

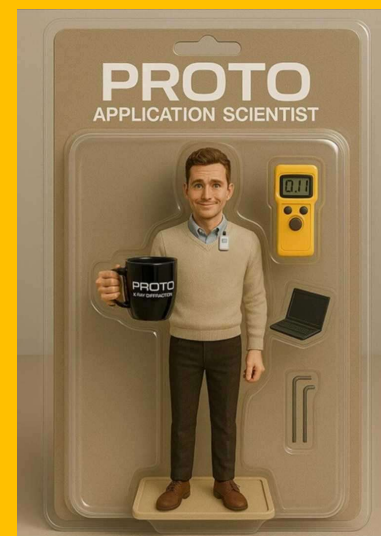
A close-up photograph of an X-ray diffraction (XRD) instrument. The image shows various mechanical components, including a goniometer with a rotating stage and a detector arm. A yellow warning label with a radiation symbol and the text "X-RAYS RAYONS X" is visible on the left. The background is dark, and the overall lighting is focused on the metallic parts of the machine.

PROTO  
X-RAY DIFFRACTION

**Canadian Powder  
Diffraction Workshop 19  
Saskatoon, SK**

July 2026

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# Everything's A Sample: Unusual Applications of Powder XRD

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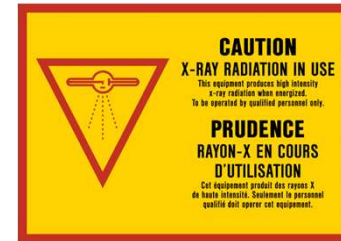
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## X-Ray Scattering

- The term “x-ray scattering” is used to describe the occurrence when the direction of an x-ray beam changes due to its interaction with electrons that orbit the nucleus of an atom.
  - **Elastic scattering** is when there is no change in the energy of the x-rays.
  - **Coherent scattering** is when the x-rays are in phase with one another.
- Diffraction is the observed result of coherent elastic scattering. Diffraction is itself an umbrella term, which encompasses **reflection** and **transmission** experiments.
- The data set obtained is often referred to as a “diffraction pattern” or “diffractogram”.

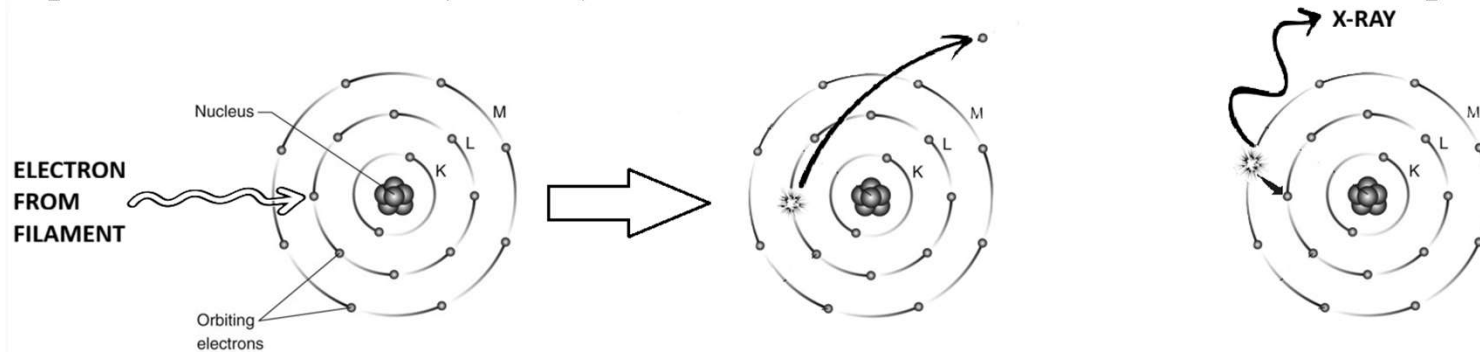
## Common X-ray Techniques

- There exist several types of methods that exploit the scattering and/or fluorescence of x-rays. These include scattering, reflectivity, diffraction, and fluorescence.
  - **Scattering:** SAXS, USAXS, WAXS
  - **Reflectivity:** XRR
  - **Diffraction:** Laue, Crystallography, Powder Diffraction, Residual Stress
  - **Fluorescence:** XRF
- They all benefit from being non-destructive techniques.



# What Are X-rays Used For?

- Structure
  - Imaging (CT, Radiography): shows internal structure.
  - X-ray Scattering (SAXS): used to measure nanoscale particles.
  - X-ray Diffraction (PXRD): reveals atomic structure
- Chemical Composition
  - X-ray Fluorescence (XRF): identifies elements and chemistry



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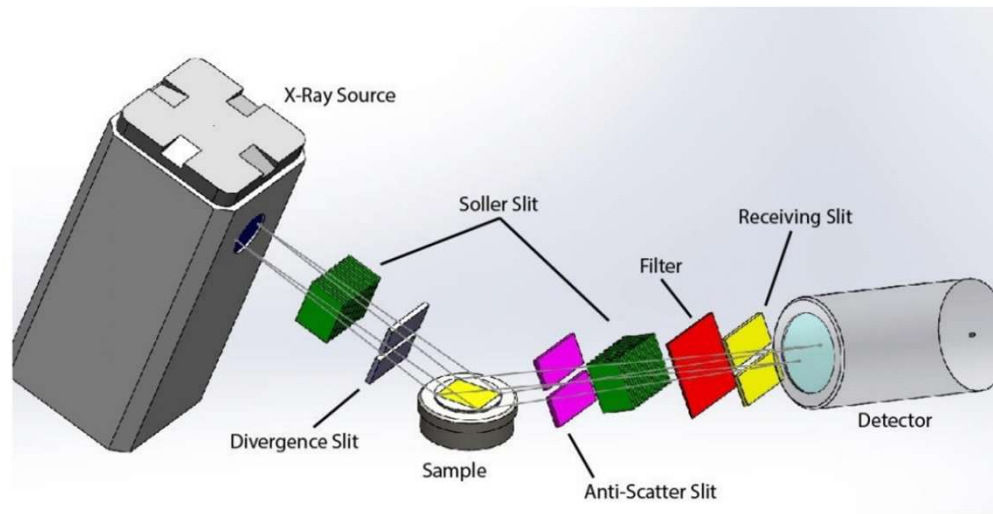
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## Powder X-Ray Diffraction (PXRD)

