Thermal Physics Project: Analysis of Cu_3Au across OD transition.

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Abstract

!!!

1 Introduction

This report aims to analyse the experimental measurements taken from [1]. In the article, the authors investigated the specific molar heat capacity of Cu_3Au as it varied with temperature. Here we are focusing on the order-disorder (OD) transition between 500 K and 720 K. [2]

2 Theory

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3 Methods

3.1 Plotting Figures

To produce Figure 1a and Figure 1b, data for the project was taken from [1], and code 5 was written to plot these figures.

3.2 Entropy Calculation

Entropy change can be calculated using [3]:

$$\Delta s = s_2 - s_1 = \int_{T_1}^{T_2} \frac{c_p}{T'} dT' \tag{1}$$

In code this is translated as [4]:

$$\int_a^b f(x)dx \approx \sum_{i=a}^{b} f(x_i)\Delta x_i, \Delta x_i = x_{i+1} - x_i \tag{2}$$

In the code, this approximates an integral sum of specific molar heat per kelvin by temperature element dT from $T_1 \approx 500K$ to $T_2 \approx 720K$ as a sum of specific molar heat per kelvin multiplied by the difference in subsequent temperature measurements.

3.3 Uncertainty Calculations

The uncertainty in the temperature measurement was given as an equation in the data-set provided in [1]:

$$\sigma_T = 0.01T + 9 \times 10^{-7}T^2 \tag{3}$$

Uncertainty in specific molar heat per kelvin was calculated as a combination of the original uncertainty in specific molar heat capacity and the uncertainty in temperature:

$$\sigma_{c_p} = c_p[-0.198 + 9.4 \times 10^{-4}T - 9.2 \times 10^{-7}T^2] \tag{4}$$

$$\sigma_{\frac{c_p}{T}} = \frac{c_p}{T}\sqrt{(\frac{\sigma_{c_p}}{c_p})^2 + (\frac{\sigma_T}{T})^2} \tag{5}$$

Uncertainty in the molar entropy change was calculated by:

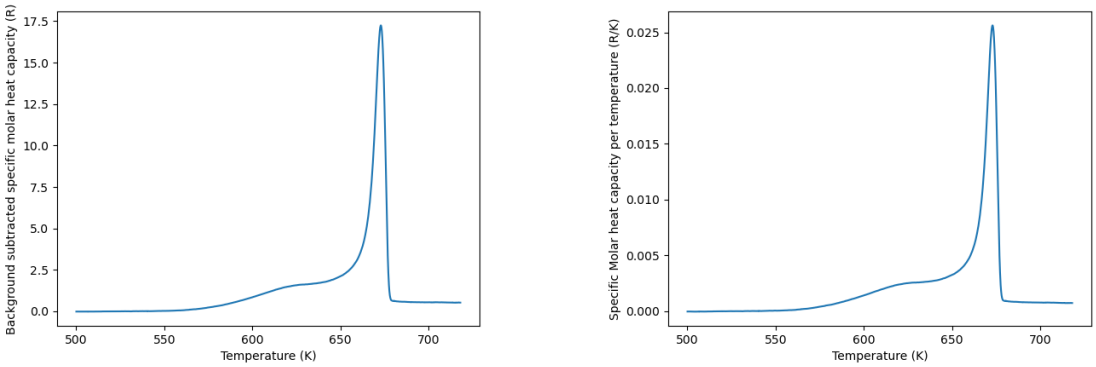
$$\sigma_{s_i} = s_i\sqrt{(\frac{\sigma_{\frac{c_p}{T}}}{\frac{c_p}{T}})^2 + (\frac{\sigma_T}{T})^2} \tag{6}$$

$$\sigma_s{}^2 = \sum_{i=1}^{N} \sigma_{s_i}{}^2 \tag{7}$$

Where s_i is the molar entropy change element from equation 2.

4 Results

The calculated value for the molar entropy change over the full temperature range S = 0.45 (1) R



(a) c_p against T.

