A Study on the Appearance of Quartz

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Abstract

The purpose of this report is to gather mineralogical and physical information relevant for future research aimed at the modeling of the appearance of quartz. Initially, we review the basic characteristics of minerals, with an emphasis on aspects that can be applied in the representation of different types of quartz. We then examine some of the key optical properties of quartz, such as light reflection and transmission, that affect its appearance. Finally, we provide a concise survey of previous works on the simulation of minerals, which can provide practical insights for future efforts towards the photorealistic rendering of quartz.

Contents

List of Figures

Table of Symbols

V_v	Velocity of light in a vaccuum.	28
V_m	Velocity of light in a material.	28
n	Index of refraction.	28
θ_1	Angle between incident ray and surface normal.	29
θ_2	Angle between propogated ray and surface normal.	29
n_1	Index of refraction in incident material.	29
n_2	Index of refraction in material.	29
T	Intensity of light as seen by the viewer.	34
r	Reflection coefficient at exit point.	34
R	Intensity of specular light as seen by the viewer.	34
F	Intensity of light from source.	34
c	Absorption rate.	34
I	Intensity of light source.	34
I'	Intensity of light due to inclusions seen by the viewer .	34
$\bar{L}$	Ray from inclusion to light source.	35
k	Reflection coefficient for inclusions.	35
H	Bisector vector between incident light and reflected light.	35
ψ	Fraction of inclusion facing H.	35
L	Intensity of propagated light.	36
x	A point on the surface of a material.	36
ω	Direction.	36
x_e	An end point on a surface.	36
τ	Transmittance function.	36
σ	Scattering coefficient function.	36
κ	Extinction coefficient function.	36
ξ	Extinction coefficient.	36
$\hat{k}_o^{(2)}$	Propogation vector for an ordinary ray.	38
$\hat{s}_o^{(2)}$	Unit vector for a ray.	38
$m^{(1)}$	Refractive index of the isotropic medium.	38
$m_o^{(2)}$	Refractive index of the ordinary ray.	38
$\hat{k}^{(1)}$	Incident propogation vector.	38
$\hat{n}$	Normal.	38
$\hat{s}$	Unit Ray vector for extra-ordinary ray.	38

ϵ	Dielectric tensor.	38
$m_e^{(2)}$	Refractive index of the extra-ordinary ray.	39
κ^o	Absorption for the ordinary ray.	40
κ^e	Absorption for the extra-ordinary ray.	40
K^o	Characteristic constant of medium for ordinary ray.	40
K^e	Characteristic constant of medium for extra-ordinary ray.	40
θ	Angle between ray and optical axis.	40
n^o	Refractive index for ordinary ray.	40
n^e	Refractive index for extra-ordinary ray.	40
$\bar{r}$	Colour matching function for red.	41
$\bar{g}$	Colour matching function for green.	41
$\bar{b}$	Colour matching function for blue.	41
λ	Wavelength of light.	41
S	A given spectrum.	41

Chapter 1

Introduction

The world is filled with many wonders, from its living inhabitants, their creations and even the earth beneath our feet. From the early ages of man, we have been fascinated by things of beauty, precious metals and stones. These metals and stones occur naturally on Earth, taking millions of years to form.

Minerals are prominent in our lives. They are used in many things, from make-up to cars to the planes of glass in windows. One of these minerals is called quartz, and it is used in many household objects.

In our daily lives we do not see quartz in its natural form. We see it in window glass, oscilloscopes, pressure sensors, watches, jewelry, etc. Quartz exhibits many properties that are usefull. For instance, it can start a fire (flint) and generate electricity (piezeoelectricity).

The natural form of quartz is very beautiful and occurs naturally in most parts of the world. Prominent souces include Brazil, Canada and the United States. The appearance of quartz is not as simple as a hexagonal prism of clear stone, there are many things that effect the appearance of it.

This report shall explore minerals, quartz and how we can approach the problem of simulating naturally occuring quartz crystals.

Chapter 2 introduces the basics of mineralogy: identification and properties of rocks and minerals, and crystal growth.

Chapter 3 discusses the varieties of quartz and properties such as colour, shape and inclusions.

Chapter 4 explains properties of light such as reflection, refraction, diffraction, birefringence, and fluorescence and how they may affect the appearance of quartz.

Chapter 5 outlines algorithms and results from various papers that address the simulation of the appearance of minerals and discusses how they can be applied to the rendering of quartz.

Finally, Chapter 6 underlines practical observations made during this study.

Chapter 2

A Field Guide Introduction to Mineralogy

In this chapter, we discuss the basics of mineralogy starting with the differences between a rock and a mineral. Visual properties and methods of mineral identification and described and the chapter concludes with a basic introduction to crystals and crystal growth.

2.1 Rocks

A rock is a conglomeration of one or more distinct minerals [5]. The mineral components of a rock named ”X” may vary in quantity and type yet still bear the same name. For example, granite is composed of many minerals including quartz, feldspar, mica and hornblend, but the appearance and exact percentage of these components may vary between samples and within a given sample [8]. Figure 2.1 shows a sample of granite with large crystal components and notable salmon coloured feldspar crystals.

But what sort of rocks are composed of a singular pure material? Pure marble is a rock composed entirely of the mineral calcite. It can be formed by the errosion of calcite crystals, forming a rock known as limestone. When limestone is exposed to extreme heat and pressure, it will turn into pure marble [8][12].

2.1.1 Classification of Rocks

Despite the variety displayed in rock samples, there is a system that is used to classify and identify rocks. This classification system divides rocks into three groups according to how they were formed. These groups are named: igneous, sedimentary and metamorphic.

Igneous rocks are formed by magma that cools as it rises. The magma crystallizes and is glued together during the magmas’ upwards motion, forming rock. The crys-

Figure 2.1: A sample of granite with large crystal components and galena inclusion.

tallized minerals forming igneous rocks are sharp and angular. Granite is an example of an igneous rock (Figure 2.1) [5].

Sedimentary rocks formed by the errosion of rocks and minerals, land, soil and decaying organic materials. These materials are compressed and cemented together by crystals forming in the water between bits of sediment. The crystals seen in a sedimentary rock are small and rounded, and the rock often has a brittle and layered appearance. Fossilized remains are found mainly in sedimentary rock [5].

Metamorphic rocks are created from both igneous and sedimentary rocks. Through heat and pressure the components of igneous and sedimentary rocks are broken down and re-crystallized forming new crystal structures. For example, the sedimentary rock limestone becomes marble. Another example of a metamorphic rock is slate, which is formed from a sedimentary rock called shale [5].

2.2 Minerals

A mineral is a known chemical compound that naturally occurs (on Earth without the assistance of mankind) in a crystalline form. For example, the compound silicone dioxide is a mineral commonly known as quartz and can be found in crystal form all over the world.

2.2.1 Mineral Identification and Classification

Minerals can be identified by their colour, shininess (luster), hardness, shape and various other traits. The next few sections will briefly discuss the common means for mineral identification.

Figure 2.2: Polished and unpolished samples of sedimentary rocks. Note the layered appearance of the rock.

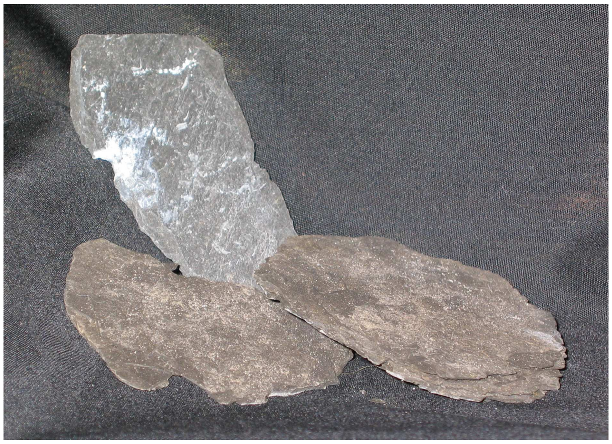

Figure 2.3: Samples of slate, a metamorphic rock.

2.2.2 Mohs Hardness Scale

A mineral can be identified in part by its hardness. Mineral hardness illustrates how easily a sample can be scratched. The Mohs Hardness Scale is composed of ten reference minerals, when using the scale to identify a mineral's hardness we start with the first reference mineral and work upwards until we find find a reference mineral that scratches the sample [12].

Mohs Hardness Scale:

1. Talc
2. Gypsum
3. Calcite
4. Fluorite
5. Apatite
6. Feldspar/Orthoclase
7. Quartz
8. Topaz
9. Corundum
10. Diamond

Talc, the softest reference mineral on the scale is so soft that its outer surfaces turn to dust when handled. The residual dust is soft and pearly. Talc is commonly used in baby powder and other beauty products.

Figure 2.4: A sample of talc, a soft and powdery mineral.

Gypsum, the second softest mineral is more stable than talc. It does not turn to dust when handled, but it can be scratched very easily. Gypsum is used in many art materials and supplies from Gesso (a type of primer) to stone carvings.

Calcite comes in at number three, a mineral that is seen in many places. Calcite is the main component of limestone and marble. It is also used in antacids and calcium supplements.

Fluorite is a colourful mineral that is used as flux for manufacturing steel. Fluoride is an additive to water and toothpaste for the prevention of tooth decay. Figure 2.6 shows a variety of fluorite called Blue John, found only in Devonshire, England.

