ESRF	**Experiment title: Mechanical properties of Ta under high pressure by single-crystal X-Ray diffraction**	**Experiment number**: HS-1361
Beamline: ID30	**Date of experiment**: from: 10/26/00 to: 10/31/00	**Date of report**: 02/01/01
Shifts: 18	**Local contact(s)**: M MEZOUAR	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

*Dewaele, Agnès

CEA/DPTA/SPMC
BP 12; F-91680 Bruyères le Châtel

*Loubeyre, Paul, same address

*Occelli, Florent, same address

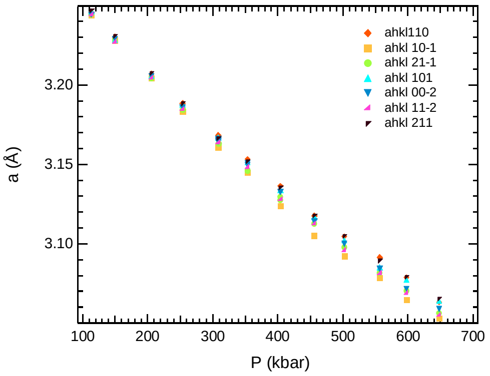
Report:

White beam single crystal X-Ray diffraction on Tantalum samples has been performed up to 65 GPa. The samples were deformed (a) under quasi-hydrostatic conditions (embedded in helium pressure medium), cell 1; (b) under uniaxial stress (sample embedded in helium but in contact with the diamond anvils), cell 2. This experiment had two goals: (1) the determination of a reference equation of state (EoS) under ultra-high pressure and ambient temperature; (2) the determination of pressure effect on the maximum deviatoric stress sustained by the sample before plastic yielding (i.e. the yield stress).

Experimental method: Lattice parameters values of several planes of Ta (bcc crystal), with different orientations towards the compression axis, have been measured for cells 1 and 2 (figure 1). From these values, the hydrostatic lattice parameter and the deviatoric stress $\tau=\sigma3-\sigma1$ ($\sigma3$ and $\sigma1$ are respectively the principal stresses parallel and perpendicular to the compression axis) have been calculated for each pressure step. For cell 2, approximate plastic deformation ε^P (function of t, the thickness of the sample) has been measured by interferometric method in the pressure transmitting medium (helium).

(1) **EoS of tantalum to 65 GPa:**

The measured EoS of tantalum is presented on figure 2, together with literature data [1], [2], [3]. The failure of cell 1 diamond, caused by helium diffusion, prevented us from performing hydrostatic measurements for pressures higher than 45 GPa. Measurements performed under non-hydrostatic conditions, after analysis, lead to a compression curve that shows a much smaller scatter than literature data. Third-order Birch Murnaghan EoS fit parameters are the following: ao= 3.3034 Å, Ko= 195 GPa, K'o=3.03, where these parameters are the lattice parameter, incompressibility and its pressure derivative in the reference state. The K'o obtained is lower than the parameter obtained by the most recent study results [1]: K'o=3.4. This low value has to be confirmed by higher pressure compression experiments.



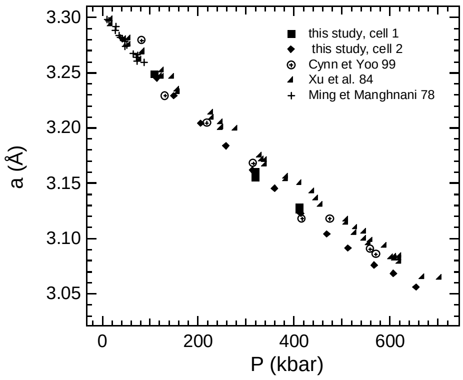


Figure 1 (left): evolution of $a_{hkl}=d_{hkl}*\sqrt{(h^2+k^2+l^2)}$ for several planes as a function of pressure (ruby florescence jauge) in cell 2.
Figure 2 (right): measured hydrostatic equation of state, compared with literature data.

(1) Evolution of yield stress with pressure to 65 GPa:

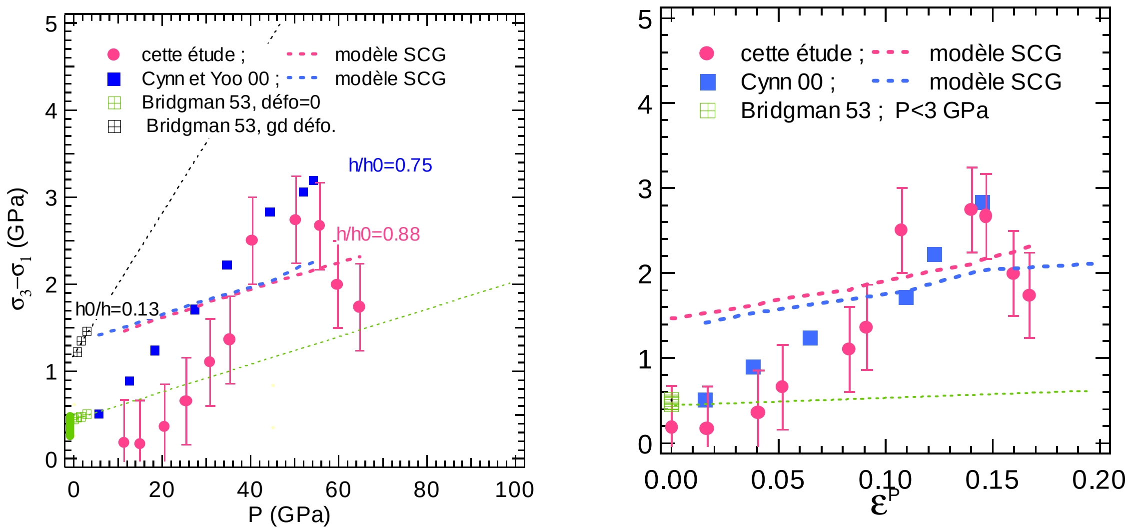


Figure 3: evolution of $\tau=\sigma 3-\sigma 1$ with plastic pressure and plastic strain. Literature data, see [4] and [5]

In our experiments, the yield stress depends mainly on the amont of plastic deformation ε^P (hardening) and the hydrostatic pressure. The evolution of $\tau=\sigma 3-\sigma 1$ with these parameters is plotted in figure 3. The main comments are:

- the large hydrostatic pressure effect on the yield stress (more dramatic than the scaling law τ proportional to shear modulus, called SCG model on the figure), observed for the first time on a single crystal
- the good coherence of our measurements with those performed on polycrystal tantalum by an other method [4], which shows that intergranular plasticity seems negligible in that metal.
- the possibillity of a decrease of yield stress under ultrahigh pressure, that must be confirmed by higher pressure measurements.

References:

[1] H. Cynn and C.-S. Yoo, Phys. Rev. B, 59, 8526-8529 (1999)
[2] J. Xu et al., High Temp.-High Press., 16, 495, (1984)
[3] L.Ming and M.H. Manghnani, J. Appl. Phys., 49, 1, 208-212 (1978)
[4] H. Cynn and C.-S. Yoo, to be published in Phys. Rev. B (2000)
[5] P.W. Bridgman, J. Appl. Phys., 24, 5, 560-570 (1953)