box is $2r$. There is a ball in the box:

$$PE\ (\text{simple cubic}) = \frac{\frac{4}{3}\pi r^3}{8r^3} \times 100 = \frac{\pi}{6} \times 100 \approx 52.4\% \quad (3)$$

For the fcc structure, the volume of the unit cell is $16(\sqrt{2})r^3$ because the edge length of the cubic cell is $2\sqrt{2}r$. There are four balls in the unit cell. It is important for students to understand that the PE value is independent of the radius of the ball because the term r^3 disappears in the formula of eq 3:

$$PE\ (\text{fcc}) = \frac{\frac{16}{3}\pi r^3}{16\sqrt{2}r^3} \times 100 = \frac{\sqrt{2}\pi}{6} \times 100 \approx 74.1\% \quad (4)$$

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Table 1. Comparison of Students' Test Answers before and after the Experiment

	Student Responses before the Experiment, N = 12		Student Responses after the Experiment, N = 12	
Question Topic	Correct Answer, N	Incorrect Answer, N	Correct Answer, N	Incorrect Answer, N
1	1	11	11	1
2	2	10	12	0
3	0	12	12	0
4	0	12	12	0

For the hcp structure, the hexagonal unit has a volume of $\{6(1/2)(2r)(\sqrt{3}r)\} \times \{2(\sqrt{(8/3)}r) = 24\sqrt{2}r^3$. There are six balls in the unit:

$$PE\ (\text{hcp}) = \frac{\frac{24}{3}\pi r^3}{24\sqrt{2r^3}} \times 100 = \frac{\sqrt{2}\pi}{6} \times 100 \approx 74.1\% \quad (5)$$

The PE value of the hcp structure is exactly the same as that of the fcc structure.

For the bcc cell, the volume of the unit cell is $(64/3\sqrt{3})r^3$ because the cell length is $(4/\sqrt{3})r$. There are two balls in the unit cell:

$$PE\ (\text{bcc}) = \frac{\frac{8}{3}\pi r^3}{\frac{64}{3\sqrt{3}}r^3} \times 100 = \frac{\sqrt{3}\pi}{8} \times 100 \approx 68.0\% \quad (6)$$

It is important to know that the PE value of the bcc cell is smaller than those of the hcp and fcc cells, but significantly greater than that of the simple cubic cell.

Experimental Results in the High School Classroom

The above experiment was conducted in a classroom in the attached Ehime University Senior High School: 12 second-year students took part in the experiment. They were divided into six groups. The students received a 50 min lesson about the crystal packing and then took a test. The question topics were as follows:

1. Number of atoms in each unit cell of the fcc, hcp, and bcc structures
2. Atomic arrangement of the two closest packings
3. Packing efficiency
4. Coordination number of each lattice structure

The averaged experimental and theoretical values are in good agreement with each other. The experimental data obtained by the six groups clearly indicated that the PE value of the fcc cell is significantly greater than that of the bcc cell, but is insignificantly different from that of the hcp cell.

After the experiment (about 100 min), the same test was taken. As shown in the third column of Table 1, the percentage of correct answers was almost 100%. Only one student had difficulty understanding the face-centered cubic lattice shown in Figure 4, panel b.

The measurement to obtain the PE values was performed three times for each cell of hcp, fcc, and bcc structures. The averaged experimental and theoretical PE values and their relative errors are reported in Table 2.

DISCUSSION

A latex ball costs twenty-one cents, and a 45 cm × 30 cm acrylic resin plate is about $5.00 (100 Japanese yen = 1 U.S. dollar). The cost is very low. Because five different colors are effectively used in the different positions in each model, it will be easier to understand the atomic arrangement in the crystal structures.

Table 2. Comparison of Measured and Theoretical Packing Efficiency Values

Lattice Type	Measured Values,[a] % (SD)	Theoretical Values,[b] %	Relative Error, %
simple cubic	53.3 (1.21)[c]	52	2.5
hcp	72.4 (1.44)	74	2.2
fcc	72.4 (1.27)	74	2.2
bcc	69.0 (1.57)	68	1.5

[a]Data obtained by six student pairs conducting three runs each of the experiment for hcp, fcc, and bcc. [b]Data calculated using eqs 2−6. [c]This value was obtained by the instructor while demonstrating the experiment.

The unit cell box made with acrylic plates should be kept after the experiment and may be reused if there remains insufficient time for the experiment.

As an extension to this experiment, students performed an experiment to measure the density of various metals. If the Avogadro number, atomic weight, and lattice type of each metal were taken from the textbook, the students can easily calculate the unit cell dimensions and the atomic radius using the density of each metal.[14] Various packing modes of atoms in three-dimensional structures and the void space between atoms are important concepts to help with the understanding of the chemical properties. This experiment will be a first step to understanding the nature of materials on the basis of atomic arrangement.

ASSOCIATED CONTENT

Supporting Information

A table of stable structures of various metal elements at room temperature and how to make the models of the simple cubic, face-centered cubic, body-centered cubic, and hexagonal closed packing structures. This material is available via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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