Figure 2.5: A sample of gypsum, the second softest mineral on the Mohs Hardness Scale.

Figure 2.6: A rhombohedral shaped crystal of reddish-orange calcite.

Apatite, is a significant component of teeth and bones. It is also used in fertilizers and dental hygiene products.

Feldspar is a main component of granite and is found everywhere. There are many varieties of feldspar with a wide range of colours, amazonite (Figure 2.7) is a lead-containing greenish-blue variety.

Quartz is one of the most common minerals on the planet. It comes in many colours and varieties. Quartz is a main component of glass, used as an abrasive, cut into gemstones and employed in oscillators and pressure sensing-devices.

Figure 2.7: Blue John variety of fluorite from Devonshire, England.

Figure 2.8: Salmon pink feldspars and greenish-blue feldspar (amazonite).

Topaz, corundum and diamond are very hard minerals that are used as gemstones and for cutting and grinding blades.

In the occasion that reference minerals are unavailable, there are common items that can be used as replacements. A steel-bladed knife has a hardness of five, a copper penny is three and a fingernail is two point five. Since glass is composed mainly of quartz, glass can be used as a household item with hardness between six and seven [12].

2.2.3 Streak

Another common method used for identification of a mineral is something called streak. When a mineral is rubbed up against a tile of unglazed porcelin, a fine powder results. The colour of this powder is refered to as the streak [12]. For example, the streak of quartz is white [12].

2.2.4 Cleavage and Fracture

Cleavage is used to describe the planes within a mineral with weak bonding. A mineral can easily be split along these planes and cleaves/breaks into specific shapes based on the mineral structure [12]. We describe cleavage based on how well the mineral cleaves. Perfect cleavage occurs if the mineral breaks into continuous planes that are smooth enough to reflect light. Calcite is an example of a mineral with perfect cleavage. It cleaves along three directions into rhombohedrons. Good cleavage produces planes that are free from fracture, but are not as continuous or smooth. Poor cleavage produces planes, but they may contain fractures and be discontinuous [12].

Another excellent example of cleavage is with a mineral called mica. Mica appears as a stack of transparent sheets. It is very easy to cleave mica simply by peeling one or more thinner-than-paper sheets from the larger sample.

Figure 2.9: A sample of mica.

Fracture describes how a mineral may break by means other than how its structure dictates. There are four main catagories of fracture: conchoidal, irregular, hackly and splintery [12]. Conchoidal which is used to describe fractures that appear curved smooth similar to broken glass. Quartz, a primary element of glass, has a conchoidal fracture. Irregular fractures are rough with random particles or points. Hackly fractures are sharp-edged. Splintery fractures look like a piece of broken wood . Malachite has both conchoidal and splintery fractures [8].

2.2.5 Colour and Luster

Another method that is used in the field to identify a mineral is the colour of the mineral. Although a given mineral may exist in a range of colours, the common

Figure 2.10: A sample of polished malachite that has broken.

ranges for many minerals are known. The colour that we see for a given mineral is due to the wavelength(s) of light that are reflected and/or transmitted [12][8].

Mineral luster describes the spatial distribution of light – reflective properties of the mineral surface. Luster is divided into two groups, metallic and non-metallic. Minerals falling under the metallic group include pyrite, and reflect large amounts of light. The metallic group is divided into two catagories, metallic (reflecting at least twenty to fifty percent of incomming light rays) and sub-metallic (reflecting twenty percent or less of incomming light rays). Metallic minerals are not usually transparent [12][8].

Figure 2.11: A sample of pyrite showing metallic luster on the faces of its crystals.

Non-metallic luster minerals are further divided into the following groups: vitreous, subvitreous, resinous, earthy, waxy, pearly and silky. Vitreous is the catagory used to describe minerals that are as reflective as a pane of glass (a pane that is not frosted). Subvitreous luster is less reflective than glass. Resinous minerals have the appearance of gum or glue. Earthy minearls have the appearance of dirt, waxy the appearance of candle wax, pearly the appearance of a pearl and silky which has the appearance of silk [12][8].

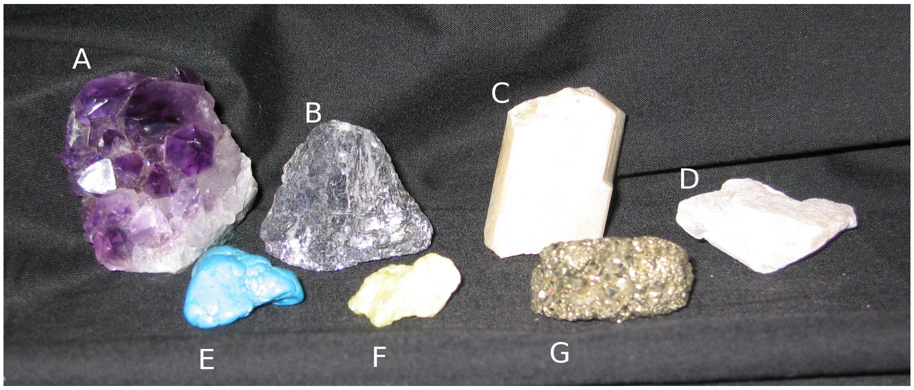

Figure 2.12: Minerals exhibiting different luster. A) Amethyst - Vitreous, B) Galena - Sub-Metallic, C) Gypsum - Silky, D) Talc - Pearly, E) Turquoise - Waxy, F) Sulfur - Earthy, G) Pyrite - Metallic.

2.2.6 Pleochroism

Pleochroism is a description of how minerals may appear to change colour when they are rotated under a light source. The colour seen is dependent on the direction of light rays hitting the polarized surfaces of the mineral. It is common in minerals that exhibit double-refraction. For example calcite exhibits pleochroism. When a clear calcite crystal is placed over an image and the viewer observes the image through the crystal, two images are seen instead of one [12].

2.2.7 Crystal Classes, Habit and System

Crystal class, system and habit are used to describe the symetry and shape of a mineral. Crystal class refers to a unique combination of reflection, rotation, inversion and rotoinversion of a crystal along its lines of symetry to form a mineral. Crystal system describes the axis of symetry present in a mineral. There are six classes for system: isometric, hexagonal, monoclinic, orthorhombic, tetragonal and triclinic [12][8].

Crystal habit is used to describe the outward appearance of a crystal, its growth patterns and intergrowth. For example, the crystal habit of corundum (more commonly known as sapphire and ruby) states that it forms tapering hexagonal crystals, basal pinacoids, and twinning may occur. This essentially means that corundum can be found with flat-top and bottom hexagonal shaped columns that may be tapered inwards near the ends and two or more corundum crystals may be intergrown in a symetrical fashion [12][8].

2.3 Crystals

In the discussion of minerals the term crystal appears frequently, but what exactly is a crystal? A crystal is an ordered arrangement of atoms in a long-range repeatable pattern that forms an orderly shape. Crystals are comprised of a homogeneous compound [5].

2.3.1 Crystal Formation

Crystals are formed by a growing process. A crystal is grown in a saturated growing solution that contains the building materials for the crystal. The growth solution may be a solid, a liquid or a gas. The building materials for a crystal are made of identical and repeatable atomic arrangements, sometimes refered to as a ”building block”. The smallest possible building block is called the ”basic block”, and it is the smallest block that can be repeated to form a crystal [5].

There are two types of ”building blocks”, an open arrangement and a closed arrangement. Figure 2.13 illustrates the difference in the arrangement of atoms between open and closed arrangements. The elements of these blocks are the atoms used to form the compound of the minerals and the arrangement refers to how the atoms are structurally packed/bonded into a building block. Crystals that are transparent typically exhibit an open-arrangement, whereas metallic (opaque) crystals are typically formed from a closed arrangement [5].

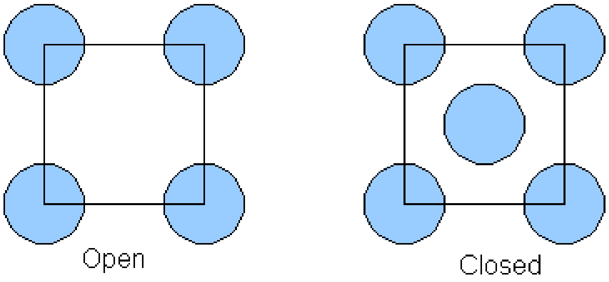

Figure 2.13: Open vs. closed arrangement of atoms in a building block.

Figure 2.14 is a diagram depicting a metallic cubic crystal with a closed arrangement of atoms. The ”basic block” is outlined, and one can see that when it is repeated it forms a larger version of the same shape [5].

The growing solution for a crystal is super-saturated, there is more solute (crystal building chemical) contained within the solvent (growing solution) than would be possible without changing the temperature or pressure of the solute. Even a slight change in a super-saturated soluction can cause the solute to separate from it.

