

Crystal Chemistry

Jennifer Dean

jennifer.v.dean@gmail.com

Julie Dick

maroonchic28@msn.com

Gabrielle Doyon

gcdoyon@yahoo.com

Ran Fan

ran_fan13@yahoo.com

Sofia Izmailov

sofiaizmailov@gmail.com

Tsz Kwok

nautti_njel721@verizon.net

Sakul Ratanaalert

LafDragon132@yahoo.com

Advisor: Nancy Twu

ntwu@eden.rutgers.edu

1. ABSTRACT

The goal of this project was to study crystalline structures: their properties, stability, practical uses, and interactions with one another. In order to achieve this goal, we investigated the general qualifications for a crystal as well as specific examples of each individual crystal system. After exploring the general structures in which crystals occur, we further explored the compositions and practical applications of various crystalline substances. These substances include Sodium Chloride (NaCl), Cesium Chloride (CsCl), Calcium Fluoride (CaF₂), Zinc Blende (ZnS), Wurtzite (ZnS), Graphite (C), Diamond (C), Boron Nitride (BN), Perovskite (CaTiO₃), Spinel (MgAl₂O₄), Beryl (Be₃Al₂Si₆O₁₈), and Zeolite (X_aAl_bSi_cO_d·eH₂O). We examined the defects which tend to occur in crystals and the benefits these “defects” have in the world of application.

2. INTRODUCTION

A crystal can be loosely defined as a solid form of matter with an internal structure of repetitive nature. Substances become crystalline structures in environments of high temperature and pressure. Under these conditions the individual atoms gain enough energy to move towards their least state of energy and most stable form. Materials are also capable of forming crystalline structures in slow-cooling conditions. For one of our experiments within this project, we experimented with growing alum crystals. We stored our specimens in warm temperatures in order to provide the optimum environment for the crystal growth.

There are 32 point groups representing different degrees of symmetry in a structure. Each of these point groups can be classified into one of the seven crystal systems. They include Triclinic, Monoclinic, Orthorhombic, Tetragonal, Hexagonal, Rhombohedral, and Cubic, listed from least to most symmetric. These systems differ in their arrangement of atoms within a plane, more specifically by bond lengths and angles. Planes are defined

with the use of Miller Indices. The points within each plane are depicted using a set of numbers (hkl), which represent the reciprocals of the intercepts on each axis. One of the defining characteristics of a crystal is the regularity in the placement of the planes within the structure. Certain planes divide crystals into symmetrical pieces and are therefore termed “planes of symmetry.” Another name for such a plane is “mirror plane,” because the plane acts as a mirror within the crystal. An additional form of symmetry is the axis of symmetry. This involves the basic structure repeating as a rotation around a central axis. Further elements of symmetry include n-fold rotation and inversion, in which the crystal assumes a congruent position in various different arrangements.

In order to explore the various systems and symmetrical elements possible in crystal formation, we used orbital model kits to create 3-D replicas of various crystals.

There are instances in which these symmetrical systems can be disrupted. Such occurrences are known as dislocations, namely screw dislocation and edge dislocation, both of which are elaborated on in Section 4.

3. CRYSTAL SYSTEMS AND MODELS

3.1 Cubic Crystal Systems

The cubic crystal system is the most symmetric of the seven crystal systems where the unit cell is in the shape of a cube. The distance between all the particles within the crystal structure is equal to each other. Referring to Figure 1 on the next page, the lengths of a, b, and c are equal to each other and all angles are equal to 90 degrees. The cubic crystal system was the first structure that we learned about. In addition, the first three structures we built—sodium chloride, cesium chloride, and calcium fluoride—were cubic crystal systems.

