Equation of state for rhenium

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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. It is known that Re has the second-highest bulk modulus value after Os. Since Re is used as gasket material in diamond anvil cell experiments, there is considerable interest in its high-pressure behavior. 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. Therefore, we used first-principles molecular dynamics calculations to investigate the thermal properties of Re, and performed high-pressure experiments to determine the room temperature EOS for Re. This combination of two methods allowed us to determine reliable values for the thermoelastic properties over a wide range of pressures and temperatures. The room-temperature bulk modulus of Re was measured in the pressure range 0 to 115 GPa using a laser-annealing diamond anvil cell and the synchrotron X-ray diffraction method. Thermal properties of Re were investigated up to 4000 K based on first-principles molecular dynamics calculations, and the EOS for Re was determined using experimental and calculated data. A Vinet equation of state fitted to the 300 K data yielded a bulk modulus of K_{T0} = 384 GPa and a pressure derivative of K'_{T0} = 3.26. The fit to the data yielded $\alpha K_T(Va)$ = 0.0056 GPa/K. In contrast, the volume dependence of the thermal pressure was very small, and fitting yielded a value of $(\partial KT/\partial T)_V$ = -0.00042.

[1] S. Ono, Equation of state determination for rhenium using first-principles molecular dynamics calculations and high-pressure experiments, Adv. Condens. Matter Phys., (in press)

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