The solute is attracted to ”seeds” (small, already crystallized particles). If no seed is present, as the solute begins to evaporate, seeds will form in the solution, causing

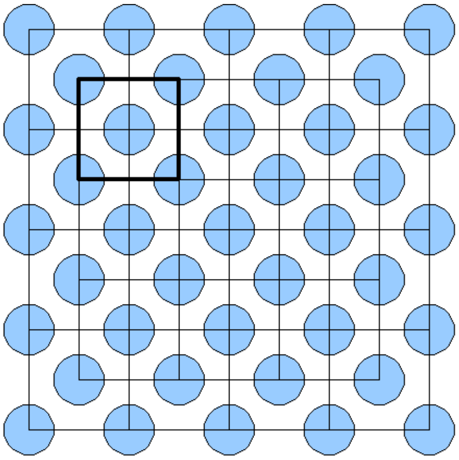

Figure 2.14: A diagram of a metallic crystal exhibiting a closed arrangement of atoms [5].

further growth of the crystal(s). However, evaporation is not the only method by which a super-saturated growing solution can form crystals. Crystallization may occur due to temperature shifts, changes in pressure and chemical reactions.

Observing how crystals are formed can be done in a kitchen with very simple materials. To grow a crystal from a seed, one can create a water based super-saturated solution of alum (Potash Alum, $KAl(SO_4)_2 - 12H_2O$)) and suspend or place a seed of alum into the solution. After a few days, the seed crystal will grow into a larger crystal.

To grow a crystal formation without a seed, one can create a water based super-saturated solution of urea $((NH_2)_2CO)$. Withing seconds (as the solution begins to cool), the solution should crystallize into tall, thin needle like crystals[1].

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[1] The mentioned experiments were conducted by Lesley Northam in 1996.

Chapter 3

Quartz Properties and Varieties

In this chapter, we explore the varieties and properties of quartz. The presentation concentrates on the crystalline varieties of quartz, and on properties such as streak, fracture and colour.

3.1 Identification

Quartz is a common mineral chemically defined as SiO_2, silicon dioxide. It is found in many parts of the world, and it is the main component of many types of rock (such as granite). There are many varieties of quartz that occur in both crystalline and microcrystalline forms [8]

3.1.1 Basic Properties

Table 3.1 shows the general identification points for quartz. Data about specific varieties may vary from what is listed.

3.1.2 The α and β Forms of Quartz

There are two unique forms of quartz, called α and β. Both α and β quartz are SiO_2, but the symetry differs due to distortions in the lattice. The α-quartz is a member of the rhombohedral-hexagonal crystal system. It has three-fold symetry, less planes of symetry than β quartz and a higher specific gravity. Most quartz samples found are α-quartz [8].

The crystal system of β-quartz is hexagonal, and has six-fold symetry. The β-quartz exists in very high-temperature environments (the higher symetry makes it stable in high heat). When the temperature drops below 573 degrees Celcius the lattice of β-quartz is destroyed, creating the three-fold symetry lattice that is α-quartz. In the remainder of this report, only α-quartz will be considered [8].

Table 3.1: The Properties of Quartz [8]

Property	Value
Chemical Formula	SiO2
Hardness	7
Colour	clear, white, red, orange, yellow, green, blue, purple, brown, black
Luster	vitreous
Streak	white
Cleavage	none
Fracture	conchoidal
Crystal System	trigonal, hexagonal
Crystal Habit	six-sided pyramid topped hexagonal prisms growing in any formation
Specific Gravite	2.65
Index of Refraction	1.544 - 1.5553

3.1.3 The Varieties of Quartz

Quartz, despite being known as SiO_2, has many varieties. The variations are caused by impurities.

Not all variations of quartz form crystals. Those varieties that do not form crystals are said to be microcrystalline quartz, a sample made up of microscopic crystals of the parent mineral (in this case, quartz). Among these varieties are agate, chalcedony, flint, and jasper.

Agate appears as a banded, glass-like mineral that is often found on the inside of geodes.[1] Agate is comprised mainly of the chalcedony. It is often used a decorative mineral. Agate is often dyed brilliant colours for decorative purposes as shown in Figure 3.1.

Chalcedony is a variety of quartz that is formed by fibrous crystals of quartz merging together. It is known to be blue, white and brown, and it is often seen as a component of agate. The hardness of chalcedony is less than crystalline quartz, and it has a the specific gravity varies depending on the distance between crystals. A pale blue and white banded sample of chalcedony can be seen in Figure 3.3.

Jasper is a reddish brown variety of microcrystalline quartz that is often used in jewelry. Flint is a gray to black variety that is used to start fires.

The remainder of this report will focus more strictly on those varieties of quartz that are found in crystal form in nature. Among these varieties is: amethyst, ametrine, citrine, milky quartz, rock crystal, rose quartz, and smoky quartz.

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[1] A geode is an ordinary looking stone that when opened is lined with crystals as seen in Figure 3.2 [8].

Figure 3.1: Three samples of agate, a thin sheet of blue-dyed agate and two pieces of natural agate displaying the characteristic banding. All samples have been polished and/or tumbled.

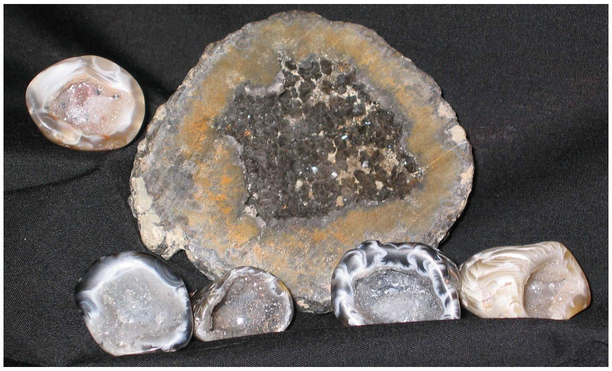

Figure 3.2: Samples of geodes filled with agate and quartz crystals.

Amethyst is a purple variety of quartz that is mined in many places, notably Canada (Northern Ontario) and Brazil. The colour of amethyst may range from a light purple to a deep reddish-purple. It is found in crystal form on its own and inside geodes. Figure 3.3 shows a sample of amethyst in a rich purple colour that was found in Brazil.

Ametrine is a type of quartz that contains two colours. As its name might suggest – ametrine has both amethyst and citrine within the same crystal. Ametrine was

Figure 3.3: A pale blue and white banded sample of chalcedony.

Figure 3.4: Amethyst from Brazil.

originally found in Bolivia, but may also be found in India and Brazil.

Citrine is a yellow to brown variety of crystalline quartz. Although citrine may occur naturally, it can be created by heating amethyst.

Milky quartz is milky-white in colour, and it is not perfectly transparent.

Rock crystal could be called pure quartz as it has no colour and it is very transparent (like looking through glass) – there are no noticable impurities in this variety of quartz.

Rose quartz, as its name indicates, is a rosy pink coloured variety of quartz. It is rare to find rose quartz in crystal form, but when it is found it is transparent. Non-crystalline rose quartz is milky in appearance (refer to Figure 3.4).

Figure 3.5: Non-crystalline rose quartz (please ignore the hot glue on the top and bottom of the sample).

The last variety, smoky quartz, obtains its name from its gray to black appearance. Smoky quartz may also appear in grayish-browns [8][12][10].

Figure 3.5 illustrates a few varieties of microcrystalline and crystalline quartz.

3.2 Colour

Pure quartz, SiO_2, is clear in colour. But there are other varieties of quartz that occur in a rainbow of colours. Are these coloured varieties of quartz not actually quartz? Or is there some impurity or process that has happened to cause our eyes to percieve the rainbow that we do? This section will discuss the current theories on how quartz exists in its array of colours, starting with the outline of the general theories on how minerals exhibit colour.

3.2.1 Substitutional and Interstitial Sites

In order to understand some of the following material, it is important to know what a substitutional and interstitial site is. Given a crystal lattice of atoms, a substitutional site is a site where an atom ”X” replaces one of the atoms ”Y” in the ordered lattice. For example, if we have a crystal of lead (Pb), when one of the Pb atoms is replaced

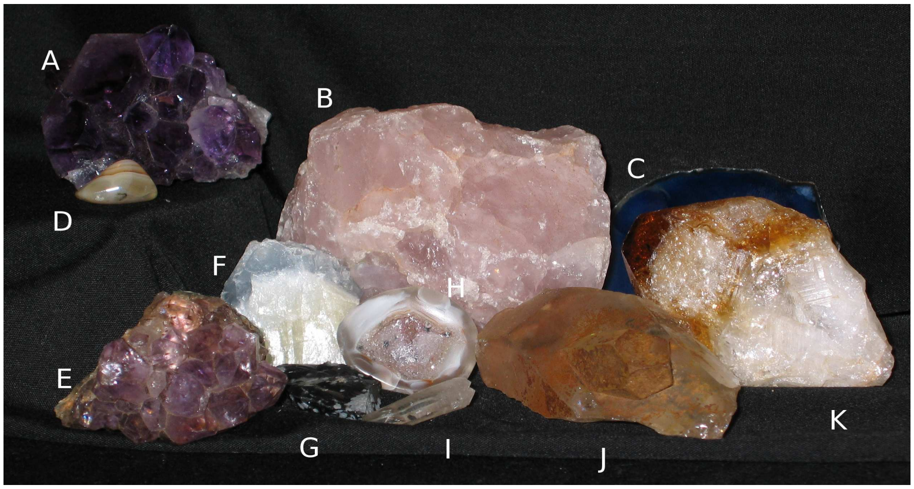

Figure 3.6: Some of the varieties of quartz: A) Deep purple brazillian amethyst. B) Milky pink rose quartz. C) A slice of agate dyed blue. D) A polished stone of natural agate. E) Amethyst (possibly ametrine) cluster from an unknown mine. F) Blue and white chalcedony. G) A piece of onyx. H) Agate geode with quartz crystals. I) A single rock crystal. J) Two fused crystals of rock quartz covered by a thin layer of rust. K) A dark crystal of citrine on a milky base.

or substituted by another atom, say iron (Fe), the site is called a substitutional site [5][10].