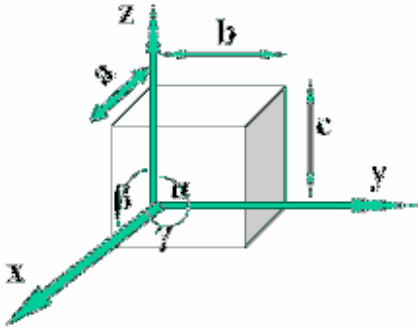


Figure 1: Cubic Crystal System

The cubic structure system is the easiest and simplest structure, as well as the one most commonly found in metallic crystals. It can be broken down into three different groups: simple cubic, body-centered cubic and face-centered cubic. The simple cubic has one lattice point on each corner of the cube, each of which is then shared by eight other points on the cube. The body centered cubic system has one lattice point in the center of the unit cell in addition to the eight corner points. It has in total two lattice points per cell. Finally, the face centered cubic lattice has lattice points on the center of each face of the cube, giving a total of four lattice points.

3.1.1 Sodium Chloride

Sodium chloride, or better known as common table salt, is made when positive charged sodium ions come together with negative charged chlorine ions. This forms a simple cubic structure. Sodium chloride can exist as a colorless, white, or a transparent crystal. This salt is extremely common and can be found around the world in Great Britain, France, India, the United States, Germany, and Russia.

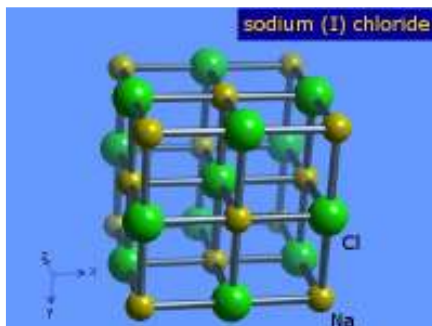


Figure 2: The crystal structure of sodium chloride

3.1.2 Cesium Chloride

Cesium chloride is an ionic compound that possesses many different reactions when placed in various environments. The cesium chloride structure is a body-centered cubic, which is a 1:1 cube. The atom in the middle of the structure is slightly smaller than the atoms surrounding it. It is usually colorless or white. Cesium Chloride is also the most common multi-compound element for interpenetrating simple cubic.

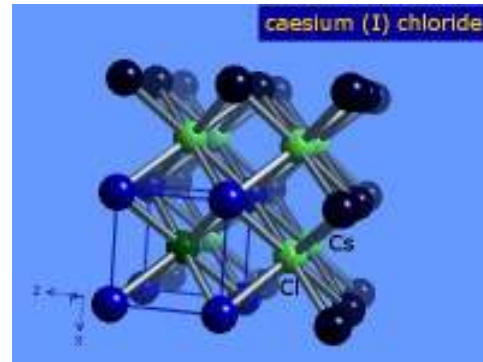


Figure 3: The crystal structure of cesium chloride

3.1.3 Calcium Fluoride

Calcium fluoride is an insoluble ionic compound made up of the elements of calcium and fluorine. CaF_2 . As seen in Figure 4, Calcium atoms are surrounding the surface of the molecule. The main purpose of Calcium Fluoride is to help transmit infrared and ultraviolet wavelengths. It is usually a white solid, but color is sometimes added to it.

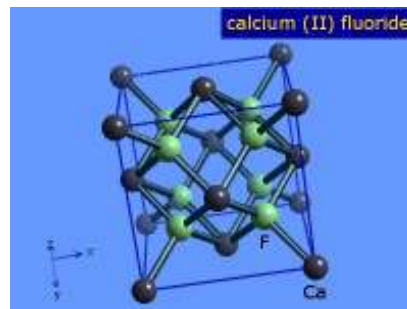


Figure 4: The crystal structure of calcium fluoride

3.2 Zinc Blende and Wurtzite

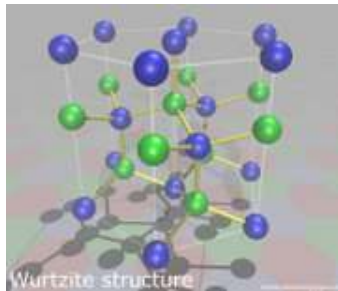
The chemical compound zinc sulfide (ZnS) is a white to yellow colored powder or crystal. A covalently bonded solid, zinc sulfide crystallizes in two different forms: wurtzite and zinc blende. Structurally, it can typically be

found in the more stable cubic form, known as the mineral sphalerite, (zinc blende). The other form is hexagonal, named wurtzite. Because both forms share the same formula, but different properties, they are polymorphs of each other.