- Expectation: Jack Of All Trades.
- Perhaps the most widely used technique for the identification and structural characterization of materials.
- Powder x-ray diffraction is based on constructive interference of monochromatic x-rays with a crystalline sample.
  - Samples are typically crystalline but information can still be gained from semi-crystalline or amorphous samples.
  - Often times, it is much easier than single crystal diffraction since it does not require individual crystals.

## Powder Diffraction (PXRD)

- A powder diffractometer consists of three main elements: a x-ray tube, a sample stage, and a x-ray detector.
- Scanning through a range of  $2\theta$  angles, all possible planes in the lattice should be detected due to the random orientation of the material.



Reference: Proto Manufacturing.

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## Powder Diffraction (PXRD)

- Qualitative (for example, Phase ID) and quantitative (for example, Rietveld) analysis is possible.
- Applications include:
  - Characterization of materials, including distinguishing between polymorphs or understanding phase transitions.
  - Determination of unit cell dimensions, lattice parameters.
  - Measurement of sample purity.
  - Characterization of thin films.
  - Size and strain broadening.
  - Plus many more!

## “Dana”

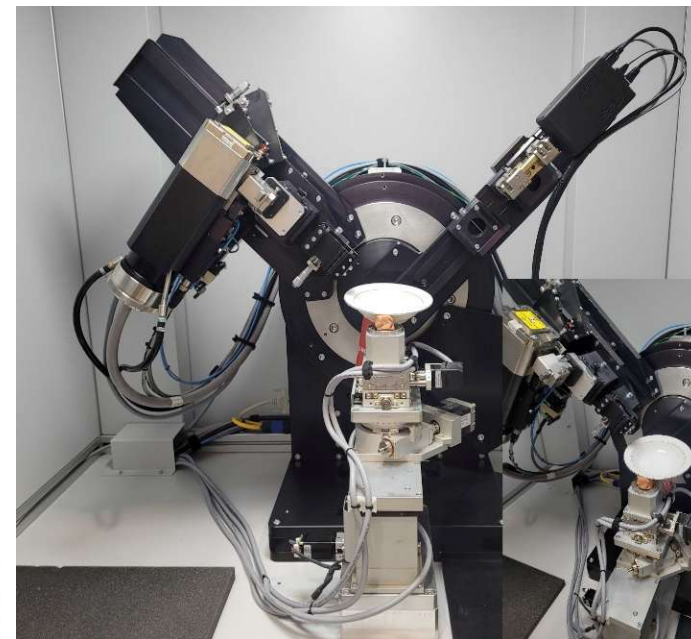
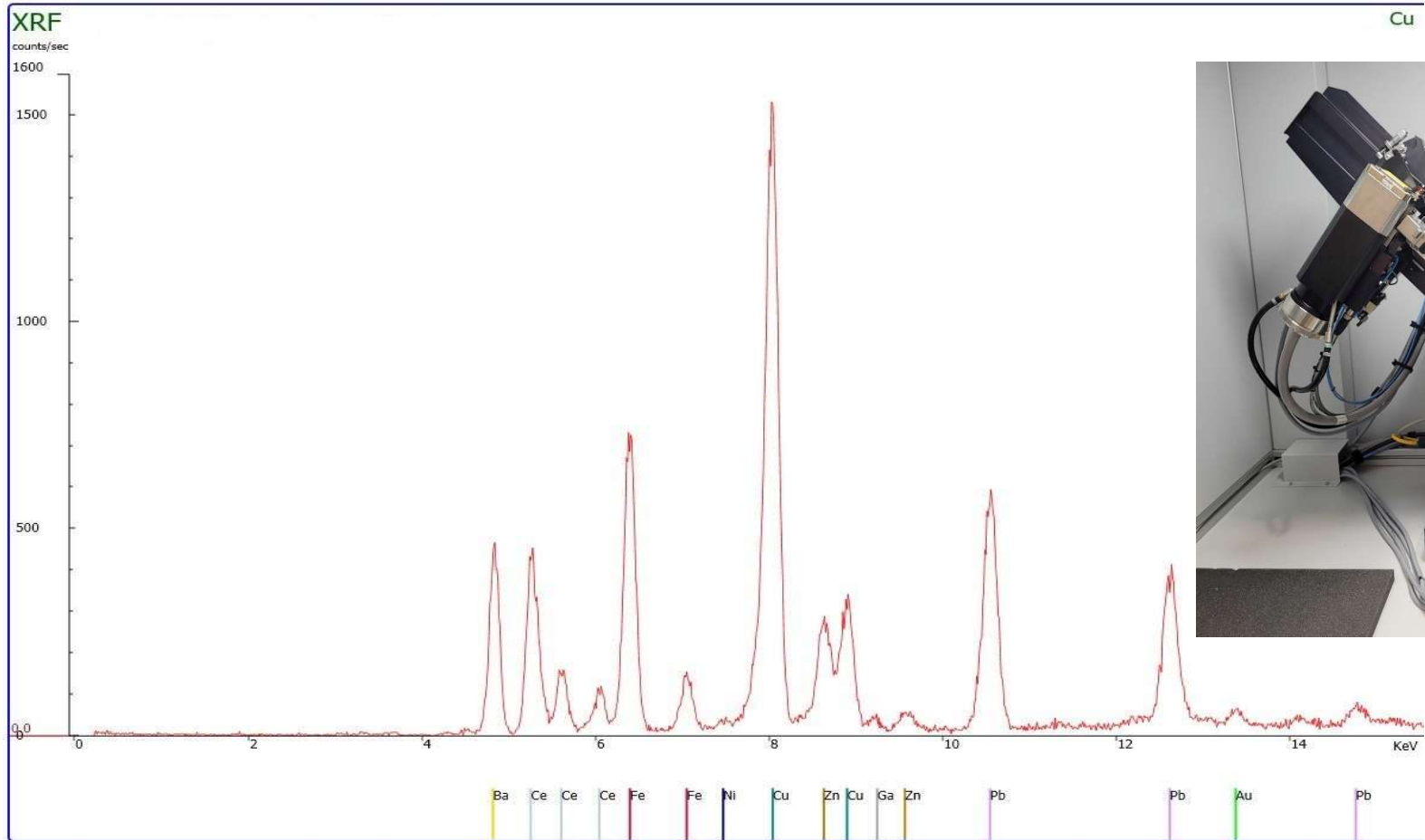
- Applications of lead in chinaware, glassware, and cookware date back centuries.
  - Traditional pottery and ceramicware is made using a porous form of clay called “earthenware”.
- In order for the pottery to hold food or liquid, it must be glazed.
  - The process of glazing applies and fuses a thin, glass-like coating to the surface of the pottery, which seals the pores of the clay. The glaze fuses to the pottery when it is fired in a kiln.
  - Lead (added as lead oxide) was primarily used as a flux to create glaze that was easy to use, available in a wide range of colours, and resulted in a smooth and brightly glazed product.

