ESRF	**Experiment title:** Lattice dynamics of vanadium under high pressure: search for electronic topological transition	**Experiment number**: HS-3749
Beamline: ID28	**Date of experiment**: from: 02.07.2008 to: 14.07.2008	**Date of report**: 22 April 2009
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Report:

We carried out inelastic x-ray scattering (IXS) measurements on vanadium single crystals compressed in diamond anvil cells (DAC) up to 45 GPa.

High quality V single crystals have been prepared by laser cutting, with subsequent chemical etching. This last step served as well for crystal size adjustment. Samples of ~30 μm diameter and ~15 μm thick have been loaded in DACs equipped 300 or 350 μm culets diamond and rhenium gaskets. Helium or neon have been used as pressure transmitting medium.

IXS measurements have been performed on ID-28, using the Si(9,9,9) instrument configuration, which provides an overall energy resolution of 3 meV full-width-half-maximum (FWHM). The direction and size of the momentum transfer were selected by an appropriate choice of the scattering angle and the sample orientation in the horizontal scattering plane. The momentum resolution was set to 0.28 nm^{-1} and 0.84 nm^{-1} in the horizontal and vertical planes, respectively. The focused x-ray beam of 30 x 90 μm^2 FWHM was further reduced in the vertical by slits to match sample dimensions. Measurements have been performed in transmission geometry, with the incoming x-ray impinging along the cell axis, across the diamonds.

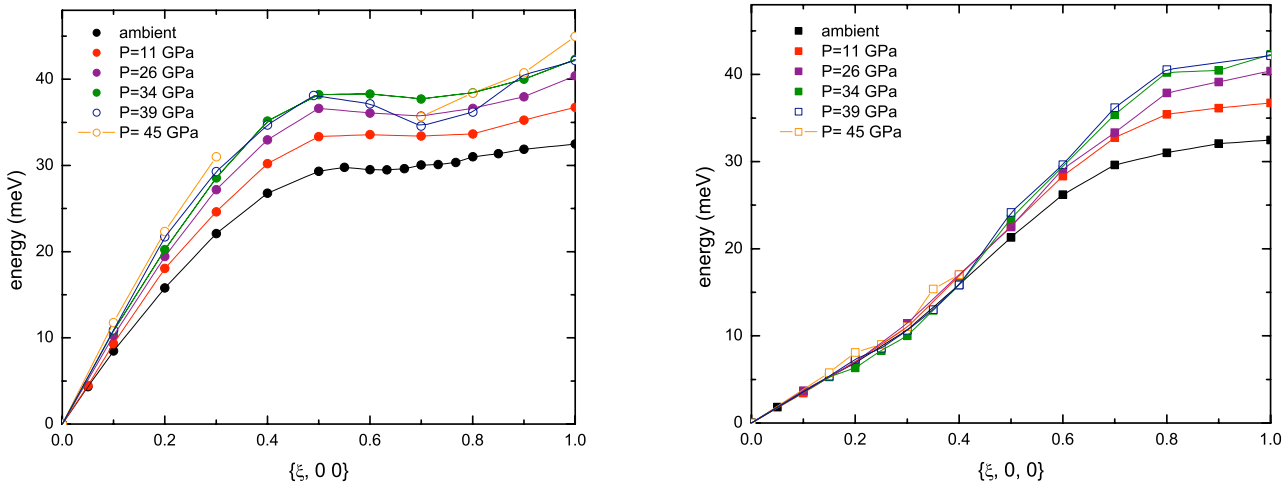

Figure 1: Phonon dispersion of LA (left panel) and TA (right panel) modes along [100] direction for increasing pressures. Ambient conditions results are from [1]. Lines are interpolation to the experimental data as guides to the eyes.