Zinc blende and wurtzite are wide-band gap semiconductors. The cubic formed zinc blende has a band gap of 3.54 eV at 300 K. Wurtzite, the hexagonal form, has a band gap of 3.91 eV. A transition from the sphalerite form to the wurtzite form occurs at around 1293.15 K. Sphalerite melts at 1991 K. It has a standard enthalpy of formation of -204.6 kJ/mol at 298 K. The ionic radius of the zinc(II) ion is 0.74 angstroms and that of the sulfide ion is 1.70 angstroms. The ratio of radii for the cation and anion is 0.44. The zinc(II) ions occupy tetrahedral holes. Again, if the sulfide ions have a hexagonal closest-packed structure, the ZnS crystal is wurtzite. If the sulfide ions originally adopt a cubic closest-packed structure, the ZnS crystal is zinc blende.

ZnS, in the early years of nuclear physics, was used by scientists such as Ernest Rutherford as a scintillation detector, because it emits light on excitation by x-rays or electron beam, making it useful for x-ray screens and cathode ray tubes. It also exhibits phosphorescence due to impurities on illumination with blue or ultraviolet light. Copper doped zinc sulfide (ZnS:Cu) is used in electroluminescent panels. It can be doped as both n-type semiconductor, which has an excess of electrons, and p-type semiconductor, which has a lack of electrons.

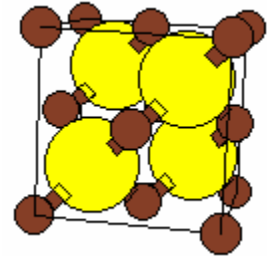
Wurtzite is a less frequently encountered mineral form of zinc sulfide. The sulfide ions lie in a hexagonal closest-packed arrangement, as seen in the image to the right. The zinc(II) ions are much smaller than the sulfide ions. The crystal structure is a member of the hexagonal close-pact (HCP) crystal system and consists of tetrahedrally oriented zinc and sulfur atoms, which are stacked in an ABABAB pattern. The structure is closely related to the structure of



lonsdaleite, or hexagonal diamond. The insertion of zinc(II) ions into the tetrahedral holes causes the structure to expand so that the sulfide ions are not in contact with each other.

Only one half of the tetrahedral holes are occupied by zinc(II) ions. The ionic solid is electrically neutral and the unit cell itself must also be electrically neutral. Because the sulfide ions adopt a HCP structure, there are two sulfide ions in the unit cell. Consequently there must also be two zinc(II) ions in the unit cell. Wurtzite has (4,4)-coordination. Several other compounds can take the wurtzite structure, including ZnO, CdS, CdSe, GaN, AlN, and other semiconductors.

Sphalerite, or zinc blende, is the chief ore of zinc. It consists largely of zinc sulfide in crystalline form but almost always contains variable iron. When iron content is high it is an opaque black variety known as marmatite. Miners have also been known to refer to sphalerite as zinc blende, mock lead, false galena and black-jack.



The sulfide ions lie in a cubic closest-packed (CCP) arrangement, shown to the right. Again, the zinc(II) ions are much smaller than the sulfide ions. The structure expands such that the sulfide ions do not touch each other and only half of the tetrahedral holes are occupied by zinc(II) ions. The ionic solid is electrically neutral and the unit cell itself must also be electrically neutral. Because the sulfide ions adopt a CCP structure, there are four sulfide ions in the unit cell. Consequently, there must also be four zinc(II) ions in the unit cell. Zinc blende has four sulfur atoms and four zinc (II) atoms per unit cell.

The mineral crystallizes in the cubic crystal system. In the crystal structure, zinc and sulfur atoms are also tetrahedrally oriented. The structure is closely related to the structure of diamond. The lattice constant for zinc sulfide in the zinc blende crystal structure is 0.542 nm.