## “Dana”

- At the proper temperature and for the proper amount of time in the kiln, essentially all the lead becomes bound within the glaze (if it is part of the glaze), resulting in an insignificant amount migrating into foods placed inside the pottery.
  - If not properly fired, however, the lead may not fuse to the earthenware and may contaminate any food placed inside the pottery.
- Aside from being used in the glaze, lead was also a popular additive to decorative elements of ceramic and glass products.



# “Dana”



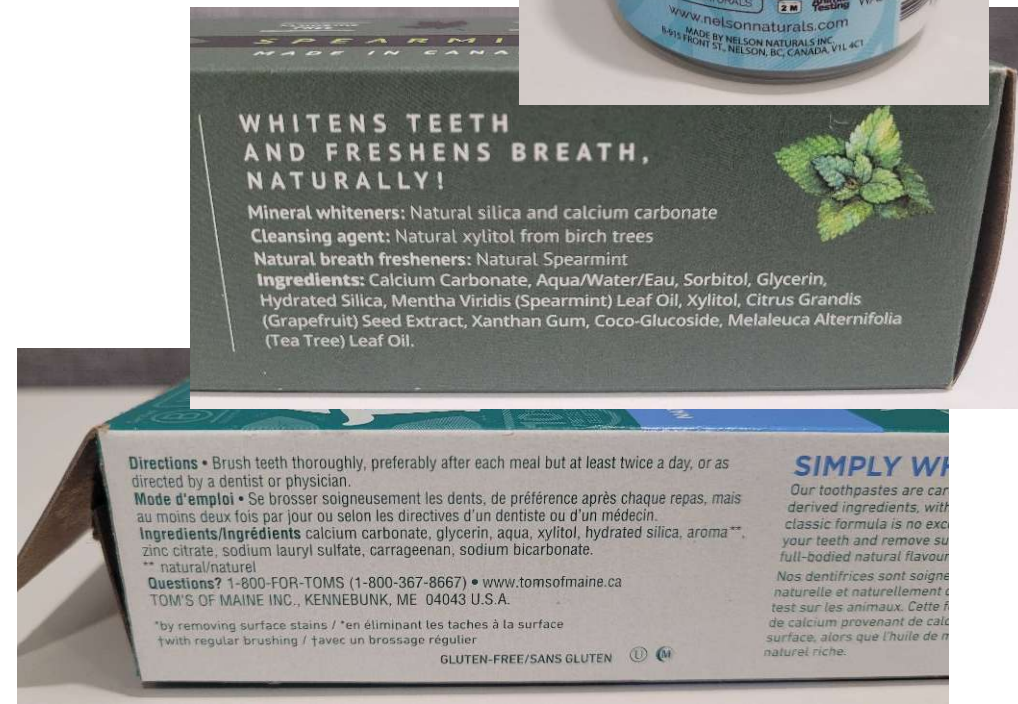
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## Non-fluorinated Toothpaste

- Non-fluorinated toothpastes often rely on natural, earth-derived ingredients like *bentonite clay*, *kaolin*, *calcium carbonate*, *(hydrated) silica*, or *hydroxyapatite*.
  - These minerals are sourced from the earth, frequently carrying trace elements of soil, which contain lead and other heavy metals.
- Health Canada (as well as the FDA) classify fluoride-free toothpastes as cosmetics rather than drugs, subjecting them to different safety thresholds and less stringent heavy metal testing requirements.
  - Health Canada classifies fluorinated toothpaste as a **Natural Health Product** (NHP), thereby requiring authorization by Health Canada.

