ESRF	**Experiment title:** Liquid-Liquid phase transition in bismuth: High pressure high temperature study	**Experiment number**: HD-506
Beamline: ID27	**Date of experiment**: from: 29/10/2010 to: 2/11/2010	**Date of report**: 11/3/2011
Shifts: 12	**Local contact(s):** Dr. Mohammed Mezouar	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

***Eyal Yahel**: Physics Dept., NRCN, POB 9001, Beer-Sheva 84190, Israel

***Aviva Melchior**: Physics Dept., NRCN, POB 9001, Beer-Sheva 84190, Israel

***Yaron Greenberg**: Physics Dept., NRCN, POB 9001, Beer-Sheva 84190, Israel

***Ori Noked**: Physics Dept., Ben-Gurion University, POB 653 Beer-Sheva, 84105 Israel

***Guy Makov:** Material Engineering Dept., Ben-Gurion University, POB 653 Beer-Sheva, 84105 Israel

Report:

Bismuth metal is suspected to have transformations in the liquid state [1]. Previously, we found evidence for a temperature-driven structural transformation in liquid bismuth at 740^0C and ambient pressure [2]. **The aim of this experiment was to study the structural nature of transformations proposed for liquid Bi**.

The structure of molten bismuth was investigated, as function of pressure (P) and temperature (T), at ID27 beamline using the Paris-Edinburgh (PE) high pressure apparatus. The selected thermodynamic conditions (P and T) were attained by compressing a high purity bismuth sample, confined in a boron-epoxy cell and DC current directly applied to a graphite heater surrounding the sample. The sample, 0.6mm in diameter and 2mm height, was encapsulated in a boron nitride (BN) tube and inserted into a cylindrical graphite heater. The boron-epoxy capsule was pressurized using a 3mm truncated WC toroidal anvil. The PE apparatus was combined with an X-ray diffraction MAR image plate detector to collect diffraction patterns from the sample. Soller slits, mounted between the pressurized cell and the imaging plate, were used to reduce peripheral diffraction patterns from structural materials (BN-pressure medium and C-graphite heater).

Special attention was paid to accurate determinations of pressure and temperature by using two internal calibration materials. The first is BN which also acts as a pressure medium and container structure material. The second material used was platinum, which was placed adjacent to the BN container. The diffraction pattern of each of these materials was measured at every P-T point. Rietveld analysis of the diffraction retrieved the lattice parameters of the calibration materials. By using known thermal equation of states (EOS)

of BN [3] and Pt [4] a cross-calibration analysis calculated the exact pressure and temperature of the sample. An initial estimate of the pressure and temperature calibration accuracy is better then 0.1GPa and 10^0, respectively. A typical P-T point is presented in Fig. 2.

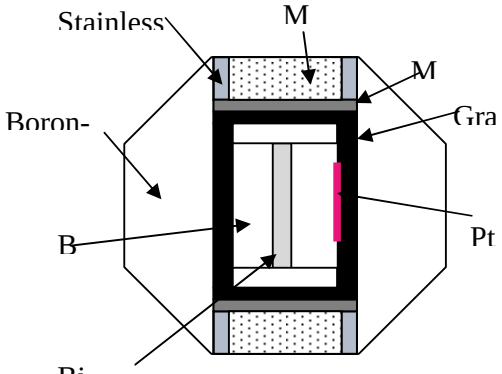


Fig.1: Schematic draw of Sample capsule

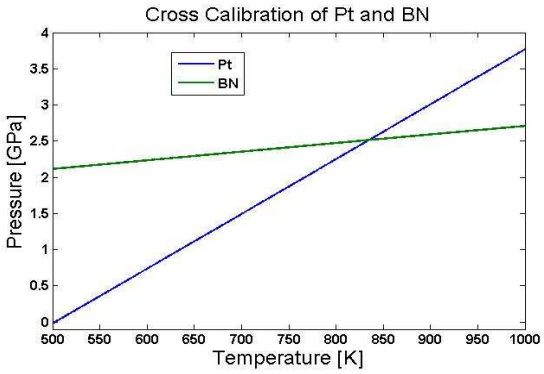
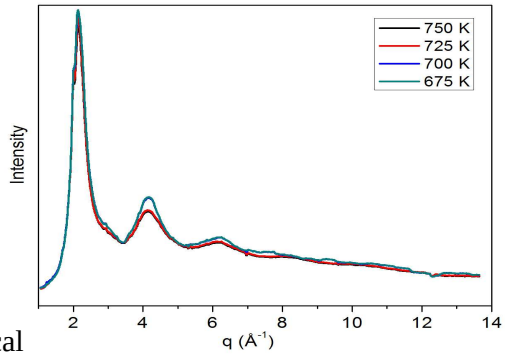


Fig.2: Cross-calibration of BN and Pt EOS

Diffraction images were taken at 3 pressures with dense sampling in temperature of approx. 25^0. Fig. 3 presents a change in the structure factor found at 2.47GPa and 800K in reasonable agreement with previously identified transition lines [1]. Furthermore, this change in liquid structure is similar to that observed previously at a different point in phase space [5].

Fig. 4: XRD from liquid Bi at 4 temperatures (P=2.47GPa**)**



Preliminary results and perspectives

Initial results suggest that liquid Bi exhibits changes in its structure at a point consistent with transition lines determined by thermophysical measurements. These results will undergo further analysis in an attempt to determine the nature of the structural rearrangement in the liquid which will assist in understand the nature of the transition in liquid Bi. In the future we propose to perform an additional set of measurements to determine the position of the transition line in phase space of liquid Bi.

References

[1] A. G. Umnov et al., J. Phys.: Condens. Matter, **4**, 1427 (1992).

[2] Y. Greenberg *et al*.., Europhys. Lett. **86**, 36004 (2009)

[3] W. Crichton and M. Mezouar, High Temperatures - High Pressures **34**, 235 (2002).

[4] M. Matsui *et al.*, J. Appl. Phys. **105**, 013505 (2009).

[5] K. Yaoita *et al*., J. Non-Cryst. Sol. **150**, 25 (1992).