The colors of the crystal include yellow, brown, or gray to gray-black as seen to the right. Its



degree of reflection may vary. It has a hardness of 2.5 to 4, and a specific gravity of 3.9 to 4.1. Some specimens have a red iridescence within the gray-black crystals called "ruby sphalerite." The pale yellow and red varieties are translucent because of the lack of iron. Thus, the darker unclear versions have more iron. Some specimens are also fluorescent in ultraviolet light. The refractive index of sphalerite (as measured via sodium light, 589.3 nm) is 2.37. Sphalerite crystallizes in the isometric crystal system and possesses perfect dodecahedral cleavage.

Gemstones are made from crystals of suitable size and transparency. For instance, sphalerite has a high dispersion of 0.156 (B-G) interval—over three times that of diamond, and would make a good gem. The luster of a freshly cut gemstone could be mistaken for a fancy-colored diamond in passing, but due to sphalerite's softness and fragility the gems are best left unset as collector's or museum pieces. Others have been set into pendants. The crystals used to make these gems are usually a yellowish to honey brown, red to orange, or green. The two most important sources are the Chivera mine, Cananea, Sonora, Mexico; and the Picos de Europa, Cordillera Cantabrica, near Santander on Spain's northern coast.

3.3.1 Graphite

Graphite is one of the two best known allotropes of carbon, its polymorphs being diamond and C_{60} , the "buckyball". It is classified as a native element because it occurs in nature uncombined to other elements, and therefore has the chemical formula of C. Even though graphite is one of the softest minerals known to man, it is best known for being the most stable and the purest form of carbon discovered yet. Due to the unpaired fourth electron in each carbon atom, graphite is a very good conductor of electricity. Graphite powder is also extremely useful as a dry lubricant due to the loose interlamellar coupling between sheets in the structure.

Each carbon atom in graphite is covalently bonded to four other carbon atoms and forms a hexagonal crystal system. The different layers of graphite are each joined by weak forces called van der Waals forces. All of the carbon atoms lie on the same plane and are

only weakly connected to the sheets above or below therefore making graphite easily fragile and soft.

The most common uses for graphite include lead for pencils, lubricants, crucibles in reducing environments, to toughen steel and high strength composites. The most noteworthy occurrences include Greenland, India, Mexico, Russia, and New York and Texas in the United States.

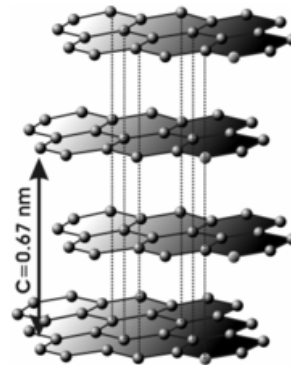


Figure 5: Carbon layers and interactions of graphite

3.3.2 Diamond

Diamond is the second best known allotrope of carbon, and is a polymorph of graphite because it has the same chemical formula of C. In contrast to graphite, which forms at low pressures, diamonds only form in extremely high pressure conditions. In addition, the diamond is well-known for its score of ten out of ten on the relative Mohs scale of mineral hardness; one of the hardest minerals known to date. This is much different from the one or two hardness of graphite. Diamond is also an excellent electrical insulator and ultimately abrasive.

Diamond has a greater density compared to that of graphite due to the more compact formation of the carbon atoms. Similar to graphite, each carbon atom in diamond is bound to four other carbon atoms having instead a tetrahedral appearance. Diamonds form in the face-centered cubic crystal system. The diamond structure is very compact and therefore very strong.

Most deposits of diamonds are found in Africa: South Africa, Namibia, Botswana, the Democratic Republic of Congo, Angola,

Tanzania, and Sierra Leone. Diamonds are also commonly found in Northwest Territories of Canada, Siberia, Brazil, Australia's Northern Territory, and Western Australia. The most common use for diamonds is gem stones and jewelry and making cutting tool tips.