# Non-fluorinated Toothpaste



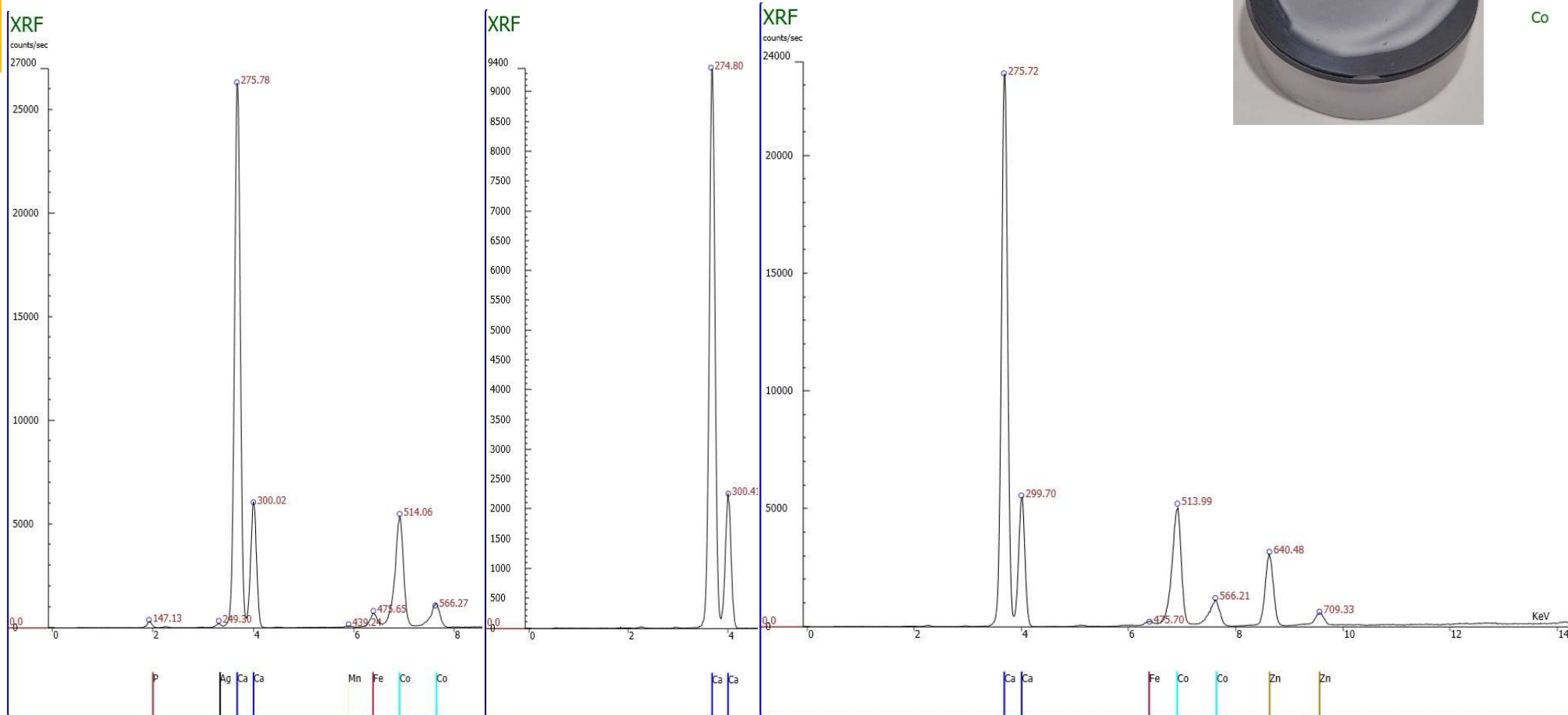
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# Non-fluorinated Toothpaste