An interstitial site is when at atom ”X” bonds with the ”Y” atoms of the crystal lattice. There are two ways that this may occur. The first way is that the atom ”X” may fit into the tiny open spaces of a closely-arranged (usually metallic) lattice. The second interstitial site is found in an openly-arranged lattice (often transparent minerals like quartz). The atom ”X” fills in one of the vacant spots that would have been previously occupied had the lattice been closely-arranged. It is also possible that during the formation of the mineral, some of the lattice was not filled in and the ”X” atom may fill in the vacant spot [5][10][8].

3.2.2 Band Theory

In a metallic mineral, the energy levels of the valence band (highest level of electrons that cannot be used in bonding) overlaps with the conduction band (lowest level of electrons that is used in bonding). Light from all visible spectrums is absorbed (the mineral is not transparent), and re-radiated when electrons fall from high-energy positions to low-engery positions. If the mineral is a semiconductor, then there is a gap between the valence band energy and the conduction band energy. This gap absorbs light from the visible spectrum if the energy of the wavelength is greater than the energy of the gap. Thus it is possible to have minerals absorbing all wavelengths of visible light (appearing black) and minerals absorbing none (appearing clear or white) [8].

3.2.3 Charge Transfer Transitions

Suppose two positively charged ions ”cations” are beside each other in a crystal lattice and one cation, ”X”, has a lower charge than the other cation, ”Y”. When the mineral is exposed to electromagnetic radiation an electron from cation, ”X”, transfers to a high-energy orbital of cation, ”Y”. Since ”X” lost an electron, its positive charge increases. The difference in energy levels between cations ”X” and ”Y” absorbs light typically in the red region (700nm) of the visible light electromagnetic spectrum [8].

3.2.4 Crystal Field Theory

A crystal field is an electric field produced by negatively charged anions that have been placed in a coordination polyhedra (a crystal building block that is greater than one atom in size) with a transition element (elements like iron with unpaired electrons in their outer orbitals). A crystal field is split when orbitals in the 3d subshell[2], have varying energy levels. When the coordination polyhedra attach during mineral growth, the difference between the higher and lower engery levels (within the 3d subshell) absorbs wavelengths of light that are between the yellow (580nm) and green (500nm) regions of the light spectrum, but also wavelengths in the violet (400nm) region [8] (refer to Chapter 4 for more details on light).

3.2.5 Colour Centers

Colour centers occur when electrons are in the wrong spot of the crystal lattice structure. There are two kinds of colour centers. The first is an electron colour center which occurs when an anion is missing from the crystal lattice. This hole could be filled by another electron supported by the crystal field. If this electron is excited, it may cause the absorption of light. The second colour center, a hole colour center, occurs when an electron disappears (it may have been attracted to another part of the crystal). The energy level of the hole may absorb visible light. Minerals that exhibit colour due to colour centers lack colour-fastness[3] [8].

3.2.6 Amethyst

Amethyst is a beautiful variety of quartz that appears in shades of purple – from pale lavender, to a deep royal purple. Impurities of iron in quartz are thought to be the

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[2] A subshell is an area around an atoms nucleus where an electron of a certain energy level has a probability of being present [9].

[3] Colour-fastness refers to the ease at which colour can be bleached from an item [10].

cause of this brilliant purple colour. The amount of iron present ranges from 10 ppm to 350 ppm [8].

It is believed that light is absorbed by amethyst due to colour centers. Three iron centers have been identified in samples of amethyst. There are many theories and models as to which positive ions of iron fill these centers and how they cause the absorption of light. One of these suggested models proposed by Lehmann in 1967 proposes that substitutional Fe^{3+} when exposed to gamma-radiation oxidizes to Fe^{4+}. The ”freed” electron becomes trapped by an interstitial Fe^{3+} which then reduces to Fe^{2+}, all together producing the brilliant purple colour of amethyst [10].

The colour of amethyst is not stable. If a sample is exposed to light (such as sunlight) the colour may disappear. For example, a sample of amethyst left in direct light may lose all of its colour within three years [10]. The colour of amethyst can also disappear when a sample is exposed to heat in the range of four hundred degrees celcius. Exposure to such heat may cause a sample of amethyst to turn into citrine. It is also possible to return the purple colour to a sample of amethyst that was previously bleached (turned clear) by exposing it to radiation (gamma rays and/or x rays) [10].

Figure 3.7 shows two small amethyst formations. The sample of the left side is from an uknown origin, has a paler shade of purple and may contain citrine. The right sample is from Brazil and displays a bold purple colour.

Figure 3.7: Samples of amethyst.

3.2.7 Citrine

Citrine is a variety of quartz that is yellow, orange or brown in colour. As mentioned in section 3.2.6, citrine colours can be obtained from heating amethyst, but it can also be artificially obtained by irradiating and/or heating smoky quartz or colourless quartz. Synthetic citrine is obtained by growing synthetic quartz in the presense of iron.

Natural citrine contains substitutional Fe^{3+}, but it is not believed to be the cause for colour. However, it is believed that the colour exhibited by natural citrine is due to small (sub-microscopic) particles of iron oxide [10].

Figure 3.8 shows a crystal of citrine growing on milky quartz. It is unknown whether this sample is naturally occuring citrine, or heat treated amethyst. However, given its low purchase cost, it is most likely the latter, heat treated amethyst.

Figure 3.8: A crystal of citrine.

3.2.8 Milky Quartz

Milky quartz is a transclucent white variety of quartz. The appearance is caused by water inclusions throughout a piece of rock crystal [8].

3.2.9 Rose Quartz

The cause for the soft pink and red colours of rose quartz is unclear. Observations have indicated that the source for colour in non-crystallized (vein) rose quartz may be different from crystals of rose quartz [10].

A prominent suggestion for the colour of vein rose quartz is that the pink is seen due to the fact that rose quartz contains inclusions of a red to pink mineral called dumortierite. The colour of vein rose quartz will fade with exposure to heat, but it is unknown if the fading occurs in the quartz or the dumortierite.

The colour of crystalline rose quartz is delicate, when exposed to two hundred degrees Celcius or ultra-violet radiation it fades. It is thought that the colour is due to a hole colour center formed from the removal of an electron from a substitutional aluminum-oxygen-phospate group. The colour of crystalline rose quartz can be enhanced by ionizing radiation [10][8].

3.2.10 Smoky Quartz

Smoky quartz appears in shades of transparent brown, and gray to black (like the colour of smoke). This colour is due to substitutional aluminum. Smoky quartz may contain a few thousand atoms of aluminum per million atoms of silicon.

A hole colour center is produced at a substitutional aluminum site when an electron is removed from a pair of electrons in a neighbouring oxygen. It is unknown where this freed electron gets trapped.

The smoky colour can be synthetically produced by passing a current through a heated sample of clear quartz, or by irradiating or heating a sample of clear quartz. However, the colour of smoky quartz is not stable, and can fade with heat exposure [10].

3.3 Fracture

Quartz has no cleavage, but it does have an interesting fracture [8]. The fracture for quartz is classified as conchoidal. A conchoidal fracture has the appearance of broken glass, *i.e., the surface is smooth and rounded, free from sharp edges*. In samples of clear rock-crystal, it is easy to see the fractures at the base of the crystal (if it was broken off of a group of crystals or another mineral specimen), and on inside of a crystal.

Fractures on the surface of the crystal reflect light in a rainbow of colours. Fractures on the interior of the crystal effect how light interacts with the crystal by creating additional planes of reflection. These properties are observed from sample set of rock crystals. It is easier to see these properties in rock crystal since it is colourless.

Figure 3.9 shows a small crystal of rock crystal that was broken off of a larger crystal. The fracture is very smooth to the touch. The reddness is caused by a rust formation on the exterior surface of the crystal faces.

3.4 Striation

We have covered the basic properties of quartz, the colours and inclusions, and fracture. But when observing a crystal of quartz, the faces appear to be cracked or misformed. These bumps are not fractures or cracks, they are called striation. Specifically striations are as small furrows and ridges on the faces of crystals [5].

Striations occur during growth when the chemical concentration of the growing solution increases or decreases. In quartz, striations are caused by the intergrowth of dominant prismatic and subsidiary rhombohedral crystals. When quartz is observed, it is noted that striations occur on the prism faces of the crystal (and not the pyramidal caps).

Figure 3.9: Quartz fracture.

Chapter 4

Light and Quartz Interactions

Light is what makes the world visible. But what is light? Light is considered to be the visible portion of the electromagnetic radiation spectrum. Electromagnetic radiation could be described as an oscillation of perpendicular electric and magnetic fields that together produce photons. Simplistically, these photons (or particles of light) travel in waves and create what we call light. The wavelength of a single ray determines the type of electromagnetic radiation, and in the case of visible light – the colour [3]. In this chapter, we introduce light related phenomena and how they may affect the appearance of quartz.