3.3.3 Boron Nitride

Boron Nitride is commonly referred to as "White Graphite" due to its similar layer structure to graphite. It is a binary chemical compound consisting of equal portions of boron and nitrogen; hence the chemical formula of BN. Boron Nitride has an extremely high heat tolerance, superior dielectric strength, and impressive thermal conductivity. It also has wonderful lubricant properties and is one of the hardest materials in the world behind the diamond.

The three most common crystal forms of boron nitride are hexagonal boron nitride (h-BN: graphite-like structure), cubic boron nitride (c-BN: diamond-like structure), and wurtzite (closed packed hexagonal). At lower temperatures and pressures hexagonal boron nitride has a similar structure to graphite, but is slightly shifted. At high temperatures and ultrahigh pressures, cubic boron nitride has a similar structure to the diamond.

Boron nitride is typically used to manufacture, contain, and process metals and also for industrial applications such as the production of electronic parts, low friction seals, CVD and vacuum melting crucibles, electrical insulators, and hard abrasive materials.

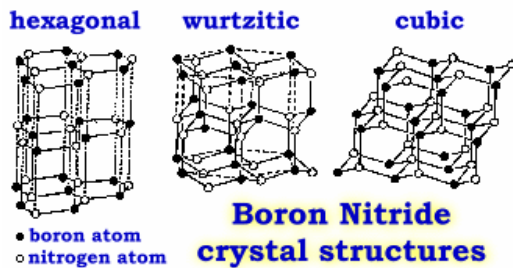


Figure 6: Boron Nitride crystal structures

3.4 Perovskite

Relatively rare, the mineral Perovskite (calcium titanium oxide, CaTiO_3), is found in Tanzania, Brazil, and Canada. It is often in contact with metamorphic rocks and associated with mafic intrusives, nepheline syenites, and rare carbonatites. Although its

crystals appear cubic, in actuality, it has orthorhombic symmetry. Due to its rare earth metal content, perovskite is becoming increasingly valuable to industry; the versatility of such a structure ranges within technological applications such as ferroelectrics, catalysts, and superconductors. Ferroelectrics are materials possessing an imbalance with ions, resulting in a spontaneous dipole moment in their structure. This imbalance can be reversed under the application of an electric field. The most important technological application of ferroelectrics is found among oxides with a perovskite structure.

The property of piezoelectricity, the ability of crystals to produce a voltage due to mechanical stress, is also observed in perovskite. Ceramics with perovskite structures contain tetravalent metal ions in a larger lattice containing divalent metal ions. When temperatures are above the critical temperature, perovskite crystals within a fired ceramic element exhibit a cubic symmetry without a dipole. However, at temperatures below the Curie point, the crystals each take on tetragonal or rhombohedral symmetry and possess a dipole moment. Mechanical tension applied to a piezoelectric ceramic element causes a change in the dipole moment, which creates a voltage. The piezoelectric effect, or the theory that compression and tension generates voltage of opposite polarity and in proportion to applied force, is utilized in sensing applications, including in displacement sensors. In contrast, the inverse piezoelectric effect, which is the converse relationship, is used in actuation applications; some examples of such applications include motors or devices that precisely control positioning and in the generation of ultrasonic signals.

Furthermore, the perovskite structure is adopted by many oxides, with ABO_3 as the general formula. A and B represent cations of varying sizes. However, the differences in ratio between the cations can cause distortions. The most common is tilting, the twisting and bending of the natural members of the group, which results in a variety of symmetries ranging from isometric to tetragonal to orthorhombic to monoclinic, depending on the degree of distortions. Generally, the crystal contains the A-cation in the center of the cube, the B-cation in the corner, and the anion,

which is often oxygen, in the center of the unit cell faces. Bonding within the structure is predominantly ionic with smaller cations octahedrally coordinated with the anions. These perovskite-like structures are often present in many ceramic superconducting materials.

The physical characteristics of perovskite are also distinctive. Among these properties are opacity of crystals, variable color, and imperfect cleavage in one direction. Perovskite structures also share the property of ferroelectricity with garnet and olivine.