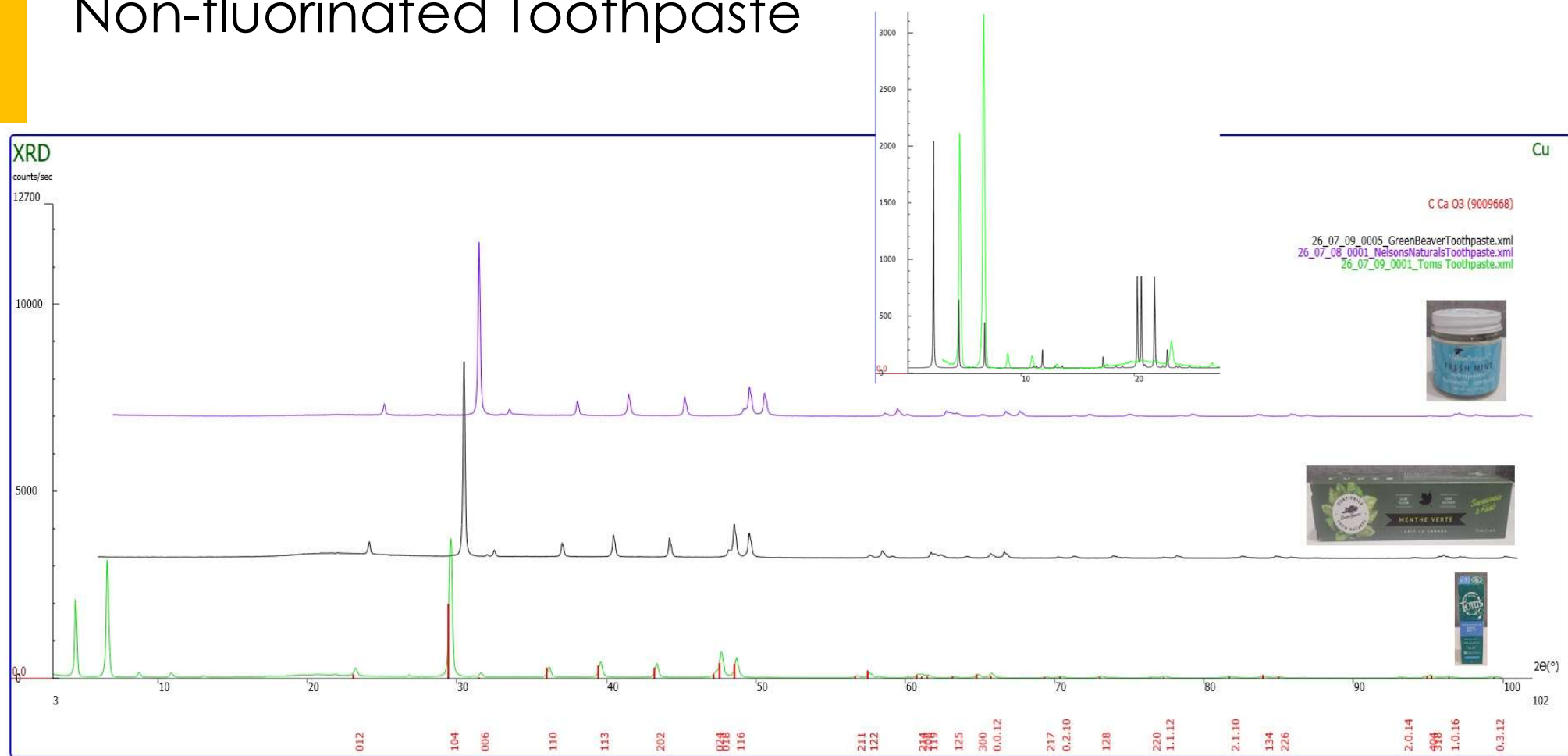
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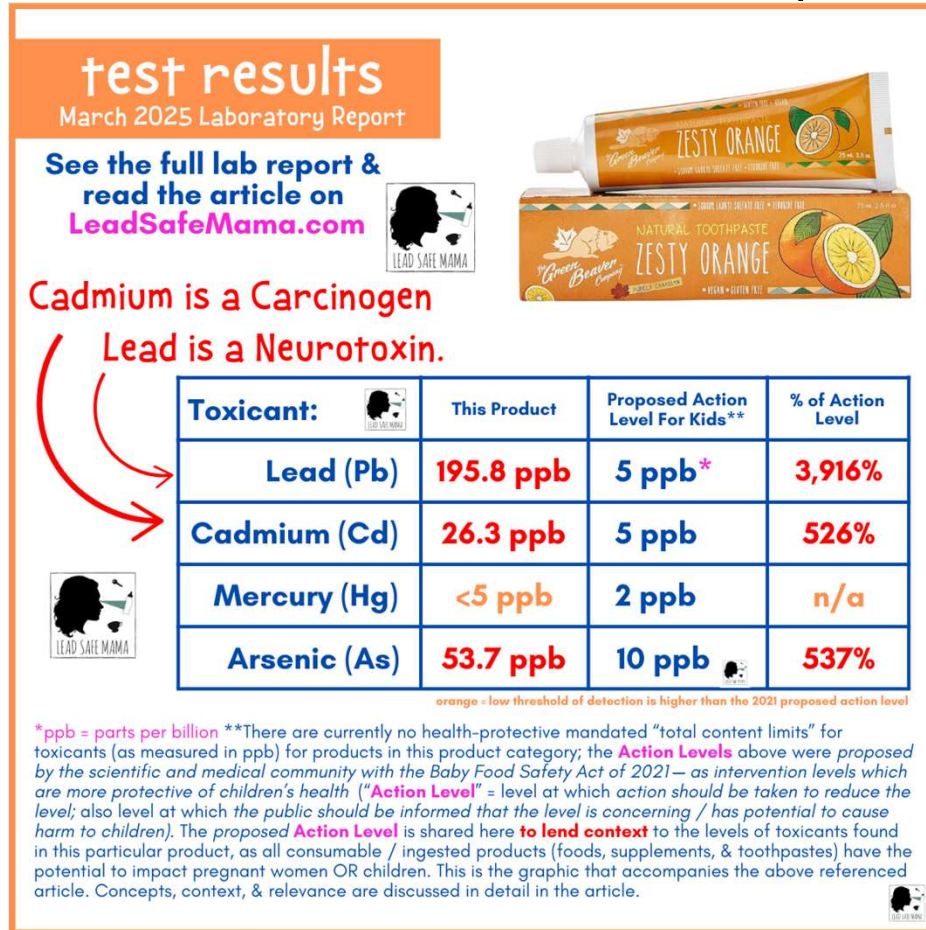
# Non-fluorinated Toothpaste



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# Non-fluorinated Toothpaste



- Opinions on whether Lead Safe Mama is legit are mixed.
  - It is, however, cited often, so should we worry about non-fluorinated toothpaste? .... 🤔
- Possible PXRD is not sensitive enough.
  - Supplement data with additional analytical techniques, such as ICP.

Source: Lead Safe Mama. <<https://tamararubin.com/2025/04/canadian-the-green-beaver-company-fluoride-free-toothpaste-in-zesty-orange-flavor/>> Accessed 10 July 2026.

# Lessons Learned from “Dana”

## Charm and Risk: Navigating Lead in Vintage Items and Homes

Lead is a chemical element, represented as **Pb** on the periodic table (for *plumbum*), that is naturally found in the earth’s crust. This naturally occurring metal, found in rock and soil samples, is shiny bluish-grey in colour when fresh and dull grey when tarnished, and is known for being soft, malleable, and corrosion-resistant<sup>10,19</sup>. Lead’s high density, low melting point, ductility, and relative inertness have been exploited in a range of applications over the centuries, however, modern day uses are typically limited to batteries, ammunition, electronics (solder), construction, and leaded enclosures, shields or vests (for example, for preventing x-ray exposure and occasionally in a weighted vest used for training)<sup>19</sup>.



