Anisotropic Compression Effects in Uranium Metal at High Pressures

K. M. Hope¹, Y. K. Vohra¹

¹University of Alabama at Birmingham, Birmingham, Alabama, United States

Introduction

The light actinides (Th-Pu) exhibit a complexity of crystal structures not seen in simple and transition metals [1]. Simple sp-metals and transition metals tend to adopt relatively high symmetry crystallographic structures bodycentered cubic hexagonal closed packed and face-centered cubic The presence of 5-f electrons causes the light actinides to adopt open, lower symmetry structures such as orthorhombic and tetragonal. Uranium has received extensive theoretical and experimental study and published data to 100 GPa and 4500 K shows the existence of orthorhombic, body-centered tetragonal and body-centered cubic phases [2-5]. At room temperature, the orthorhombic phase of uranium is known to be stable up to 100 GPa. Recent studies of uranium have shown the presence of an anisotropic compressibility of the orthorhombic phase. This anisotropy has been seen in energy dispersive x-ray diffraction in the absence of a pressure medium conducted earlier by our research group [6]. Since the energy dispersive x-ray data had a dearth of data in the range of 40 GPa to 70 GPa, further experiments were needed in order to better quantify the anisotropy. The goal of the angular dispersive x-ray diffraction (ADXD) data collected at the Advanced Photon Source is to reproduce the data with ADXD and compare the results. Analysis of this data is still ongoing and results are preliminary, final analysis of the data will appear in a PhD dissertation by Kevin Hope entitled, "Crystallographic Phase and Anisotropic Compression Effects in Light Actinide Metals at High Pressures."

Methods and Materials

Angular dispersive x-ray diffraction was conducted on a sample of commercially available uranium foil of 99.98% purity. The foil was loaded into a diamond anvil cell with a copper pressure marker. A pressure medium was omitted due to the softness of the material. After loading, the diamond anvil cell was sealed in Kapton tape to insure sample containment in case of diamond failure. Diffraction images were collected using an image plate detector and exposures of ten seconds were usually sufficient to obtain excellent diffraction data. The images were integrated using the ESRF FIT2D software, which generates files for data analysis by Rietveld refinement with the GSAS program.

Results



Figure 1: Comparison of b/a axial ratio from ADXD data with previously collected EDXD data. The line represents the EDXD data and is there to guide the eye.

c/a axial ratio for ADXD uranium data



Figure 2 : Comparison of c/a axial ratio from ADXD data with previously collected EDXD data. The line represents the EDXD data and is there to guide the eye.

Discussion

GSAS analysis of the data conducted to data shows an increase in the b/a axial ratio also observed in earlier experiments, and excellent agreement with previous data for the c/a axial ratio. Further analysis of the data is still ongoing and will provide data up to approximately 70GPa. In summary, we have measured the crystallographic anisotropy effects in the compression of the orthorhombic phase of uranium metal. We observe very interesting variation in both axial ratio (b/a) and (c/a) with increasing pressure to100 GPa. Our results indicate that the c-axis in the orthorhombic cell is the least compressible in the entire pressure range to 100 GPa and there is a crossover point in the compression of a-axis and b-axis of the orthorhombic cell at 83 GPa. Our detailed analysis of all available experimental data also indicates that the observed axial ratio trends are independent of pressure media used or non-hydrostatic stresses on the sample. The measured static equation of state of Uranium is presented to 100 GPa and a good level of consistency is obtained with three different pressure markers in the diamond anvil cell experiments.

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