3.5 Spinel

Those among the class of minerals that crystallize in the isometric system with an octahedral habit are known as spinels. Found in metamorphic mineral, it also acts a primary mineral in basic rocks. The formula of spinel is often interpreted as $MgAl_2O_4$, but other species may adopt the structure as well. Within the structure, the oxygen anions are in a closely-packed cubic formation. Furthermore, trivalent cations are present within half of the octahedral holes, and one eighth of the tetrahedral holes are filled with divalent cations. Inverse spinels also exists, where one eighth of the tetrahedral holes are filled with half of the trivalent cations, while half of the octahedral holes are filled with divalent cations along with the remainder of the trivalent cations. Found in the gravel of Sri Lanka and in the limestones of Myanmar and Thailand, spinel often occurs as isometric crystals, such as octahedrons.

The spinel structure is generally based on the structure of the diamond. Due to the position of the A ions being practically identical to the position of the carbon atoms in the diamond, there is a rather high degree of hardness and density in the group. Furthermore, the arrangement of other ions in the structure also conforms to the symmetry of the diamond structure. However, they disrupt the cleavage due to the lack of cleavage directions within any member of this group.

As for the other physical characteristics of spinel, it can be of varying colors, ranging from colorless to shades of red, yellow, green, blue or black. Typically, however, spinel takes on a red color, resembling the shade of rubies. Thus, this resemblance causes spinel to be

used as a substitute for the gemstone. Famous among such "impostors" is the *Black Prince's Ruby*, a spinel found on the Imperial State Crown in the British Crown Jewels. Besides their physical likeness, ruby and spinel are also chemically similar; spinel is magnesium aluminum oxide, while ruby is aluminum oxide. Properties shared among the two include similar luster, density, and hardness.

The Spinel Twin Law also makes the mineral famous. This form of twinning produces a twin plane, which is parallel to one of the octahedral faces. Acting as a mirror, the plane produces left and right sides that are mirror images of each other, but this plane is not parallel to any of the other planes; instead it appears to lower the symmetry of the crystal. During this process, the plane collapses in the center of the crystal, dividing it in half and causing the two octahedron faces parallel to the twin plane to become equilateral triangles. Despite being rare, the popularity of twin spinels leads to their availability on the market.

3.6 Beryl

Beryl, also known as beryllium aluminum cyclosilicate, has a hexagonal crystal system, with a chemical formula of $Be_3Al_2Si_6O_{18}$. Its structure is a series of rings with 6 SiO_4 each, interconnected with alternating beryllium and aluminum atoms to form a "sun-like jewel" unit cell structure that can connect to others to compose the beryl crystal's hexagonal structure (see Figure 7).

When pure, beryl is colorless, but with the introduction of various impurities, different species with different colors can form. For example, trace chromium and/or iron impurities in the beryl crystal taints the mineral green, forming emerald. Other members of the beryl family include bixbite (red; also known as red emerald or scarlet emerald), aquamarine (blue), and goshenite (white).

Because of the way each unit cell connects to another, there is no clear-cut cleavage plane as in sodium chloride or other simpler crystal structures. Instead, beryl exhibits conchoidal fracture, which means it fractures to form curved ripples, much like the shell of a mussel (a conchoid).

There are not many applications for this crystal, except for jewelry and an ore source for beryllium and beryllium oxide.



Figure 7: Beryl crystal structure

3.7 Zeolite

The zeolite crystal structure refers to the mineral family characterized by porous and spherical structures. It belongs to the cubic crystal system. Each unit cell has six regular octagons, eight regular hexagons, and twelve squares. They are among a variety of hydrated aluminosilicates, which are composed of aluminum, silicon, and oxygen atoms, as well as water molecules trapped between the crystal lattices. The atoms in the crystal arrange themselves in a sphere-like arrangement with apertures that allow cations (positive ions) to be trapped and exchanged. These cations, along with the ratios between Al, Si, O, and H₂O, are what differentiate the different species of mineral within the zeolite family. Examples include chabazite, heulandite, natrolite, and phillipsite.