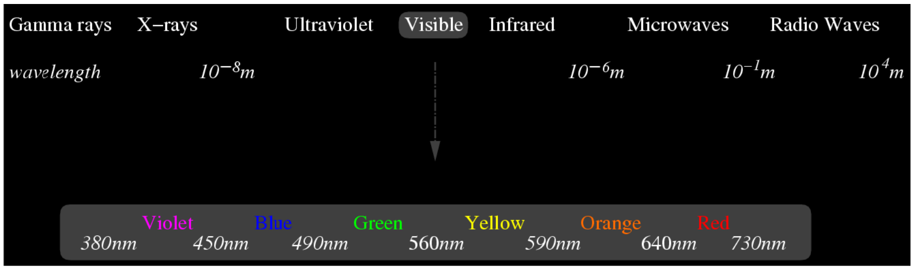

Figure 4.1: The electromagnetic radiation spectrum contains sound waves, microwaves, infrared rays, light, ultra-violet rays, x-rays and gamma rays. Light is between 730nm (red) and 380nm (violet).

4.1 Reflection

Reflection occurs when a ray of light hits a surface and bounces off it. Classically, the angle of incidence is equal to the angle of reflection. Feynman [3] has shown that although the most probable reflection occurs at the classical point of incidence, the rest of the surface may take part in reflection as well. The mineral characteristic luster described in chapter one describes qualitatively the reflective properties of a mineral. Quartz is considered to have a vitreous luster. Upon observing the faces of a quartz crystal, we can see that they are smooth and capable of reflecting light upon experimentation.

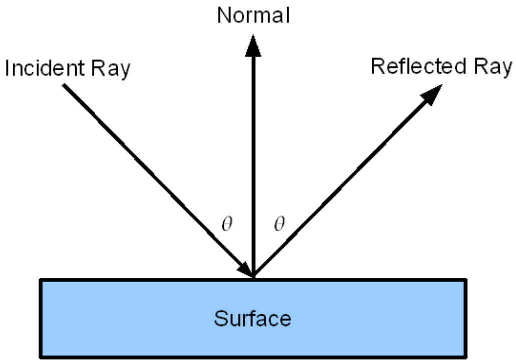

Figure 4.2: Sketch depicting classical reflection in which the angle of incidence is equal to the angle of reflection.

4.2 Refraction and Dispersion

Refraction of light occurs when light bends as it passes through a material. A value known as the refractive index is used to describe how light will bend as it passes through a material. The refractive index for a material may differ depending on the wavelength of incident light. The refractive index can be calculated as [8],

$$n = \frac{V_v}{V_m}, \tag{4.1}$$

where:

- V_v is the velocity of light in a vacuum,
- V_m is the velocity of light in the material, and
- n is the index of refraction.

Depending on the angle of incidence and the index of refraction of the materials involved, it is possible for the light to be reflected internally. When this occurs, it is called **total internal reflection**, and the angle that it occurs at is called the **critical angle** [5]. Pure quartz is a colourless, transparent mineral and is capable of refracting light. Quartz has a refractive index specific to the wavelength of incident light, it ranges from 1.55 for red (730nm) light to 1.7 for ultra-violet light (200nm) [7].

Snell's Law is a formula that allows us to calculate the angle of refraction and/or the index of refraction in a given material [8]. It is stated as:

$$\frac{sin\theta_1}{sin\theta_2} = \frac{n_2}{n_1}, \tag{4.2}$$

where:

- θ_1 is the angle between the incident ray and the normal,
- θ_2 is the angle between the normal and the propogated ray,
- n_1 is the index of refraction for the incident material, and
- n_2 is the index of refraction for the material.

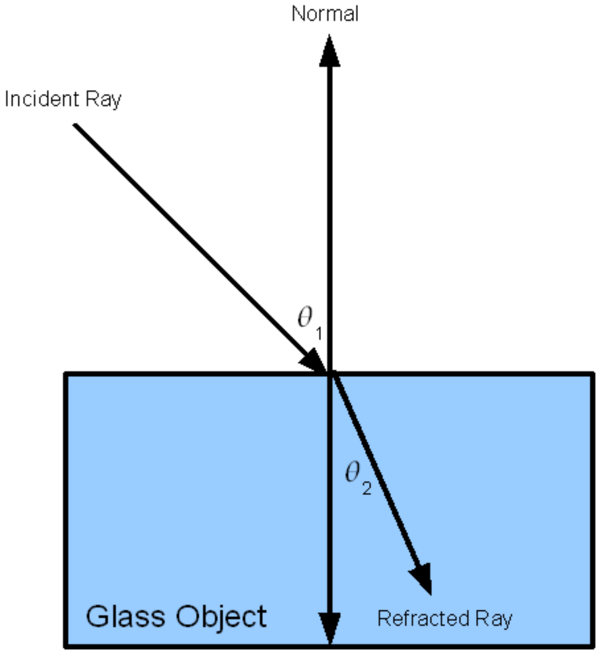

Figure 4.3: Sketch depicting refraction. When the indicent ray passes through the second material the light bends. If the index of refraction for the incident material is the same as the second object, then the light does not bend and θ_1 will be equal to θ_2.

White light is actually composed of coloured light – the full visible light spectrum from red to violet. When you shine a white light through a triangular prism, it will seperate into the full spectrum. This behaviour is called dispersion, and it occurs because the refractive index for each wavelength of light is different causing each colour to bend a unique amount. This experiment is illustrated in Figure 4.4.

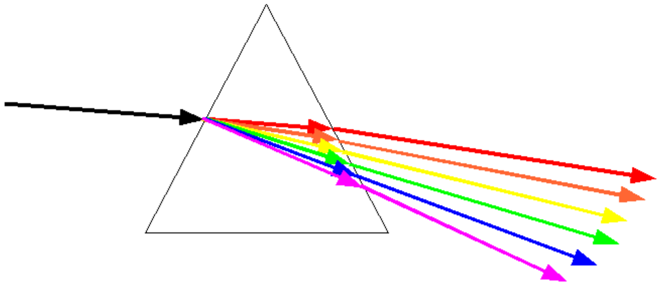

Figure 4.4: Sketch depicting dispersion. When a ray of white light travels into a prism, the different colours of light composing white are refracted differently, thus causing the white light to split into the ”rainbow”.

4.3 Polarization

Light is considered to be a wave composed of electric and magnetic field oscillations. It is propagated from some source towards the world, this direction is called the propagation vector, or direction. Unpolarized light oscillates on any plane that is perpendicular to the propagation vector. Polarized light, oscillates in a single plane perpendicular to the propagation vector [8][12].

4.4 Birefringence

A ray of light passes through an ansiotropic material and splits into two rays, the ordinary ray and the extra-ordinary ray. The ordinary ray follows Snell’s Law as shown above, however the extra-ordinary ray does not. Both the ordinary and extra-ordinary rays are polarized and oscillate on planes perpendicular to each other [8][12].

4.5 Isotropy

In the study of mineralogy, an isotropic material is considered to be a material such that the index of refraction for the material is the same throughout. That is, given a crystal C any ray of light from any source intersecting with C will have the same velocity as it travels through the crystal. The density and the strength of the electric feild (of the lattice structure) is uniform [8].

4.6 Ansiotropy

In mineralogy, an ansiotropic material is a material where the index of refraction may differ throughout the crystal. For example, suppose a crystal C is a rectangular prism and we shine a ray of light through through a thin section and then a long section. The index of refraction for these two directions is different. This is because an ansiotropic mineral's lattice structure differs in electron density and electrive feild strength, thus effecting the index of refraction. Quartz is an ansiotropic material [8].

4.7 Fluorescence and Phosphorescence

When a material is irradiated by ultraviolet light, it may re-emit visible light. A material is called fluorescent if it emits visible light only when the ultraviolet light hits the material. A material that continues to emit visible light after the source of ultraviolet rays is removed is called phosphorescent. For example, fluorite is a mineral that glows brilliantly under a black (ultraviolet long range 366nm and short range 254nm) lamp [8]. In addition, rubies may fluoresce under visible light.

Chapter 5

Related Rendering Work

In this chapter, we will discuss various papers relevant to the rendering of stone, crystals and minerals. How these papers apply or could be applied to the simulation of the shape and appearance of quartz will also be discussed.

5.1 The Appearance of Quartz

As discussed in Chapter 3, there are many varieties of quartz. But let us consider pure quartz for the moment. Chapter 3 discussed the physical properties of appearance, most importantly that quartz belonged to the hexagonal crystal system.

More simply, we can describe qualitatively the appearance of quartz as a hexagonal prism capped with a six-sided pyramid, with occasionally the odd extra face. It is noted (in Appendix B) that the shape is not perfect, the hexagonal prism appears stretched, squashed and even skewed amongst a sampling of crystal points. Even the faces of the crystal are not perfectly smooth – they are covered in striations. The striations on the sides (hexagonal prism) are rectangular, and on the pyramidal caps they appear smoother and nearly triangular.

When we look inward, into the substance that forms the crystal we note that it is not clear like a plate of glass or cup of water. There are many particles, cracks, fractures, phantoms, and cloudy inclusions that yield a natural and imperfect appearance.

