

MEASURING CHANGES IN LATTICE PARAMETERS AND DENSITY DUE TO ALLOYING

Introduction

Vegard's law is often used to estimate the effect of substitutional impurities on the lattice parameters. It states that there is a linear relationship between substitutional impurity concentration and the lattice parameter in cases where the solute and solvent have similar bonding properties. In these cases the lattice parameter is influenced only by the relative sizes of the atoms and has been shown to be valid in ionic salts and compounds such as CdSe where sulfur substitutes for the selenium [1]. Vegard's law does not apply in the cases of interstitial solid solutions and in cases where the bonding in the solute and solvent are different. Positive and negative deviations from Vegard's law may be seen in fcc and hcp metals [2]. Note that pure copper has the fcc structure and zinc the hcp structure.

The solubility of zinc in copper can be as high as 39 weight percent. There are many brasses within this range (see table 1) and a common one is the C26000 alloy, or as it is more commonly known, 70/30 or cartridge brass. It is a single phase α brass which should be an excellent candidate for investigating the effects of impurity content on changes in the lattice parameter of pure copper and to experiment with Vegard's law.

Procedure

The procedure has three parts:

1. Budget and cost analysis
2. Modeling and feasibility
3. Laboratory measurements and data analysis

For the budget/cost analysis part of this experiment work up a budget for doing this experiment by making a best estimate of how much instrument time and labor is needed. Ask your instructor about the current recharge rate for the diffractometer and decide how much your time is worth. Add up the instrument, labor, and incidentals costs then add overhead at a rate of 48.5%, the current NUD rate at U.C. Davis.

For the modeling phase obtain the PDF files for copper and any brasses found in the ICDD database then use spreadsheets, Math Lab, Mathematica, or similar software to do the following:

- Calculate and plot the density and lattice parameters of copper as a function of zinc content.
- Calculate and plot the diffraction angles for all peaks in copper's diffraction pattern as a function of zinc content.
- Determine the peak shifts, $\Delta 2\theta$, one can expect to measure in the upcoming experiment.
- Calculate the corresponding densities for copper and each brass.

These calculations will provide a basis for deciding if Vegard's law applied in the case of brass and to be able to anticipate how much peak shift to expect in the diffraction measurements.