The general formula for a zeolite species would be $X_aAl_bSi_cO_d \cdot eH_2O$, where the lowercase letters are numbers and X is a cation-forming element. For example, the chemical formula of Chabazite-Sr is $SrAl_2Si_4O_{12} \cdot 6H_2O$.

Zeolite is made of interlocking SiO₄ and AlO₄ tetrahedrons, making a 3D network solid. It is one of the most complex tetrahedral combinations, simplest being a straight chain, followed by a branched chain, and so on.

Zeolite is one of many members of the family of “molecular sieves,” in which the crystal is used as a filter to allow only certain sized particles to pass through its apertures and tunnels but prevent other larger particles from entering.

The properties of being able to exchange ions, being selectively permeable, and having regular pores are what make zeolite so applicable to many fields. Commercially, the ion-exchange and small chamber capabilities allow for extraction of a certain molecule for closer analysis, or a confined area for catalytic usage. Agriculturally, the zeolite chambers can be loaded with a certain molecule, atom, ion, or other particle for a slow and steady release of that particle to its surroundings (i.e. slow release of potassium into the soil for treatment.) Medically, the sieve properties create a collection of oxygen pure enough to be used for medicinal purposes; for example, the vast amount of oxygen able to be concentrated allows for quicker blood clotting.

The origins of the name zeolite are derived from its discovery. In the 1700s, Swedish mineralogist Axel Fredrik Cronstedt heated a mineral, freeing the water trapped within the crystal structure. As the stones began to shake with steam being emitted, Cronstedt called it a “stone that boils”, and using the Greek words for stone (*lithos*) and boil (*zein*), he named it “zeolite”.

4. DEFECTS IN CRYSTALS

While a crystal is a very ordered structure it is not perfect and has imperfections. These imperfections add to the entropy or disorder of the crystal. Only at 0 Kelvin is it possible to have a perfectly ordered crystal with zero entropy. Since absolute zero is unattainable, so is the perfect crystal. The different types of crystal defects can be defined and classified. These crystal defects can be classified according to the three categories: point defects, line defects, planar defects, and bulk defects.

A point defect is a defect in which a single atom is missing or misplaced within the crystal lattice. One type of point defect is a self interstitial atom. Interstitial refers to the empty spaces in a crystal lattice which are empty in the theoretical perfect crystal. So this type of

defect refers to an extra atom which is located in an interstitial space in the crystal structure.

Substitution impurity atoms are atoms of elements, which differ from the atoms in the main crystal. These atoms fit within the crystal lattice as the normal atoms since they are of similar size. Interstitial impurity atoms are also atoms that differ from the main composition of the crystal. However, due to their small size relative to the other atoms, these impurities fit in the interstitial space of the lattice.

Vacancies are another type of point defect which is simply an atom missing from the crystal lattice. It may shift around as neighboring atoms move into it. Vacancies cannot just disappear because the neighboring atoms move into the vacancy because they are too strongly bonded to their neighbors so the crystal surrounding the vacancy remains highly ordered.

Point defects for ionic solids can also be classified for specifically ionic solids. Frenkel defects occur when a lattice has a vacancy of one type of ion and the same type of ion interstitial in the lattice. This way, the net charge of the entire crystal remains neutral unlike what would occur if there was just a vacancy or just an interstitial atom.

Schottky defects also involve pairs of defects, which maintain the neutrality of the overall crystal. Schottky defects are paired vacancies of anions and cations. This maintains the overall neutral charge since equal amounts of positive and negative charge leave the crystal.

Line defects or dislocations are defects where areas atoms are in the wrong position. These occur when a stress is applied to a crystal. An edge dislocation results when an extra plane of atoms appears to be partially wedged in between two of the planes of atoms that are present in the ideal crystal lattice. From the side, the planes which would normally appear to run in a straight line are now bent out of shape hence the classification as a line dislocation. Line dislocations can move throughout the crystal using relatively little energy because only a few bonds at a time need to be broken.

