AR-NE1A/2023G021/2021G019

Equation of state for rhenium

Shigeaki Ono [1,*]
[1] Research Institute for Marine Geodynamics, Japan Agency for Marine-Earth Science and Technology (JAMSTEC), Yokosuka 237-0061, Japan

1 Introduction

Rhenium (Re) is a group VII transition metal that crystallizes in a hexagonal close-packed (hcp) structure. The high-pressure behaviors of Re have been studied widely, as Re has a high bulk modulus value (~350 GPa) compared with other metals. Since Re is used as gasket material in diamond anvil cell experiments, there is considerable interest in its high-pressure behavior. Recently, the double-stage and the toroidal diamond anvil cells have extended the pressure range over 600 GPa. In such experiments, the equation of state (EOS) for Re has often been used as a pressure marker at extremely high pressures. An investigation of EOS could therefore improve the reliability of high-pressure experimental studies. Reliable data for high temperatures are still not available, as the uncertainty in the temperature is nonnegligible in high-pressure experiments. We performed high-pressure experiments to determine the room temperature EOS for Re.

2 Experiment

High-pressure X-ray diffraction experiments were carried out using a diamond anvil cell (DAC) with a laser-annealing system. Powdered sample was sandwiched between pellets of NaCl powder, which was used as the pressure-transmitting medium and the pressure reference. The starting material was compressed at room temperature using a symmetrical DAC. An angle-dispersive X-ray diffraction method was used to investigate the sample on a synchrotron beamline: AR-NE1A at the Photon Factory. The powdered X-ray diffraction patterns were obtained on an image plate system. The observed intensities on the imaging plates were integrated as a function of 2θ to obtain conventional, one-dimensional diffraction profiles. Sample pressure was calculated from the NaCl unit cell volume, using the EOS for NaCl. EOS parameters for Re were obtained from a least-squares fit to the pressure-volume data of the Vinet EOS. The sample was compressed to the desired pressure at room temperature, which was confirmed by the pressure scale of the Raman spectra from the diamond. Since the differential stress during room temperature compression causes a significant systematic bias in the relationship between the pressure and structural properties, the samples were heated after each change in pressure using an infrared laser, to reduce any differential stress in the sample.

3 Results and Discussion

The room-pressure unit-cell parameters of the starting material were a = 2.7620(1), c = 4.4592(2) Å, and V = 29.460(2) $Å^3$, values that are in good agreement with those from previous studies in the literatures. Typical diffraction data are shown in Fig. 1. After compression to the desired pressure, stress broadening of each diffraction peak was observed (Fig. 1a), which decreased drastically after laser annealing (Fig. 1b). This indicates that the differential stress under compression was released on annealing. Diffraction data after annealing were used to determine the EOS, since the differential stress often causes bias in the relationship between volume and pressure. The volumes and pressure data were fitted to the Vinet EOS using the least-squares method, yielding values of V_0 = 8.878(12) cm^3/mol, K_{T0} = 383(13) GPa, and K'_{T0} = 3.26(30). The value of the bulk modulus obtained in our experiments differs slightly from those reported from previous experiments without annealing [1].

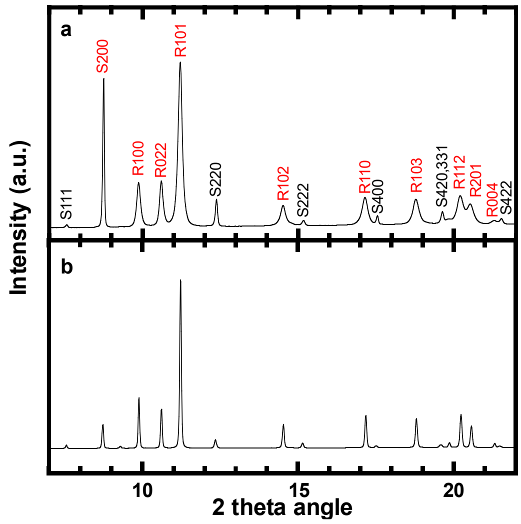

Fig. 1: Comparison of powder X-ray diffraction data, before and after annealing. The upper and lower data show the results before and after annealing, respectively. Labels for the diffraction peaks are as follows: R – Re with hexagonal structure; S – B1-type NaCl. Numbers on the labels correspond to the indices of hexagonal or cubic symmetry. Monochromatic incident X-ray beam wavelength: λ = 0.4110 Å.

Acknowledgement

This work was partially supported by JSPS KAKENHI Grant Number JP18K03792.

References

[1] S. Ono., *Advances in Condensed Matter Physics* **2022**, 7545777 (2022).

* sono@jamstec.go.jp