ESRF	**Experiment title:** P-V-T equation of state of tungsten by means of single-crystal diffraction and new heating techniques	**Experiment number**: HS-4050
Beamline: ID09A	**Date of experiment**: from: 07.04.2010 to: 10.04.2010	**Date of report**: 23.08.2010
Shifts: 9	**Local contact(s)**: Michael Hanfland	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Thomas Pippinger *, Institut für Geowissenschaften, Universität Heidelberg
Ronald Miletich *, Institut für Geowissenschaften, Universität Heidelberg
Natalia Dubrovinskaia, Institut für Geowissenschaften, Universität Heidelberg
Pascal Schouwink *, Institut für Geowissenschaften, Universität Heidelberg
Leonid Dubrovinsky*, Bayrisches Geoinstitut, Universität Bayreuth

Report:

Modern science and technology rely on the fundamental knowledge of matter that is provided by structural studies. Most reliable information about crystal structures and their response on variable pressure and temperature comes from single crystal diffraction experiments. *In situ* pressure and temperature calibration in diamond-anvil cell experiments remains always a challenge considering required accuracy. Several methods are described in literature, but often afflicted to large errors in measurement or simply unsuitable to experimental setup. A promising strategy to apply an internal standard are equations of state of physically stable and chemically inert materials, such as platinum, gold or tungsten.
Simultaneos high-pressure and high-temperature conditions favours tungsten as a promising candidate to be applicable as standard material, for reason of the extremely high melting point, pressure stability even to highest pressures, simple structure and the well known equation of state at 300K.

Single-crystal x-ray diffraction images were collected during ω-scans of the DAC and laser heating device [1] (Fig. 1). To achieve homogeneous heating conditions the whole assembly was moved simultaneously resulting in a restricted ω-scan range of -20° to 10°. Collected data was used to determine unit cell parameters of tungsten and neon in a measuring range up to 43 GPa and 2500 K (Fig.2). The isothermal Birch Murnaghn EOS was fitted using 18 datapoints at pressures between 4.5 GPa and 46.6 GPa, and is in good agreement with literature data.

Fig. 1. Universal laser-heating head (UniHead) (1) with a π-shaper (2) mounted for single crystal X-ray diffraction experiments in diamond anvil cell at ID09a beam-line at ESRF (Grenoble). (3) – the optical fiber connected to the 100 W laser light source, (4) – the silver-coated carbon mirror, (5) – the diamond anvil cell; green arrow in inset shows the direction of the laser beam.

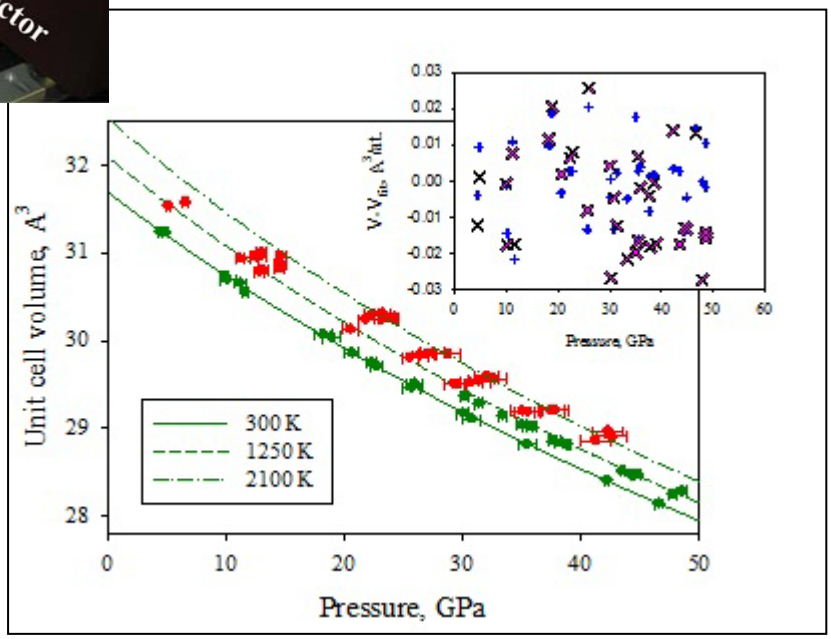

Fig. 2. Measured unit cell volume of tungsten at different pressures and temperatures. Green points were used to fit thermal equation of state with Ne as pressure gauge-pressures for red points and for lines were determined using fitted thermal EOS. Insert shows the difference between measured and fitted atomic volumes for thermal equations of state obtained in the present study (blue pluses) and predicted based on *ab initio* calculations.

[1] Dubrovinsky, L., Glazyrin, K., McCammon, C., Narygina, O., Greenberg, E., Uebelhack, S., Chumakov, A. I., Paskarelli, S., Prakapenka, V., Bock, J. & Dubrovinskaia, N. Portable laser-heating system for diamond anvil cells, *J. Synchrotron Rad.* 16, 737-741 (2009).