ESRF	Experiment title:  Phase transformation of magnesite at very high temperature and megabar pressures studied by angle dispersive X-ray diffraction	Experiment number: HS622
Beamline: ID9	<b>Date of experiment:</b> from: 21/01/99 to: 21/01/99	<b>Date of report:</b> 01/03/99
Shifts:	Local contact(s): Michael Hanfland	Received at ESRF:

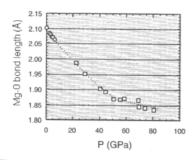
## Names and affiliations of applicants (\* indicates experimentalists):

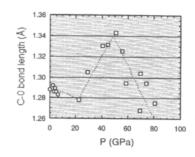
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## Report:

We report here X-ray diffraction experiments that have been carried out to determine the compression properties of a natural MgCO<sub>3</sub> magnesite. Magnesite has been reported to be a important potential host for oxidized carbon in the Earth's mantle. It is thus of primary importance to study its stability to the greatest pressure and temperature known at these depths (130 GPa, 3500 K). Angle dispersive X-ray diffraction experiments were carried out at the high-pressure beamline ID09 of the ESRF (Grenoble, France). X-ray beam at a wavelength of 0.41259 Å was used in association with imaging plates to collect data over a 2-theta interval from 4 to 25°, suitable for structural refinements.

X-ray diffraction pattern were recorded to 113 GPa on a mixture of magnesite and platinum powders, loaded in a diamond-anvil cell and annealed with an infrared YAG laser. As shown in Figure 1, Rietveld structural refinements show that the principal structural change with increasing pressure is a very large compression of the MgO<sub>6</sub> octahedra on the cost of a slight expansion of the CO<sub>3</sub> groups. Above 60 GPa however, MgO<sub>6</sub> octahedra almost stop compressing and the overall compression is in turn accommodated by a compression of the CO<sub>3</sub> groups.





**Figure 1**: variation of M-O bond lengths and C-O bond lengths with pressure in magnesite. Circles: data from [Ross, *Amer. Mineral.*, 82, 682, 1997]; squares: this work.

Above 80 GPa, the magnesite pattern progressively disappears and new features can be noticed on the 2-dimensional pattern recorded at 90 GPa (see below).

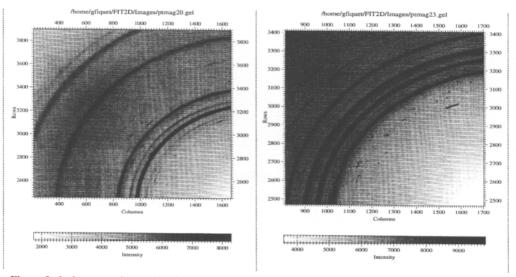


Figure 2: Left: magnesite sample after compression above 90 GPa, continuous lines are those of platinum and those of rhenium, used as gasket material. A few spots at low angle correspond to the most intense 104 reflection of magnesite. Right: at 130 GPa, one notices new features at low angle as well as new spots for diffraction angle exceeding those of the most intense lines (Pt and Re).

These new spots develop with laser heating at 130 GPa, which clearly indicates a recrytallization of the MgCO<sub>3</sub> magnesite in a new structure, which has not been identified yet.