**Figure 1:** Lead sulphide (galena). Lead is rarely found in its free form in nature<sup>18</sup>.

As one of the earliest metals worked by humans, lead dates back to as early as the seventh century BCE<sup>16</sup>. It spread widely across early civilizations due to its association with silver ore and eventually found uses in tools, currency, cosmetics, warfare, writing, architecture, and alchemy,

# Goldschläger

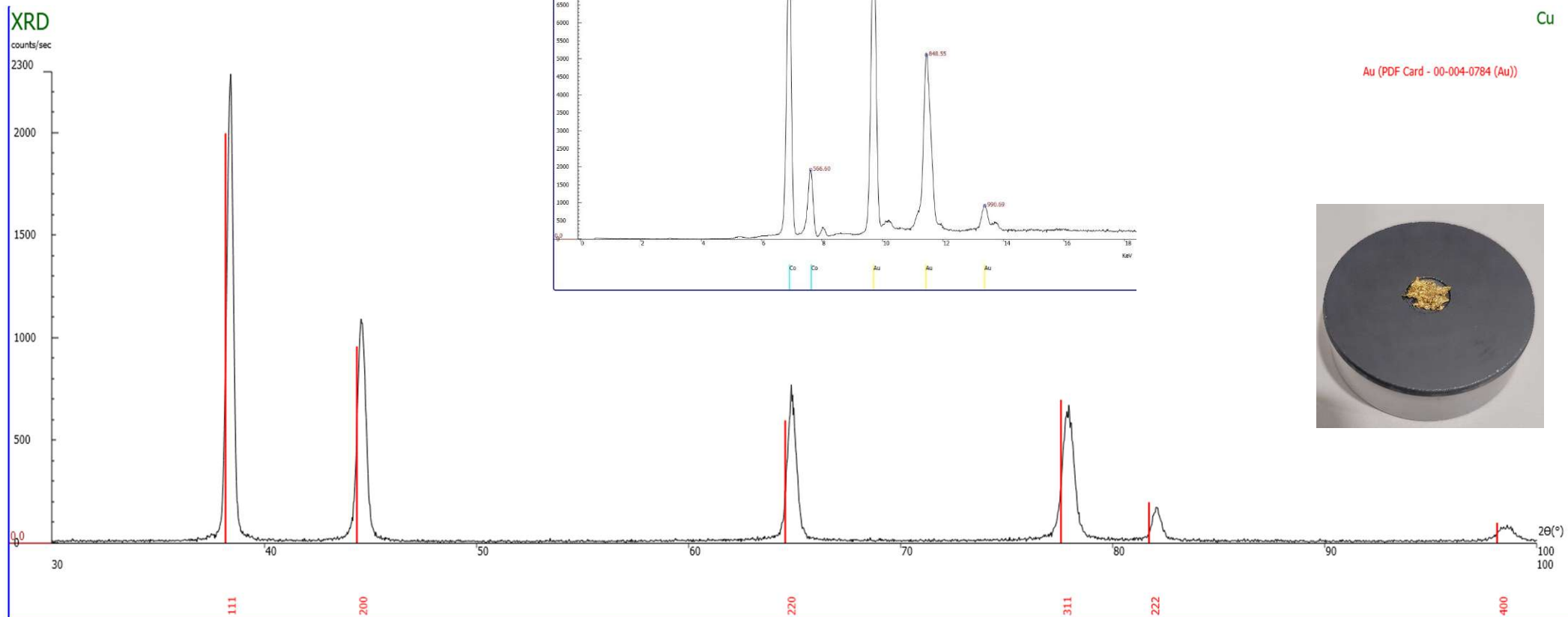
- Goldschläger is a cinnamon-flavoured liqueur with very thin, yet visible, 24-karat gold flakes floating in it.
  - Inspired by Goldwasser, a gold-infused liqueur first created in Poland in the early 1600s.
  - The amount of gold per 1-litre bottle is approximately 13 milligrams.



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# Goldschläger



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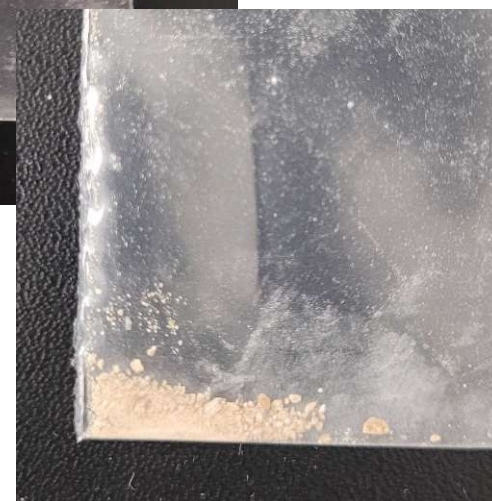
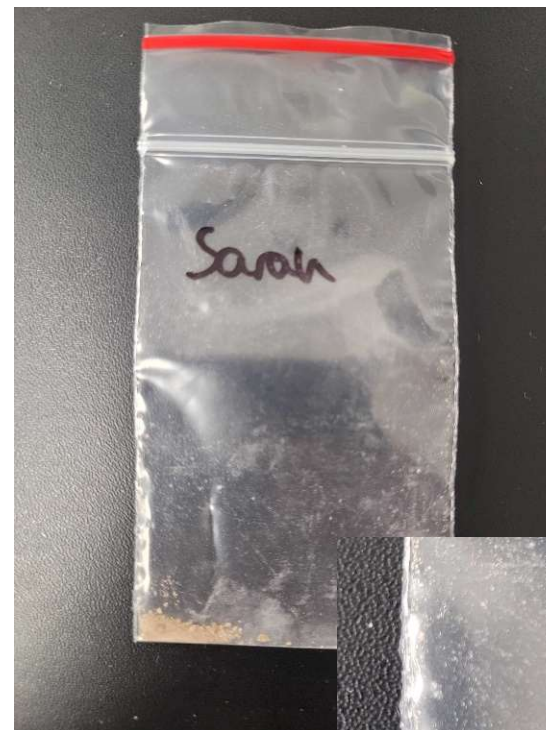
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## Lessons Learned from Goldschläger

