ESRF	**Experiment title:** Short Range Order in Liquid Tellurium: an X-Ray Absorption Study	**Experiment number:** HE-156
Beamline: BM29	**Date of Experiment:** from: 14-02-1997 to: 18-02-1997	**Date of Report:** 28-02-1997
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Report:

During beam time allocated for experiment HE-156 we performed a successful x-ray absorption spectroscopy (XAS) study on crystalline (s-Te) and liquid (ℓ-Te) tellurium.

To probe the local structure of ℓ-Te particular care was devoted to prepare suitable sample for XAS measurements. In order to achieve the optimal thickness ($\sim 20\ \mu$m) and requested homogeneity, both in solid and liquid state, samples were prepared as follows: fine precursor compound (TeO_2) powder was ball-milled together with inert matrices powder (either ultra-pure graphite or BN) in 1:20 dilution, and then pressed into pellets. *In situ* reduction to crystalline Te was performed by means of thermal treatment under controlled atmosphere during several cycles and was monitored looking at the near edge structures.

Because of the peculiar thermal treatment we characterized the experimental samples using the reflectometer available at beamline BM29 and we performed x-ray diffraction (XRD) analysis both at the beginning and the end of thermal sample history. RT powder diffraction patterns of a Te reference in amorphous matrix and of a sample before, as TeO_z grains confined in inert matrix, and after the reduction are shown in Fig. 1 where the excellent agreement of Te peaks assure the actual reduction of precursor.

The occurrence of a sharp melting transition characteristic of a high purity bulk sample was verified by a single energy temperature scan in the range room temperature (RT)-800 K. The absorption coefficient shows an hysteresis cycle with discontinuity at the known Te melting point on the heating stroke and reveals an undercooled state during the cooling period.

XAS measurements were performed in the transmission mode with Kr filled photodiode detectors in the energy range 31.5 - 32.8 keV and with constant k spacing of 0.02 $Å^{-1}$. Spectra were collected at various temperature from 20 K to RT in a closed cycle He cryostat and from RT up to 800 K in an oven with graphite crucible.

In Fig. 2 XAS oscillations of s-Te and ℓ-Te at several temperatures are shown. With respect to previous

x-ray absorption measurements on similar systems [I], our data show an improved energy resolu
together with an excellent noise-to-signal ratio (better than 10^{-4}): the overall quality of measurem
was extraordinary.
Data analysis has been performed along the line traced in previous works [2] using *ab initio* mult
scattering calculations and correctly taking into account the medium range structure evaluated
previous neutron scattering studies [3].
The main results obtained in present experiment are going to appear in a forthcoming letter [4], w
a more complete work is under preparation. Reliable radial distribution function g(R) for ℓ-Te u
about 3.5 Å have been determined and information have been extracted on atomic arrangement
electronic structure of ℓ-Te, explaining the semiconductor to (semi)metal transition observed ir
upon melting.

References:

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[2] A. Filipponi J. Phys.: Condens. Matter 6, 8415 (1994).
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[4] S. De Panfilis and A. Filipponi, Europhys. Lett. (in press, 1997).

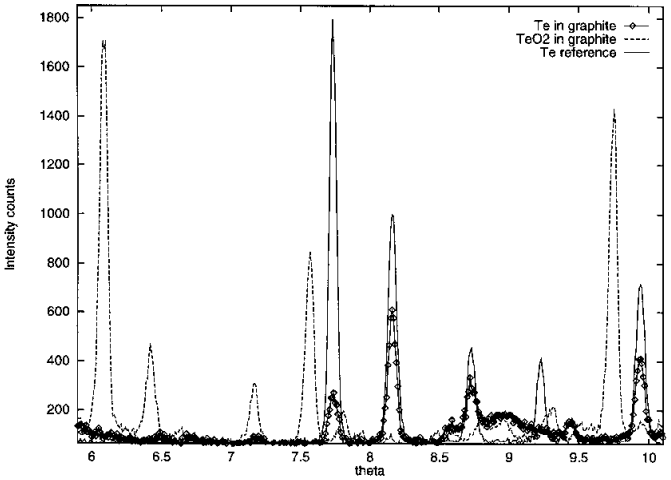

Figure 1: XRD patterns of Te and TeO_2 powders diluted in graphite and a Te reference.

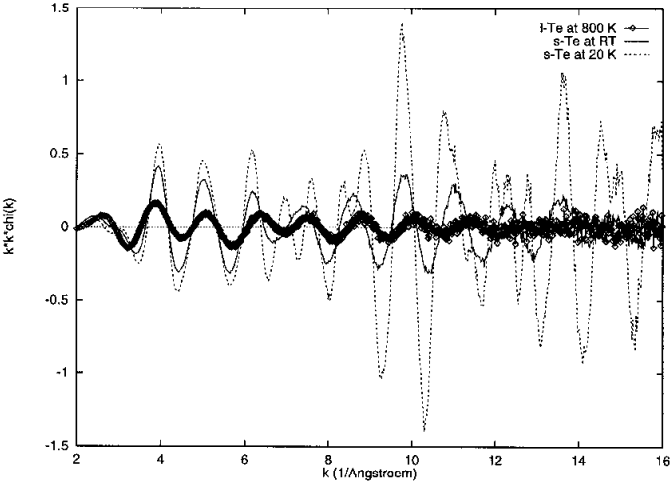

Figure 2: $k^2\chi(k)$ of ℓ-Te at 800 K and of s-Te at RT and 20 K.