Angell and Moore [1] discuss a graphics package for teaching crystal morphology. The software package allows the user to input descriptive information about the crystal: system, lattice information, class and facet information. From there, the program generates the facet structure defining the crystal shape and generates a stereogram illustrating the symetry of the crystal. It then constructs a data structure for storing the surface shape of the crystal and creates a pictoral representation of the crystal in orthographic and clinographic views. Finally, it generates a growth-sector representation of the crystal.

To store the surface shape, Angell and Moore start with a large tetrahedron and using the users input as a guide, the program creates the habit planes. The habit planes

”cut” portions of the tetrahedron, and when all habit planes are added the remains of the tetrahedron is the crystal shape.

Written in Fortran IV for a D.E.C. VAX 11/780, this program is quite old. However, the program would be usefull for creating and storing the crystalline shape of quartz.

Yokoi, Kurashige and Toriwaki [11] presented an algorithm for rendering the desirable inclusion that creates star sapphires.

Minerals exhibiting asterism or chatoyancy are filled with ”needle-like inclusions”. When light refracts and reflects in a sample, it is scattered by the inclusions yielding brilliant star-like patterns.

Yokoi, Kurashige and Toriwaki devised a method for rendering asterism and chatoyancy by introducing thin cylinders with micro-faceted surfaces into the sample. The cylindrical inclusions are placed homogeneously throughout the crystal. Their algorithm can be summarized as follows:

- Compute the ray distribution map inside the gem by generating all rays from light source to the stone. The points of intersection, refracted ray and transmitted coefficients are calculated and stored in a table.
- For each pixel x, consider the ray T connecting x to the eyepoint.
- For ray T: Compute the absorption of light. Compute I’, the light seen by the viewer due to reflection caused by the inclusions.

The light intensity seen by the viewer is expressed as:

$$T = r \cdot R + (1 - r)Fexp(-cl_0) + I', \tag{5.1}$$

where:

- T is the intensity of light that is seen by the viewer,
- r is the reflection coefficient at exit point,
- R is the intensity of specular light as seen by the viewer,
- F is the intensity of light from the source of light,
- c is the absorption rate,
- I is the intensity of the light source, and
- I' is the intensity of light due to inclusions seen by the viewer, which is given by:

$$I' = \int_{\bar{L}} (1-r)(1-r') \cdot I \cdot k\psi(H) \cdot exp\{-c(g(l)+l)\}dl, \tag{5.2}$$

where:

- $\bar{L}$ is a ray from the inclusion to the light source,
- k is the reflection coefficient for inclusions,
- H is the bisector of incident and reflected light vectors, and
- $\psi(H)$ is the fraction of inclusion facing H.

Yokoi, Kurashige and Toriwaki [11] presented the results of their algorithm by means of a series of images. The first set of images from the paper depict a stone commonly refered to as Cat's Eye, which is treasured for its chatoyancy effects. The second set of images show a star sapphire with asterism from various viewing angles. Visual inspection indicates that the effects of chatoyancy and asterism have been acheived. The authors conclude by stating the algorithm is not fast enough to be used in any commercial rendering product.

Although quartz crystals do not exhibit chatoyancy or asterism, they do have needle-like, fibrous and particle inclusions as well as phantoms and internal fractures. The discussed algorithm can be a starting point for creating a method of rendering the various inclusions common to quartz.

Dorsey *et al.* [6] presented an algorithm for generating and rendering weathered stone. Stone or rock as described in Chapter 2 is composed of particles from one or more minerals. Weathering of stone can occur by the travel of water or liquids over the stone surface, dissolving and recrystallization of mineral components caused by water, chemical alterations caused by forces such as oxidation and heat, and deposits made by pollution [6]. The algorithm includes methods for representing rounding sharp surface edges, yellowing, scabbing and salt crystallization on stone surfaces.

An input mesh is required by the algorithm to describe the original object. This mesh is passed to the ”Voxelizer” which covers the mesh surfaces in rectangular volumes called ”slabs”. At each vertex in the slab, water and dirt constances are stored for later use. After a slab has been created, it goes into the ”Quarry” to generate a clean peice of un-weathered stone. The clean stone slabs are sent to a simulator to be weathered, and are then rendered.

In rendering the weathered stone, Doresey *et al.* [6] noted that light scatters inside the stone due to inclusions of water and other particles. To model this subsurface scattering they first note that light transport in a medium can be calculated with the following formula [6]:

$$L(x, \overrightarrow{\varpi}) = \int_{x_e}^{x} \tau(x', x)\sigma(x') \int_{\Omega} \int (x', \overrightarrow{\varpi}', \overrightarrow{\varpi}) L(x', \overrightarrow{\varpi}') d\omega' dx' + \tau(x_e, x) L(x_e, \overrightarrow{\varpi}) \tag{5.3}$$

where:

$$\tau(x', x) = e^{-\int_{x'}^{x} \kappa(\xi) d\xi} \tag{5.4}$$

and:

- L is the intensity of propagated light,
- x is a point on the surface of a material,
- $\overrightarrow{\varpi}$ is the direction,
- x_e is an end point on the surface,
- τ is the transmittance function,
- σ is the scattering coefficient function,
- κ is the extinction coefficient function, and
- ξ is the extinction coefficient.

To simulate scattering by air and water bubbles, cracks and other inclusions, Dorsey *et al.* [6] uses an approximation to Mie scattering called ”two-lobed Schlick approximation of the Henyey-Greenstein phase function” [6]. A variant of photon mapping is used to store light that was scattered within the stone [6].

Dorsey *et al.* [6] provided results of their algorithm in the form of three sample stone carvings through increasing amounts of weathering. The first carving is a stone sphinx, the second of a roman sandstone column and the third being the bust of Diana the Huntress. The resulting images are pleasing to the eye, but the model has some limitations as stated in Dorsey *et al.*:

> Because the state of our scientific knowledge is incomplete, an exact model for stone weathering is not feasible. Therefore, our model is still a phenomenological one.

Although the form of quartz discussed in this article is in crystalline form and not stone form, Dorsey *et al.* [6] presents some interesting ideas that might be modified to suit the modelling of quartz crystals. For example, the striations on the faces of a quartz crystal could be simulated as a form of weathering – more simply than in [6] because their shape and pattern is known and definable. The paper [6] also presents a method for rendering subsurface scattering of light. A pure quartz crystal would have no inclusions, but such things do not exist naturally. Naturall quartz crystals contain water, air, and other particle bubbles, cracks and other inclusions that scatter light. Milky quartz, a variety that gets its colour from tiny inclusions of water could use the subsurface light scattering in Dorsey *et al.* [6] to achieve its milky white colour. Examples illustrating the scattering of light caused by inclusions in quartz can be seen in Appendix B.

5.2 Simulation of Light Interaction with Minerals

Quartz is a transparent material with smooth surfaces – capable of refracting and reflecting light. In order to simulate a quartz crystal, we must know how light is reflected and refracted by quartz. But what are the optical properties that affect how light may be reflected, refracted, dispersed, or emitted from quartz.

The first piece of information we need to know, is what an optical indicatrix is. An optical indicatrix is a diagram that describes the index of refraction for light passing through a medium from any direction. The diagram shows indices of refraction in elliptical forms perpendicular to the incident ray of light [8].

This indicatrix diagram is used for calculating the index of refraction for the ordinary and extra-ordinary rays as the light passes through the medium.

There are different types of optical indicatrix. The optical indicatrix of quartz (except in some rare amethyst cases), is called uniaxial positive. A positive uniaxial indicatrix is shown in Figure 5.1.

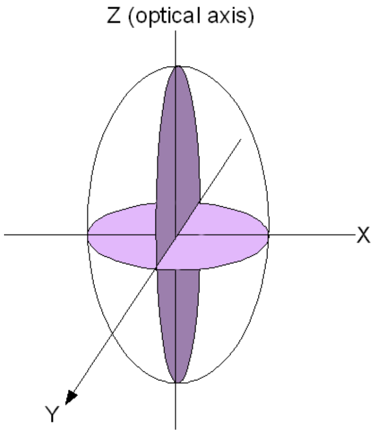

Figure 5.1: Positive uniaxial indicatrix for quartz with incident light travelling along the Y axis redrawn from [8].

But how could we calculate the refracted rays?

Beyerle and McDermid [2] described a method of calculating the ordinary and extra ordinary rays in uniaxial crystals. They first noted that in uniaxial crystals, the ordinary ray follows from Snell's law since the normal surface is spherical in the indicatrix.

They give the following formula for the ray vector and propogation vector of the ordinary ray:

$$\hat{k}_o^{(2)} = \hat{s}_o^{(2)} = \frac{m^{(1)}}{m_o^{(2)}}[k^{(1)} + (\{[\hat{n} \cdot \hat{k}^{(1)}]^2 - 1 + [\frac{m_o^{(2)}}{m^{(1)}}]^2\}^{\frac{1}{2}} - \hat{n} \cdot \hat{k}^{(1)})\hat{n}] \tag{5.5}$$

where:

- $\hat{k}_o^{(2)}$ is the propogation vector for an ordinary ray,
- $\hat{s}_o^{(2)}$ is the unit vector for a ray,
- $m^{(1)}$ is the refractive index of an isotropic medium,
- $m_o^{(2)}$ is the refractive index of the ordinary ray,
- $\hat{k}^{(1)}$ is the incident propogation vector, and
- $\hat{n}$ is the normal vector.