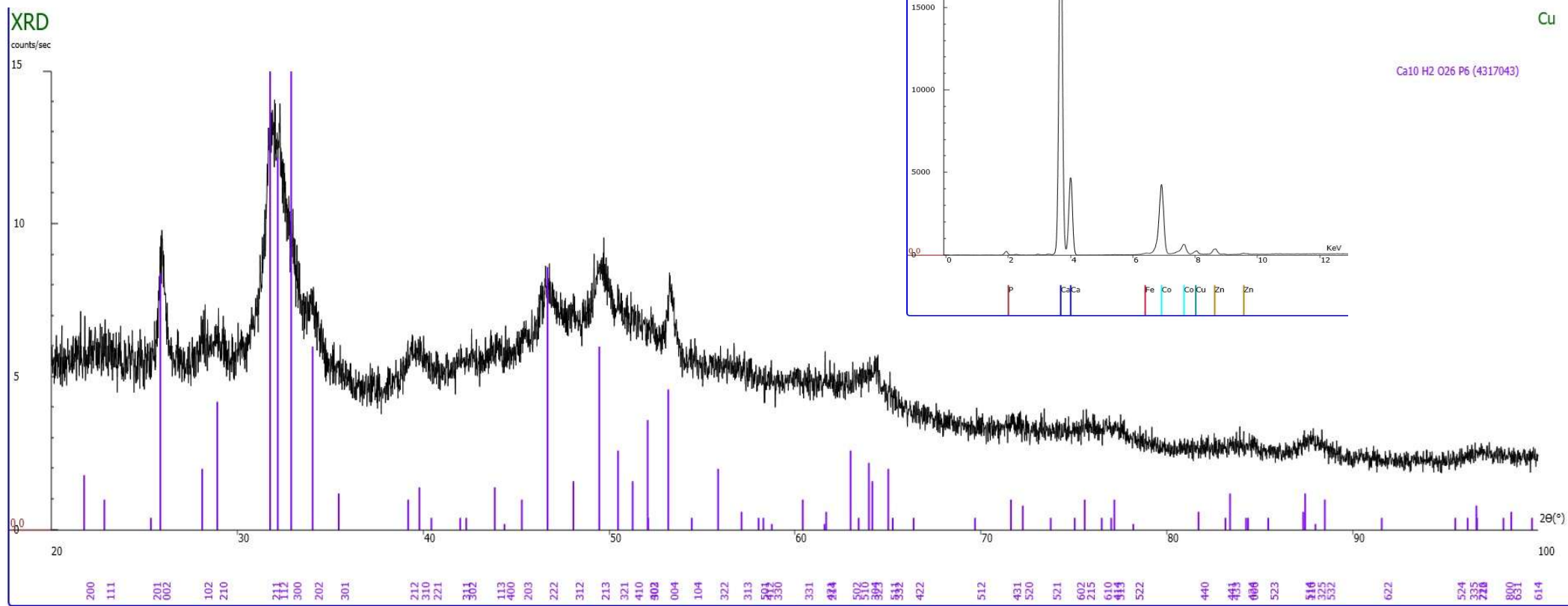
- Sample preparation is key.
- Currently, 1 gram of gold is \$131 USD.
  - 13 mg = 0.013 g of gold per Goldschläger bottle.
    - There is \$1.70 USD worth of gold in each bottle.
  - 1 bottle of Goldschläger cost \$30 CDN in Ontario (\$21 USD).
  - To get 1 gram of gold, one would need to buy 77 bottles of Goldschläger.
    - This would cost \$1,617 USD >>>> \$131 USD.

## “Sarah”

- Sarah passed two kidney stones.
  - One was donated for analysis by PXRD.
- Approximately 10% of North Americans will develop kidney stones in their lifetime.
  - 70-80% of kidney stones in North America are calcium stones – calcium phosphate or calcium oxalate.
  - Uric acid stones make up approximately 10% of cases.



“Sarah”



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# Lessons Learned from “Sarah”

## CALCIUM OXALATE vs CALCIUM PHOSPHATE KIDNEY STONES

| CALCIUM OXALATE STONES                                                                                          |                                                                                                                          | VS.                                                                                                         | CALCIUM PHOSPHATE STONES                                                                                                                                                                              |                                                                                              |
|-----------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------|
|                                |                                                                                                                          |                                                                                                             |                                                                                                                    |                                                                                              |
|                                | <b>APPEARANCE</b><br>Dark, hard, jagged                                                                                  |                                                                                                             |                                                                                                                    | <b>APPEARANCE</b><br>Light-colored, smoother                                                 |
|                                | <b>URINE pH</b><br>Usually acidic to neutral<br>(pH ≤ 7)                                                                 |                                                                                                             |                                                                                                                    | <b>URINE pH</b><br>Usually alkaline<br>(pH > 7)                                              |
|                                | <b>RISK FACTORS</b><br>Low fluid intake, high oxalate diet,<br>low calcium diet, certain<br>medical conditions, genetics |                                                                                                             |                                                                                                                    | <b>RISK FACTORS</b><br>Urinary tract infections,<br>renal tubular acidosis,<br>high urine pH |
|                              | <b>X-RAY APPEARANCE</b><br>Usually visible (radiopaque)                                                                  |                                                                                                             |                                                                                                                                                                                                       |                                                                                              |
| <b>PREVENTION (BOTH TYPES)</b>                                                                                  |                                                                                                                          | <b>IMPORTANT</b>                                                                                            |                                                                                                                                                                                                       |                                                                                              |
| <br>Drink plenty<br>of water | <br>Eat a balanced<br>diet            | <br>Limit salt<br>intake | <br>A 24-hour urine test and medical evaluation<br>can help determine the cause and the<br>best prevention plan. |                                                                                              |
| <br>Follow medical<br>advice |                                                                                                                          |                                                                                                             |                                                                                                                                                                                                       |                                                                                              |