We collected data at room temperature and pressures of 11, 26, 34, 39 and 45 GPa. At 11 and 26 GPa the complete phonon dispersion for high symmetry directions has been recorded, while at higher pressure we focused on the longitudinal acoustic (LA) and transverse acoustic (TA) modes along [100] direction. The pressure evolution of the LA (left panel) and TA (right panel) phonons along {ξ,0,0} is shown in Figure 1. If we focus on the low q part of the dispersions, we can notice a phonon hardening for the LA mode (as commonly expected with increasing pressure), while there is no sizable change in the TA mode, which slightly softens at 34 GPa, and then start to get stiffer. An analysis of the overall shape of the LA dispersion also highlights a change above 34 GPa, with a deeper minimum for ξ~0.7 clearly visible at 39 and 45 GPa (Figure 1).

The derived elastic moduli C_{11} and C_{44} as a function of pressure are reported in Figure 2.

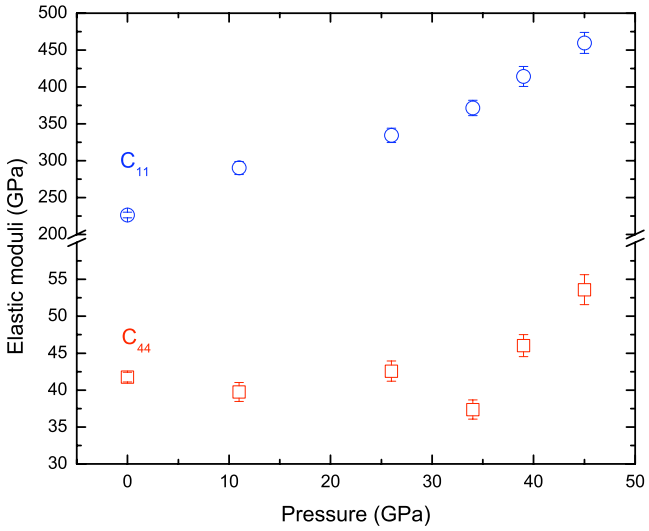

Figure 2: Elastic moduli C_{11} and C_{44} as a function of pressure

In agreement with the predictions of previous theoretical [2] and experimental [3] studies, we argue this softening of C_{44} to trigger a rhombohedral lattice distortion. However, our results clearly place the transition around 35 GPa rather than at 69 or 84 GPa as previously suggested [2,3]. Our conclusions are further supported by the compression curve obtained by preliminary x-ray diffraction measurements on V single crystals (see Figure 3), which also highlights the first-order nature of the phase transition.

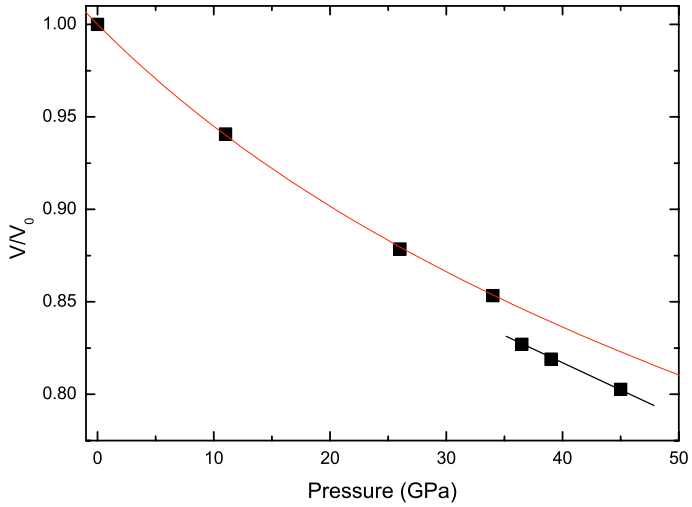

Figure 3: Compression curve of vanadium up to 45 GPa. The black squares are our data, the red line is obtained from literature equation of state [3], while the black line is a guide to the eyes.

References:

[1] Bossak et al., Phys. Rev. B 78, 020301(R) (2008).
[2] Lee et al., Phys. Rev. B 75, 180101(R) (2007); Lee et al., Phys. Rev. B 77, 134105 (2008).
[3] Ding et al., Phys. Rev. Lett. 98, 085502 (2007).