SESEY
Summer Experience in Science and Engineering for Youth

# The Experimental Determination of the Atomic Structure of Materials Using X-Ray Diffraction

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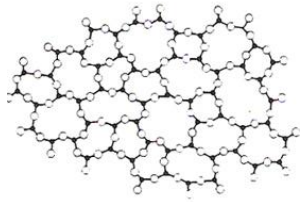
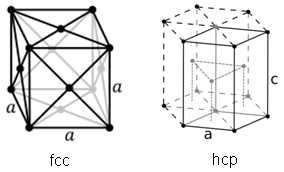
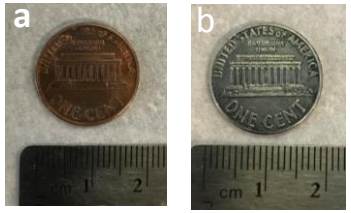
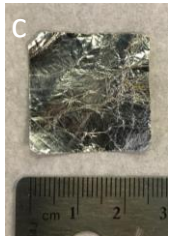


**Fig.1**
An example of an amorphous structure.

**Fig. 2**



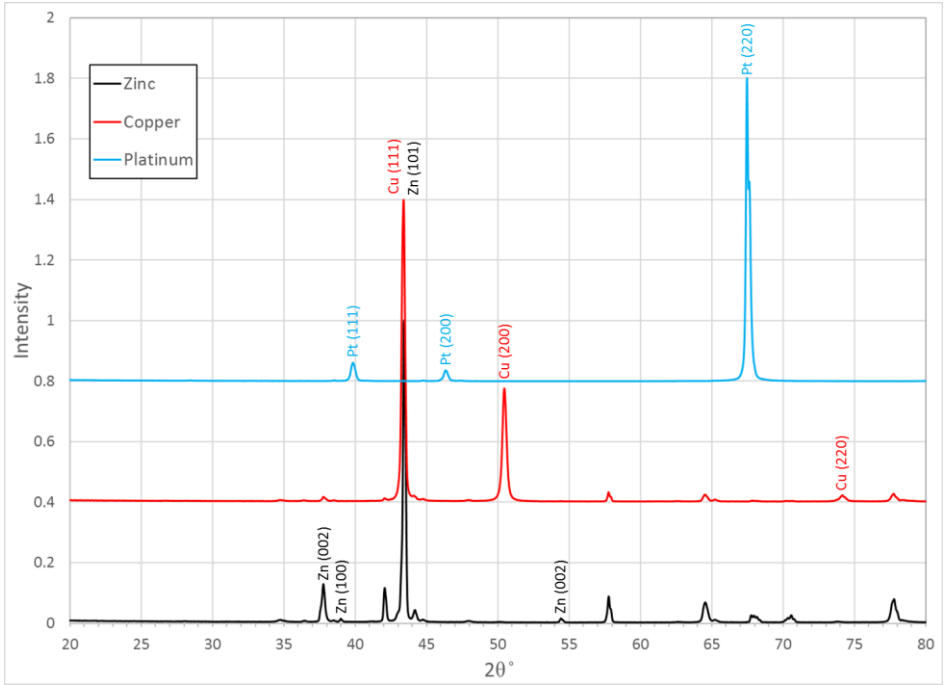

Examples of crystalline metallic structures

## Background

Metals are crystalline. Crystallinity is defined by long range atomic order. Other structures exist where this order is not present, these are amorphous materials (fig1). It has been proven that Copper and Platinum are FCC (face centered cubic) packed structures. Zinc has a HCP (hexagonal close packed) structure. (Fig. 2)

## Process

The distance between atoms of a crystal can be determined with the use of X-Rays. The Bruker-AXS D8 Discover X-Ray Diffractometer (fig3) uses x-rays to probe atomic crystal structure and record the readings. We were able to calculate the D-spacing of Copper (fig. 2a), Zinc (fig. 2b) and Platinum (fig. 2c) using these readings. D-spacing is the atomic interplanar distances that define a unit cell.




| Element | Exp. (nm) | Comp. (nm) | Lit. (nm) |
|---|---|---|---|
| Cu | .36143 | .363981 | .3597 |
| Pt | .392124 | .39723 | .3912 |
| Zn (a) | .266588 | .2622 | .26649 |
| Zn (c) | .500297 | .50025 | .49468 |

**Table 1**

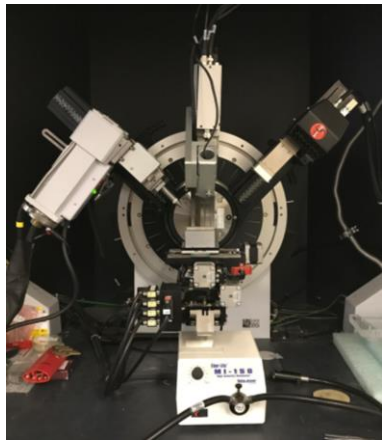


**Fig. 3**

## Results

To determine the D-Spacing Bragg's Law ($2d\sin\theta=n\lambda$) can be used. The SESEY group working with Dr. Árnadóttir determined the Lattice Parameter of Cu, Zn and Pt using computational material science. The results when compared to the results summarized in table 1 are a very good match.