The other type of line defect is the screw dislocation. This occurs when one plane of the

crystal lattice begins to slide across the plane below it. Rather than just sliding all the unit cells over at once, the plane slides over a few rows at a time. This requires less force than breaking all the bonds at the same time.

Dislocations in metals cause metals to be easily formed into new shapes since the atoms in their lattices are easily moved. Likewise, dislocations explain why ionic solids are so brittle. When atoms in an ionic solid are shifted, the ions will encounter repulsive forces. The repulsive forces cause the ionic crystal to break easily.

The third class of crystal defects is planar defects. Stacking faults are planar defects that occur when the layers in a crystal stack incorrectly. This can mean that a certain layer which would normally be there is not there or there is an extra layer within the normal pattern of layers. These stacking faults sometimes repeat for some time rather than just occur one at a time. These stacking faults are called twin stacking faults.

Grain boundaries are the other type of planar defects. Most crystals that we see are actually made up of a lot of smaller individual crystals. Grain boundaries are the divisions between the individual grains. At the grain boundaries, the direction of the crystal lattice changes. However, the grain boundaries make dislocation more difficult since smaller grains limit the amount of dislocations possible. Thus, smaller grains make the larger crystal stronger. In order to produce smaller grains the material from which the crystal is made usually must be cooled rapidly.

Bulk defects are larger scale defects than the other defects and are much more varied. Voids are one type of defect which results in a lot of atoms missing from the crystal. This may be caused due to trapped gas bubbles, known as porosity, or shrinkage of the crystalline material during solidification, known as cavitations.

Another form of bulk defects are precipitates, or impurities. Unlike substitution errors which are a single atom in one place at a time, precipitates are cluster of impurities.

Probably the most interesting and useful thing about crystal defects is that the name is a misnomer. A defect implies poorer quality.

However, these “defects” allow crystals to take on certain desirable properties that cannot be achieved in the pure crystal. Steel is an example of a crystal structure with interstitial impurity atoms. Carbon is added to iron and since the carbon atoms have a much smaller atomic radius than the iron atoms, the carbon atoms can fit into interstitial spaces. The final product is stronger and not as easily corroded as iron.

Semiconductors, such as silicon, require impurities in the crystal lattice in order to conduct electricity. Finally, some of our most prized jewelry is actually only desired for its impurities. No one makes jewelry out of pure aluminum oxide. However, when there are chromium impurities in the aluminum oxide, one gets a ruby. Or if there is titanium, iron, or vanadium in aluminum oxide, one gets a sapphire.

Occasionally, crystal defects do harm the properties of a substance or are undesirable. Too many bulk defects can make substances brittle. When diamonds are artificially produced in a laboratory from other forms of carbon, impurities may discolor the diamond and make it worthless.

Understanding crystal defects allows one to alter existing crystalline structures to make new materials such as stronger alloys and cheaper semiconductors. Understanding crystal defects allows one to alter the existing properties of existing crystalline structures while considering how crystal defects may benefit or harm the final products. Such new materials are constantly being developed with the help of engineers.

5. CONCLUSIONS

As we explored various examples of the different types of crystals, we learned about their physical properties and various uses. For one, we conducted research on aspects of crystals such as dislocations and nomenclature for various structures. Some of the dislocations include edge and screw dislocations. To learn about structural properties, we engaged in hands-on activities to build unit cells of fourteen unique crystals.

In addition to building models in class, we also grew our own crystals of alum, an ionic substance used in pickling. While the seed

crystals did get larger, few ordered crystal structures were present in the final product. This could be due to the impurity of the powdered alum used to grow the crystals. Even though the conditions were technically unfavorable, the experimental results were acceptable.

Additionally, we learned that crystal chemistry has many uses in the real world such as electronics, jewelry, and metallurgy. On the whole, since it has such broad applicability, we conclude that crystal chemistry is a worthy subject of further study and development.

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CITATIONS

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