They then provide a means of calculating the extra-ordinary ray by transforming the elliptical normal space into a spherical one. First they prove that the ray vector can be calculated using the propogation vector given by:

$$\hat{s} = \frac{\epsilon\hat{k}}{|\epsilon\hat{k}|} \tag{5.6}$$

where:

- $\hat{s}$ is the unit ray vector for the extra-ordinary ray, and
- ϵ is the dielectric tensor.

Using the principle coordinate system denoted by:

$$\{\hat{e}_1, \hat{e}_2, \hat{e}_2\} \tag{5.7}$$

and a non-orthonormal coordinate system with basis:

$$\{\hat{o}_1, \hat{o}_2, \hat{o}_2\} \tag{5.8}$$

they form a transformation matrix:

$$\gamma = O \begin{bmatrix} \frac{1}{m_e^{(2)}} & 0 & 0 \\ 0 & \frac{1}{m_e^{(2)}} & 0 \\ 0 & 0 & \frac{1}{m_o^{(2)}} \end{bmatrix} O^T, \tag{5.9}$$

where:

$$O = \begin{bmatrix} \hat{e}_1 \cdot \hat{o}_1 & \hat{e}_2 \cdot \hat{o}_1 & \hat{e}_3 \cdot \hat{o}_1 \\ \hat{e}_1 \cdot \hat{o}_2 & \hat{e}_2 \cdot \hat{o}_2 & \hat{e}_3 \cdot \hat{o}_2 \\ \hat{e}_1 \cdot \hat{o}_3 & \hat{e}_2 \cdot \hat{o}_3 & \hat{e}_3 \cdot \hat{o}_3 \end{bmatrix} \tag{5.10}$$

and:

- e is a unit vector in the principle coordinate system,
- $\hat{o}$ is a unit vector in the non-orthonormal coordinate system, and
- $m_e^{(2)}$ is the refractive index for the extra-ordinary ray.

This matrix transforms from the elliptical normal space to a spherical one, where Snell's law can be used again as it was with the oridinary ray. Leaving the following formula for the propogation vector:

$$\hat{k}^{(2)} = \frac{|\gamma\hat{n}|^2\hat{k}^{(1)} + \{S - (\gamma\hat{n}) \cdot [\gamma\hat{k}^{(1)}]\}\hat{n}}{||\gamma\hat{n}|^2\hat{k}^{(1)} + \{S - (\gamma\hat{n}) \cdot [\gamma\hat{k}^{(1)}]\}\hat{n}|}, \tag{5.11}$$

with:

$$S = (\{(\gamma\hat{n}) \cdot [\gamma\hat{k}^{(1)}]\}^2 - |\gamma\hat{n}|^2|\gamma\hat{k}^{(1)}|^2 + \frac{|\gamma\hat{n}|}{[m^{(1)}]^2)}^{\frac{1}{2}} \tag{5.12}$$

Beyerle and McDermid [2] also give us a formula for calculating the propagation vector of a reflected ray of light, which is given by:

$$\hat{k}^{(2)} = \frac{|\gamma\hat{n}|^2\hat{k}^{(1)} - 2\{(\gamma\hat{n}) \cdot [\gamma\hat{k}^{(1)}]\}\hat{n}}{||\gamma\hat{n}|^2\hat{k}^{(1)} - 2\{(\gamma\hat{n}) \cdot [\gamma\hat{k}^{(1)}]\}\hat{n}|} \tag{5.13}$$

Beyerle and McDermid [2] concluded by comparing their results obtained for an isotropic uniaxial mineral (calcite) to those generated by using formulas of Simon and Echarri, Liang, and Zhang. They claimed that the results agree, and their (Beyerle and McDermid) formulas are faster by a degree of two to three times when all methods are implemented and run in Matlab [2].

How does this apply to quartz? Quartz is a transparent uniaxial mineral so these formulas could be used to calculate the oridinary and extra-ordinary rays during refraction and internal reflection. However, quartz is ansiotropic. Hence modifications to these formulas may be required to account for that.

Guy and Soler [4] presented an algorithm for rendering cut (faceted) gemstones for use in jewelry designing software. Assuming linear polarization, Guy and Soler use a modified version of Beyerle and McDermids ordinary and extra-ordinary ray calculations. The modified formulas take into account ansiotropic materials.

To calculate absorpance of light, Guy and Soler [4], uses the following formulas for ordinary and extra-ordinary rays originally presented by Born and Wolf in 1999:

$$\kappa^o = K^o \tag{5.14}$$

and

$$\kappa^e = K^e cos^2\theta + K^e(\frac{n^o}{n^e})^2 sin^2\theta, \tag{5.15}$$

where:

- κ^o is the absorption for an ordinary ray,
- κ^e is the absorption for an extra-ordinary ray,
- K^o is the characteristic constant of the medium for an ordinary ray,
- K^e is the characteristic constant of the medium for an extra-ordinary ray,
- θ is the angle between the ray and the optical axis,
- n^o is the refractive index for the ordinary ray, and
- n^e is the refractive index for the extra-ordinary ray.

These formulas for absorbance are independent of wavelength, and do not consider fluorescence. They also treat absorption as linear when it is actually elliptical.

Instead of representing light using the full spectrum of visible light, the standard primary components red, green and blue are used. Guy and Soler [4] claim that in using the primary red, green and blue components they limit spectral sampling – possibly over saturating colours instead of darkening them. To obtain the absorbance values for red, green and blue a derivation is given starting with a formula that turns a spectrum into red, green and blue as seen by the human eye. This is done with the following formula:

$$\begin{bmatrix} R \\ G \\ B \end{bmatrix} = \int_\lambda \begin{bmatrix} \bar{r}(\lambda) \\ \bar{g}(\lambda) \\ \bar{b}(\lambda) \end{bmatrix} S(\lambda) d\lambda \tag{5.16}$$

where:

- $\bar{r}$ is the colour matching function for red,
- $\bar{g}$ is the colour matching function for green,
- $\bar{b}$ is the colour matching function for blue, and
- λ is the wavelength of light.

For red, the absorbance value is:

$$\kappa_r = -\frac{1}{R_0} \int_\lambda \kappa(\lambda) \bar{r}(\lambda) S_0(\lambda) d\lambda \tag{5.17}$$

where:

$$R_0 = \int_\lambda \bar{r}(\lambda) S_0(\lambda) d\lambda \tag{5.18}$$

Guy and Soler [4] discussed a method for rendering faceted gemstones. A stone may have thousands of facets. Guy and Soler [4] presented an algorithm for regrouping facets into a tree called the facet tree.

The rendering algorithim first generates the facet tree by starting with a given facet and tracing reflected and refracted light to other facets, then clipping them to the original facet. The level of facet reflection/refraction depth will effect the size of the tree and the quality of the image. The facet tree is then rendered by traversing it with breadth-first search and extracting the refraction and internal reflection contribution values. A comparison of refraction/reflection depths is used, and it is shown using a rendered gemstone that a depth of two to three refractions and reflections is the most needed.

Guy and Soler [4] compared the results of rendering gemstones visualizing the differences in result images between their presented hardware algorithm and a raytracer with exact refraction. They note that some of the more brilliant rainbow effects are lost in the hardware implementation.

Although the linear approximations may not be accurate for quartz, the red, green, blue absorbance formulas may prove usefull. In addition, although quartz does not occur naturally in a cut gemstone, it does occur as a faceted crystal, so the facet tree algorithm may be used after considering the level of accuracy desired.

The works by Beyerle and McDermid [2] and Guy and Soler [4] give a starting point for calculating the refraction and reflection of light in minerals. But, neither of these papers give much consideration to the fluorescent properties of quartz (or any other mineral). Guy and Soler [4] suggested that fluorescence does not need to be considered because ”it is weak and mainly affects UV light outside the visible spectrum”. However, it is a possibility that light rays hitting a crystal sample may cause the sample to fluoresce (even under sunlight), slightly affecting the percieved colour of the mineral.

Chapter 6

Concluding Remarks

The first step in attempting to simulate the shape and appearance of quartz involves learning the properties of quartz that give it the visual properties that it has. This report has covered the basics, an introduction to mineralogy was given in Chapter 2, in which simple visual methods of mineral identification and the basic formation of crystals are provided. Next, in Chapter 3 the properties and visual appearance of quartz were discussed. In Chapter 4, we outlined relevant light phenomena and how they affect the appearance of quartz.

With a background in the appearance and shape of quartz, and how light interacted with it we then set out to find existing algorithms for rock and mineral simulations. In Chapter 5 we discussed several papers that address how properties of rocks and minerals could be simulated.

A paper on optics by Beyerle and McDermid [2] yielded formulas for simulating refraction and internal reflection in uniaxial crystals. A second paper by Guy and Soler [4] presented an algorithm for rendering reflection, refraction and facets of gemstones. We found a program that renders the shape of quartz crystals in a paper by Angell and Moore [1] but later discovered that their program had been written in Fortran IV on punch cards for a D.E.C. VAX 11/780 and had sadly been lost.