(b) $\frac{c_p}{T}$ against T.

Figure 1: Plots showing specific heat capacity (R) against temperature (K) (Left) and specific heat capacity per temperature (R/K) against temperature (K) (Right).

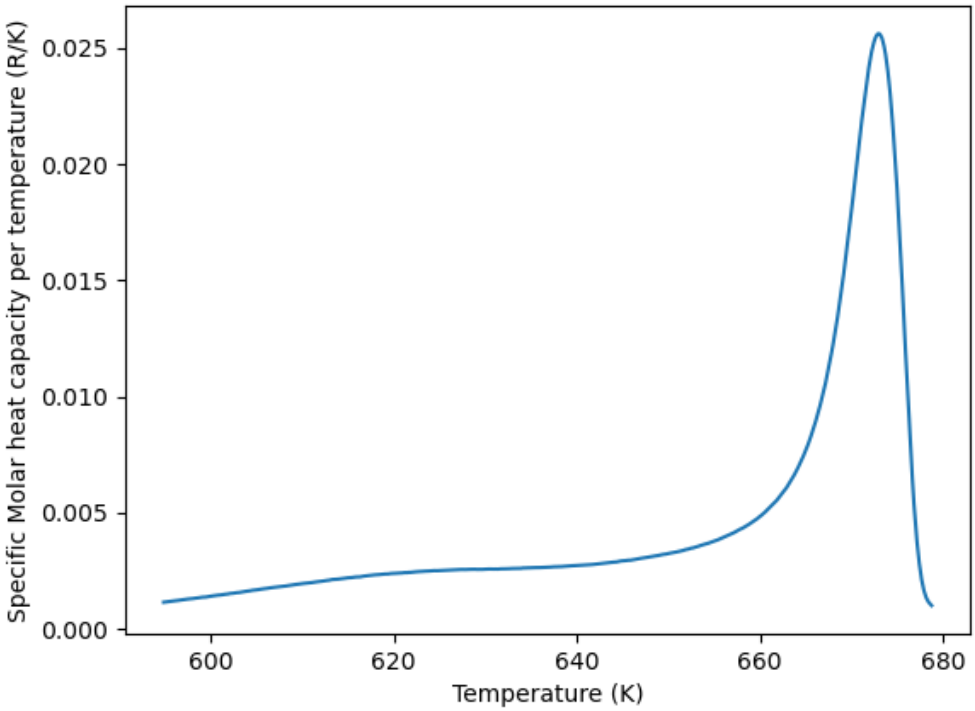


Figure 2: Plot showing specific molar heat capacity per temperature against temperature. Temperature range specific to the integration bounds of the entropy calculation.

5 Appendix

Code to plot graphs, estimate entropy change and estimate uncertainty from `https://git.ecdf.ed.ac.uk/s2153833/thermodynamics-project/-/blob/afc7295709bc6ba74f2b1b783056` `thermal_project_code.py`.

References

1. Benisek, A. & Dachs, E. The vibrational and configurational entropy of disordering in Cu3Au. eng. *Journal of alloys and compounds* **632,** 585–590. ISSN: 0925-8388 (2015).
2. Buck, T. M., Wheatley, G. H. & Marchut, L. Order-Disorder and Segregation Behavior at the $Cu_3Au(001)$ Surface. *Phys. Rev. Lett.* **51,** 43–46. `https://link.aps.org/doi/10.1103/PhysRevLett.51.43` (1 July 1983).
3. Poon, W. *Thermodynamics* 2023. `https://www.learn.ed.ac.uk/ultra/courses/_113371_1/outline/file/_9557072_1` (Oct. 15, 2023).
4. Poon, W. *Thermal Physics Semester 1 Hand-in Project* 2023. `https://www.learn.ed.ac.uk/ultra/courses/_113371_1/outline/file/_9557070_1` (Oct. 28, 2023).