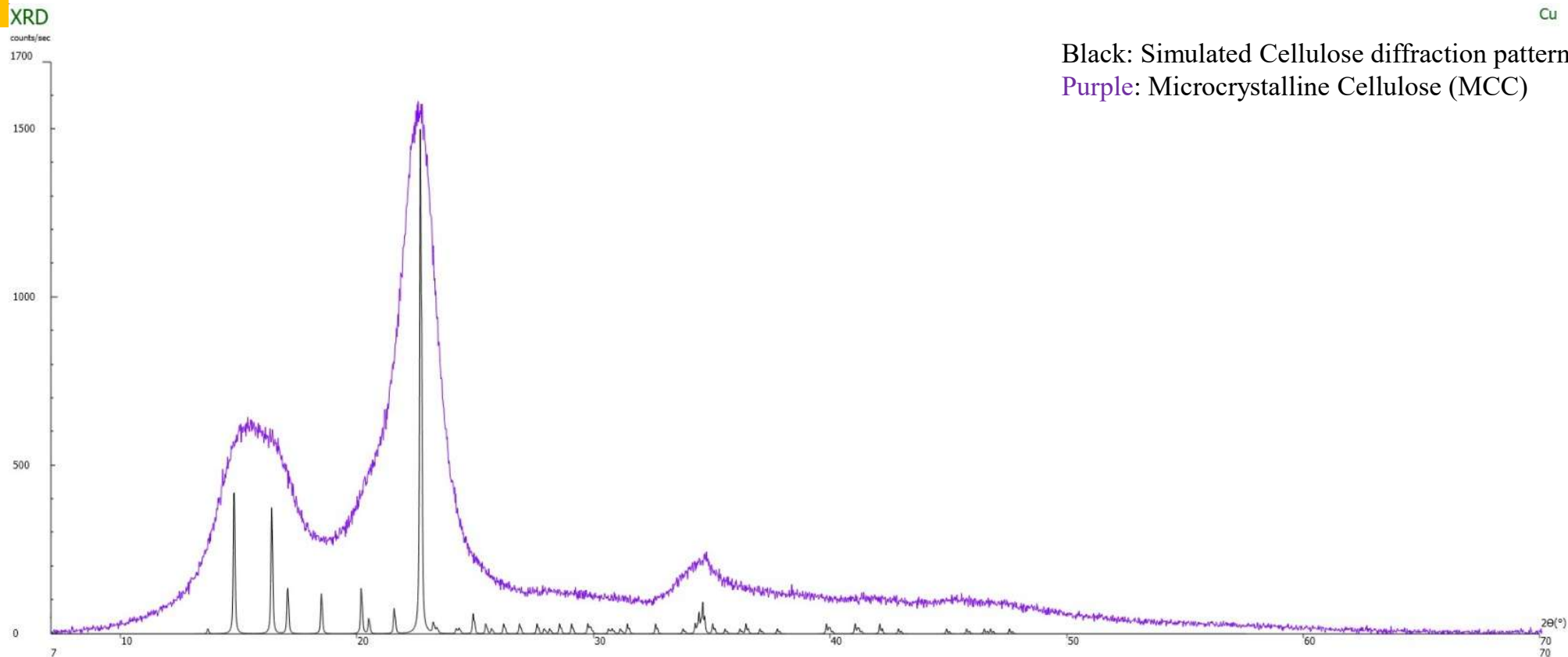
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# Cellulose

- Cellulose is a complex polysaccharide, composed of long chains of  $\beta$ -D-glucose molecules and is the planet's most abundant biopolymer.
  - The chemical formula for cellulose is  $(C_6H_{10}O_5)_n$ , where  $n$  can be hundreds or thousands of glucose units.
  - Cellulose has been characterized (via x-ray diffraction and  $^{13}C$  NMR) as existing in four different allomorphs: I (native), II, III, IV.
- The structure of cellulose is highly ordered due to the formation of linear, straight chains that are aligned parallel to each other.

# Cellulose

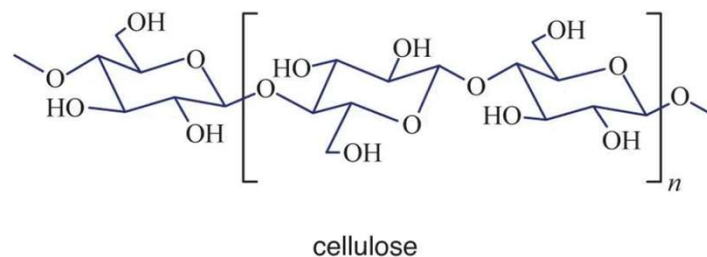
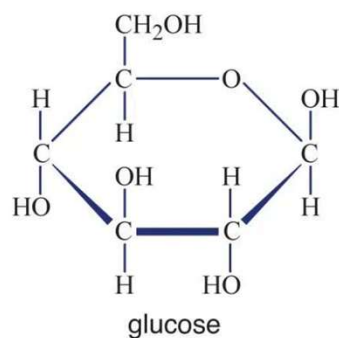


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## Lessons Learned from Cellulose

- Cotton, for example, is the purest form of cellulose; cotton fibers are composed of 90% cellulose. Wood, in comparison, is only 40-50% cellulose.
- Percent Crystallinity is (highly) subjective.
  - Results are relative, not “absolute”.
  - Can’t believe this is a hill I ended up willing to die on :/



Thank you for your attention!

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