As for rendering the inclusions and striations of quartz, a paper by Yokoi and Kurashige [11] presented algorithms for rendering asterism and chatoyancy that while not directly applicable to crystalline quartz provides an interesting starting point for rendering inclusions such as air and water bubbles. A second paper by Dorsey *et al.* [6] presented algorithms for rendering weathered stone that could be applied to the rendering of striations on the exterior faces of a quartz crystal point.

In conclusion, to the best of our knowledge, there are no predictive models of quartz appearance available in the literature to date. We hope that the information gathered in this report can contribute to form a sound scientific basis for the development of such models in the near future.

References

[1] ANGELL, I., AND MOORE, M. A computer graphics package for teaching crystal morphology. *Eurographics '82* (1982), 295–302.

[2] BEYERLE, G., AND MCDERMID, I. S. Ray-tracing formulas for refraction and internal reflection in uniaxial crystals. *Applied Optics 37*, 34 (1998), 7947–7953.

[3] FEYNMAN, R. P. *QED The Strange Theory of Light and Matter*, first ed. Princeton University Press, New Jersey, 1985.

[4] GUY, S., AND SOLER, C. Graphics gems revisited: Fast and physically-based rendering of gemstones. *ACM Transactions on Graphics 23*, 3 (2004), 231–238.

[5] HOLDEN, A., AND MORRISON, P. *Crystals and Crystal Growing*, ninth ed. The MIT Press, Massachusetts, 1960.

[6] JULIE DORSEY, ALAN EDELMAN, H. W. J. J. L., AND PEDERSEN, H. K. Modeling and rendering of weathered stone. *SIGGRAPH 99*, 1 (1999), 225–234.

[7] KIMMEL, B. W. Splits: A spectral light transport model for sand. Master's thesis, Computer Science, University of Waterloo, 2005.

[8] NESSE, W. D. *Introduction to Mineralogy*, first ed. Oxford University Press, New York, 2000.

[9] R.H. PETRUCCI, W. H., AND HERRING, F. *General Chemistry - Principles and Modern Applications*, eighth ed. Prentice Hall, 2002.

[10] ROSSMAN, G. R. Colored varieties of the silica minerals. *Reviews in Mineralogy 29*, 1 (1994), 433–467.

[11] SHIGEKI YOKOI, KOSUKE KURASHIGE, J.-I. T. Rendering gems with asterism or chatoyancy. *The Visual Computer 2*, 1 (1986), 307–312.

[12] WENK, H.-R., AND BULAKH, A. *Minerals, Their Constitution and Origin*, first ed. Cambridge University Press, United Kingdom, 2004.

Appendix A

Photography and Supplies

Photography for this report was done using the following digital cameras:

- Canon PowerShot S50
  5.0 mega pixels
  3.0x zoom

- Olympus D-550 700M
  3.0 mega pixels
  2.8x zoom

Special thanks to Austin Hung for use of the PowerShot camera, tripod, laser pointer and UV LED light source.

Amethyst/Ametrine sample (from unknown mine), large geode, and greek quartz samples courtesy of Pam Northam.

Appendix B

Case Studies

In this appendix, we describe simple experiments and studies conducted on quartz samples to provide a better understanding of the mineral.

B.1 Streak

A common mineral identification test creating a fine powder of the mineral is called the streak test. In this test, a mineral is rubbed against an un-glazed porcelain tile and the colour of the resultant powder is recorded.

The purpose of this mini-experiment is to observe the powder resulting from the streak test of quartz under a microscope, possibly comparing it to the powder of another mineral such as hematite.

Results for this experiment have not yet been gathered.

B.2 Colour Fastness

Rossman [10] states that amethys is not colour-fast, *i.e., it is possible to bleach the colour out of the mineral*. He also claims that heat and/or light is sufficient to fade and bleach amethyst samples. It also states that exposure to higher heat can turn amethyst into citrine (visually).

The purpose of this experiment is to expose small pieces of amethyst to varying temperatures and observe any colour change. If amethyst is bleached this simply, then when conducting a time-based simulation of amethyst where it is exposed to light and/or heat these colour changes should be taken into consideration.

B.2.1 Materials

A set of small amethyst chips from the same geographical location, a controlled source high heat.

B.2.2 Results

Kitchen stoves do not reach temperatures higher than 287 degrees Celcius.

A set of 10 amethyst pieces were placed into an oven at a temperature of 204 degrees Celcius for a period of one hour. There was no change in the shape or colour of the samples. According to Rossman [10], a higher temperature is probably needed.

Further results are needed.

B.3 Fluorescence

Quartz is not listed neither by Nesse [8] or Wenk and Bulakh [12] to be a mineral that fluoresces. However, some varieties of it do.

The purpose of this experiment is to create a light shielded box with an ultraviolet light source and to place various quartz samples into the box to determine if they fluoresce. If the minerals fluoresce, the colours will be recorded.

Results are not yet available for this experiment.

B.4 Study of Shape and Inclusions

Is every quartz crystal the same shape? There are many types of inclusions for quartz, fractures, phantoms, particles, water bubbles, etc. What do these inclusions look like? How do they scatter light?

The purpose of this study will observe the shape of quartz and the inclusions as seen in a test group of about sixty small sized quartz crystal points.

B.4.1 Materials

A set of sixty quartz crystal points (colourless) from the same mine were obtained. These crystal points range in size from 0.5mm to 4.5mm in length. A medium sized quartz crystal. A red laser pointer and a 380nm light source.

B.4.2 Exterior Shape

A sampling of crystals was taking from the set of points by reaching into a bag and randomly drawing a point. A sampling of ten was drawn and observed. Five of these crystals were photographed to illustrate and record any results.

Results

All ten crystals in the small sampling exhibited an imprefect hexagonal shape. That is the length of each side of the hexagonal prism was not equal. Crystals appeared squished and skewed to varying degrees – some were nearly rectangular in shape. In Figure B.1, five crystals are shown first as themselves and secondly with outlines of the hexagonal prism drawn to illustrate the level of squishing and skewing present.

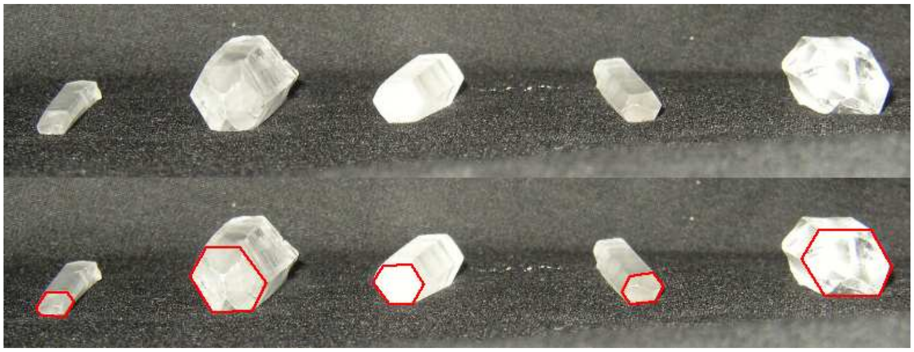

Figure B.1: A sampling of quartz crystal points illustrating the squashing and skewing. The upper image shows the points in their natural form and the lower image outlines the hexagonal shape for clarity.

B.4.3 Inclusions

A sampling was again drawn from the set of sixty points and the inclusions observed. A medium sized quartz crystal that is part of a cluster was also observed. Various light sources were shone on the medium sample to illuminate the inclusions for better viewing.

Results

The small crystal points did not contain a great deal of inclusions. Internal fractures were the most common type of inclusion. Air bubbles and a strange wisp-like cloud inclusion were also observed in some samples. These points are too small for the naked eye to detect greater details of these inclusions – they should be observed under magnification.

The medium sized crystal in the cluster contains many inclusions. It has internal fractures, wisp-like clouds and air bubbles included. To observe these inclusions better and to illustrate how they might scatter light, a room was darkened and various light sources were shone on the crystal. The first was a red laser which was shone through the crystal. Instead of passing right through the crystal, the laser beam was scattered by the inclusions illuminating large portions of the crystal with red light. A 380nm light was also shone onto the crystal. This light source illuminated the fractures and air-bubbles so that they were easily visible. Figure B.2 illustrates the affects of illuminating a quartz crystal with varying light sources.

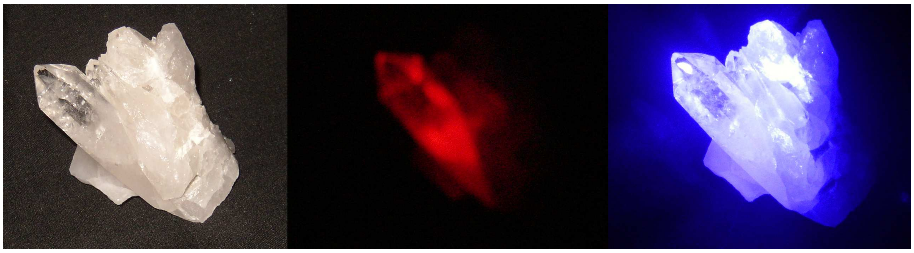

Figure B.2: The medium sized quartz crystal illuminated first with an ordinary light, second with a red laser and third with a 380nm light source. The coloured light sources cause the inclusions to become easily visible.

Index