Diamonds: Micro and Macro Scales – Peter Ashton

Purpose

The microscopic structure of a material may have significant consequences for its macroscopic properties. However, these small-scale details can be something of a "black box" to beginning students – opaque to their analyses until the correct interpretation is presented to them. In this lesson, students investigate the microscopic crystal structure of a diamond by considering some possible simple models and comparing the models' predictions with observations.

Overview

In this activity, students work through problems leading them from large-scale, easily measurable qualities of a diamond down to its microscopic properties. They are presented with simple models for how the atoms could be arranged within the diamond and asked to make predictions about what densities they would observe in a real diamond. Comparing predictions to data on a real diamond, they will be able to rule out models and draw conclusions on the necessary conditions for diamond crystal structure.

Student Outcomes

Students will be able to:

- Compute the average density of a material given a description of its internal, microscopic structure.
- Evaluate proposed models of microscopic structure based on macroscopic observable quantities.
- Explain their findings in terms of statements about "what must be true" and "what can't be true" with evidence to support both.

Standards Addressed

- HS-PS1-3. *Plan and conduct an investigation to gather evidence to compare the structure of substances at the bulk scale to infer the strength of electrical forces between particles.*
- HS-PS2-6. *Communicate scientific and technical information about why the molecular-level structure is important in the functioning of designed materials.*

Time

1-2 50-minute class periods.

Level

High school (nominally 10th grade) Regular or Honors Chemistry

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Materials and Tools

- Attached worksheet
- Calculators
- Periodic table

Preparation

Make copies of worksheets

Prerequisites

Students should have an understanding of mass and density and how the two are related/calculated. Basic stoichiometry (i.e. the mole) should have been introduced, though this lesson could serve as an early exercise using only the definition that 1 mole is the number of atoms (Avogadro's number) in 12 grams of Carbon-12. Students should be able to perform unit conversions (e.g. nanometers to centimeters, grams to AMUs). Students should be familiar with "percent error" as a means of evaluating agreement between observations and theory.

Background

In nature, carbon can take many different forms. For example, consider diamonds and graphite: both are made purely of carbon atoms, but they have very different properties. Graphite is soft and black, while diamonds are hard and clear. Both are made of carbon, but the difference is in the way the carbon atoms arrange themselves within the material.

To find the density of something, we generally divide its mass by its volume. We can also talk about the "average density" of something by dividing total mass by total volume. To see the difference, think about a heavy rock sitting in an otherwise empty room*. If we ask what the density of the rock is, we would find the mass of the rock and divide by the volume of the rock. If we want to know the average density in the room, we would find the mass of everything in the room (just the mass of the rock) and divide by the whole volume of the room (much bigger than the volume of the rock). The result we get for average density will be much smaller than the density of the rock, because we're dividing by a bigger number. Another way to think of it is that we're averaging together something that's relatively dense with a lot of empty space that's not dense.

A mole is defined as the amount of a substance that has as many particles as in 12 grams of Carbon-12. This number is called "Avogadro's Number" and is equal to 6.02 x 10^23. The mass of one mole of an element in grams can be found on a periodic table. For example, 1 mole of Lithium has a mass of 6.94 g and consists of 6.02 x 10^23 atoms. You can use these equalities to convert between moles, mass, and atoms for any substance.

*We're ignoring the mass of the air in the room in this example.

Teaching Notes

Make sure students are comfortable with the above background material, especially the concept that diamonds and graphite are both carbon but in different arrangements. The big question is how we can learn about what the individual atoms are doing if we can only measure large-scale properties like mass and volume. Distribute attached worksheets one to a student, but encourage them to work together in small groups if they get stuck on a question or want to confirm answers/methods. Teacher should walk around the room checking the progress of students/groups. An answer key is provided. Especially pay attention to the answer to problem #7, the volume of a sphere with a given radius, as some students may have trouble with a unit conversion when taken to a power, or may need to be reminded of the formula for the volume of a sphere (V = (4/3) π r^3). As students start to reach the end of the first page, stop them and reconvene the class, and ask students to explain their answer to #8 (the correct answer should be ~14 g/cm^3). It's important for all students to have this information correct before proceeding to the models on the back, or else the comparison between predictions and observations won't work.

If students have trouble understanding the physical picture being described in the models in #9 and #10, explain to them that the first is like imagining that atoms are like Lego blocks that can always fit together perfectly with no spaces in between. The second is like imagining that atoms are like hard marbles in a jar – no matter what, there will always be spaces because round things can't pack together perfectly. If time is available, show students the NYU MRSEC video "Particles and Pirates" (http://www.youtube.com/watch?v=yUeY5hSNCKc) as an illustration of the issues involved in packing efficiency.

As students continue to work on questions 9 and 10, emphasize that in their calculation of percent error, the "observed" values come from the real measurements of the Hope Diamond given at the top of the first page. What will change between the two models is the "expected" value, due to our predictions for density changing between the two models.

When students finish with question 11, they should find that the "packing factor" for diamonds is expected to be something like 25%. This is in fact remarkably close to the actual atomic packing factor for diamonds, ~34%. Show them something like the animation here: http://en.wikipedia.org/wiki/Diamond_cubic#mediaviewer/File:Diamond_Cubic-F_lattice_animation.gif, which shows the real arrangement of atoms in a "unit cell" of a diamond crystal. Note that that the atoms are nowhere near as densely packed as possible, as our models were assuming.

As a possible extension, explain to students that the way scientists learned what the diamond's crystal structure is actually like is through a process called x-ray crystallography. In this method, a beam of x-rays is focused on a sample of a substance, and the resulting pattern of bright and dark interference spots can be interpreted to obtain specific locations of individual atoms. This was the method by which the structure Rosalind Franklin found the double-helix structure of DNA, and it is also used my the Curiosity rover on Mars to identify samples of rock. Another possibility, given time, is to provide students with a beaker of marbles or other spherical objects, and let them figure out how much of the volume is occupied by the spheres. Likely they would need to find the volume of one marble by submerging it in a graduated cylinder, and compare that to the amount of water needed to submerge a larger collection of marbles. If the marbles are "close packed", they should recover the 74% figure cited in #10.

Assessment

As students complete the worksheet, the teacher should check in to make sure answers are in the correct order of magnitude, if not numerically identical. It's a good idea reconvene the class once students have calculated the average density of a carbon atom to ask them to explain their answer, so that students who have made errors can correct them before moving on to the models of the diamond structure. At the conclusion, the teacher can check the "strength" of the statements students are able to make about the crystal structure, e.g. if a student writes that "It must be true that a diamond is made of many carbon atoms," that is a true statement, but they should be directed to try to make it more specific. The class can then have a discussion on what they've concluded and how the models they considered matched observations.

Additional Information

This lesson uses data on the Hope Diamond for the sake of a concrete example. Data was taken from the Hope Diamond wikipedia page (http://en.wikipedia.org/wiki/Hope_Diamond), and the volume was estimated from the mass and a typical density for diamonds. In reality the Hope Diamond contains boron impurities, so it's a simplification to treat it as only carbon. Many students asked how much it's worth, and the answer seems to be $200 million - $250 million as of 2011. However, anyone can see it for free in the Smithsonian Natural History Museum in Washington, DC.