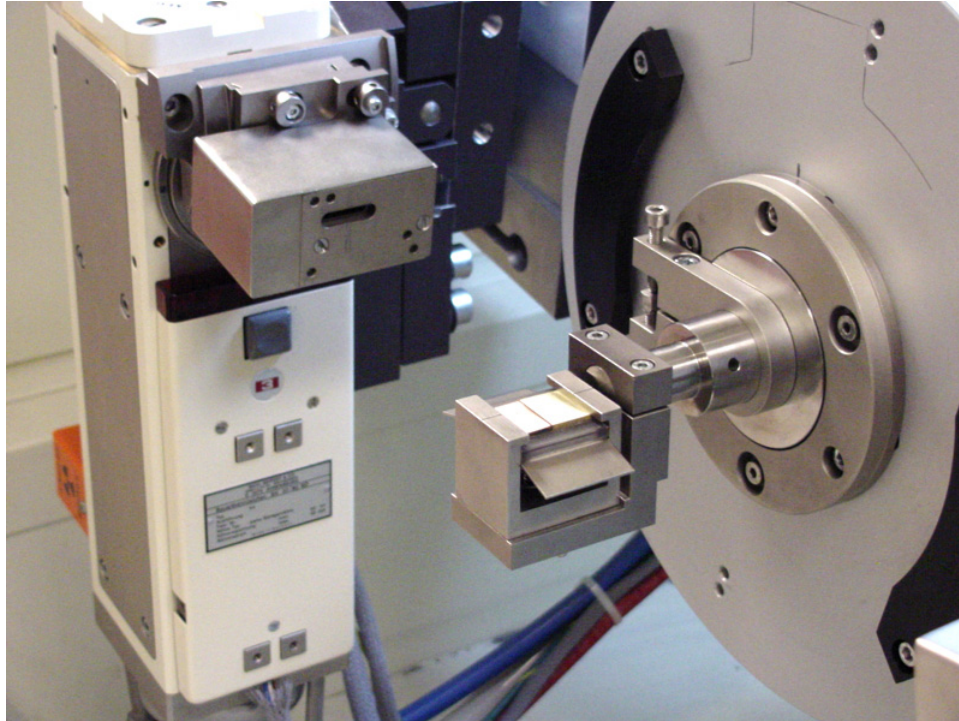


Figure 1 A view of the copper/brass sample installed in the diffractometer.

The experimental phase is very straight-forward. Select the starting and ending 2θ positions and a scan rate that will give a quality pattern containing as many peaks as time allows. The scan procedure itself is a normal θ - θ scan of the 2θ range or ranges.

The samples used in this experiment are simply small pieces of brass and copper strip (1.6 mm thick) that were annealed at 500°C for one hour to affect recrystallization and limited grain growth. They were then cut into 15 mm x 30 mm pieces and mounted side-by-side on a 30 mm x 30 mm plexiglass substrate using double-sticky tape. The mounted sample should be sanded using 600 grit SiC paper to remove oxides and to ensure that the tops of the samples were in the same plane. Figure 1 shows these samples after mounting them in the diffractometer.

Identify each peak in terms of its Miller indices, determine each peak's position by profile fitting the raw data, then calculate the d-spacing and the lattice parameter. Assuming a nominal composition for the brass, calculate the density for the copper and brass. When analyzing the results refer to the results of the modeling phase of the experiment to compare the results and to produce the desired tables and graphs that will help illustrate the results of this experiment.

To improve the results consider correcting for absorption errors. The different mass absorption coefficients of the copper and brass means that x-rays will penetrate the two samples to different depths, resulting in errors similar to those caused by sample displacement. The correction is simply:

$$\Delta 2\theta = \frac{180}{\pi} \frac{\sin(\theta)}{2\mu R} \quad (1)$$

where $\Delta 2\theta$ is the peak shift in degrees, R is the goniometer radius, and μ is the linear absorption

coefficient.

Finally, summarize the cost of performing this experiment and add this to your budget page. Include this budget/cost page in your report.

References

1. R.Jenkins and R.L.Snyder, Introduction to X-ray Powder Diffractometry, John Wiley & Sons, Inc., pp.42-43, (1996).
2. B.D.Cullity, Elements of X-ray Diffraction, 2nd edition, Addison-Wesley, Reading, Mass., pp.352-353, (1967).
3. Properties and Selection: Nonferrous Alloys and Pure Metals, ASM Metals Handbook, Volume 2, 9th Edition, ASM International, Metals Park, Ohio, pp.316-330, (1986).

Table 1. Data for brasses that could be used in this experiment [3].

Alloy Designation	Zinc Content (w%)	Density (Mg/m ³)	Lattice Parameter (nm)	Notes
C21000	5	8.86	0.3627	Gilding metal, 94.0-96.0% Cu Single phase microstructure, α (fcc)
C22000	10	8.80	0.364	Commercial bronze Single phase microstructure, α (fcc)
C22600	12.5	8.87	-	Jewelry bronze Single phase microstructure, α (fcc)
C23000	15	8.75	-	Red brass Single phase microstructure, α (fcc)
C24000	20	8.67	0.366	Low brass Single phase microstructure, α (fcc)
C26000	30	8.53	0.3684	Cartridge brass, 70-30 brass, spinning brass, spring brass Single phase microstructure, α (fcc)
C26800	34	8.47	-	Yellow brass Single phase microstructure, α (fcc)
C27000	35	8.47	-	Yellow brass Single phase microstructure, α (fcc)
C28000	40	8.39	-	Muntz metal Two phase microstructure consisting of α (fcc) and β (bcc)