Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office using the **Electronic Report Submission Application:**

http://193.49.43.2:8080/smis/servlet/UserUtils?start

Reports supporting requests for additional beam time

Reports can now be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** High-pressure elasticity of FeO	**Experiment number**: HS-3197
Beamline: ID-28	**Date of experiment**: from: 26.11.2006 to: 04.12.2006 (22.12 - 26.12 – set-up time)	**Date of report**:
Shifts: 18	**Local contact(s)**: Michael Krisch	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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ESRF

Report:

Acoustic phonon dispersion modes in a single crystal of synthetic wüstite $Fe_{0.95}O$ were measured using inelastic x-ray scattering (IXS) at elevated pressure and room temperature. We recorded the longitudinal acoustic (LA) phonon branches along the [001] and [110] directions, and transverse acoustic (TA) branches along the [111] and [100] direction. The corresponding sound velocities were determined from the linear part of the acoustic phonon branch, and the three independent elastic moduli were then derived using the Christoffel equation. The effective adiabatic bulk modulus K_S was calculated for every complete dataset using individual elastic constants, and converted into isothermal modulus K_T using the following equation:

$$K_T = K_S \left(1 + \alpha\gamma T\right)^{-1} \qquad (1)$$

In parallel to the IXS spectra, the Bragg angles of the (002) and (220) reflections were recorded in order to provide an independent determination of volume and density for each pressure point. The coefficients of a finite-strain isothermal third-order Birch-Murnaghan equation of state (EoS) were determined by fitting pressure-volume dependence.

This combined IXS and x-ray diffraction (XRD) study revealed an increasing difference in the bulk modulus determined from static (XRD) and dynamic (IXS) measurements upon compression. The effective ambient conditions bulk modulus determined from IXS and compressibility measurements coincides within the experimental error (K_T = 162 ± 3 GPa), while *K'* values differ significantly (5.3 ± 0.2 for IXS data vs. 1.79 ± 0.9 for diffraction data). At pressures of about 17 GPa (just below cubic-to-rhombohedral transition) the difference in bulk modulus reaches ~40 GPa, at least one order of magnitude larger than the associated experimental uncertainty (Fig. 1). The reanalysis of previous results put some more evidence for relative good coincidence for bulk moduli and systematic difference for *K'* between static and dynamic measurements.

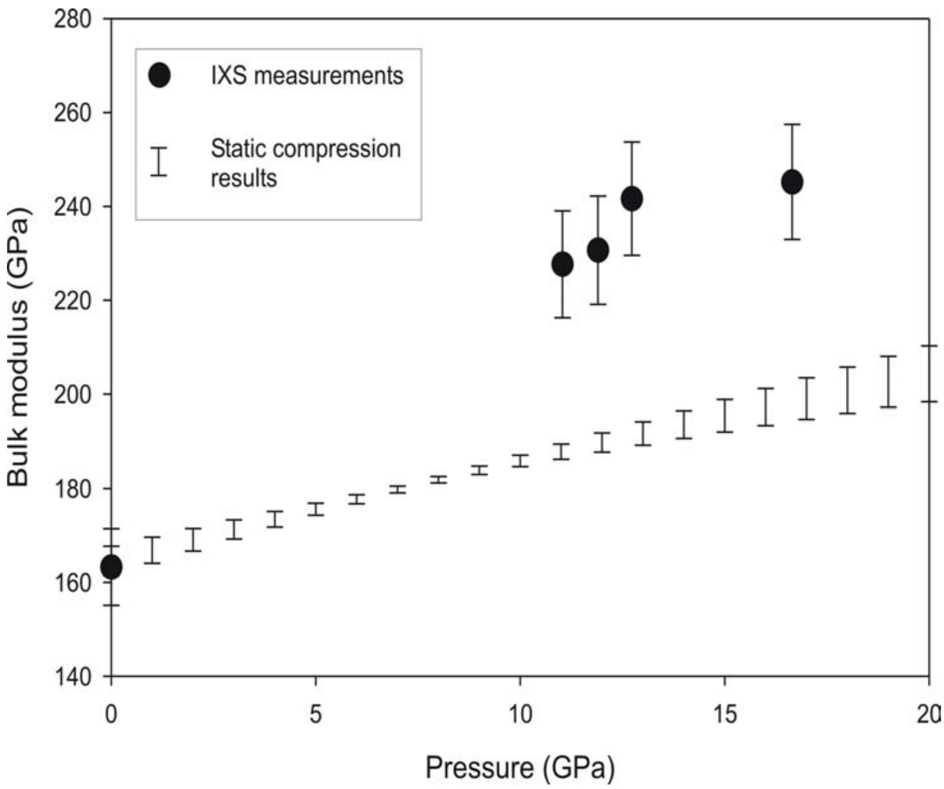

Fig. 1. Bulk modulus of $Fe_{0.95}O$ as a function of pressure.

We explain and quantitatively describe this observation by anelastic relaxation in wüstite associated with defect diffusion. We assume, that pressures, measured under static stress, reflect fully relaxed structure, and bulk moduli measured from acoustic phonons dispersion are pure elastic response. Low frequency or static measurements would reflect a sum of elastic and anelastic contributions. In the case of any internal structural relaxations, associated with atomic diffusion, a certain characteristic time τ is required to reach equilibrium state. If the inverse sampling frequency is smaller than τ, only elastic relaxation occurs, and the measured bulk modulus and *K*' are higher than the ones probed with an inverse frequency larger than τ. Our observations show that significant anelastic behaviour appears only at high pressure, when a certain strain is applied.