ESRF	**Experiment title:** Cation disorder in the system CaCO3-MgCO3-FeCO3 to 6 GPa: the thermodynamics and phase relations of the ternary carbonate solid solution at upper mantle conditions	**Experiment number**: **HS- 3709**
Beamline:	**Date of experiment**: from: 12 nov 2008 to: 17 nov 2008	**Date of report**:
Shifts:	**Local contact(s)**: Mohamed Mezouar	*Received at ESRF:*

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Report:

Dolomite occurs in a wide range of rock compositions, from peridotites, to mafic eclogites and metasediments, up to mantle depths of more than 200 km. At low temperatures dolomite is ordered (R3), but transforms with increasing temperature into a disordered higher symmetry structure (R3c). To understand the thermodynamics of dolomite, we have investigated temperature, pressure, kinetics and compositional dependence of the disordering process in Fe-bearing dolomites. To avoid quench effects, in-situ X-ray powder diffraction experiments were performed at 300-1350 K and 2.6-4.2 GPa. The long-range order parameter s, quantifying the degree of ordering, has been determined using structural parameters from Rietveld refinement and the normalized peak area variation of superstructure Bragg peaks characterizing structural ordering/disordering. Time-series experiments show that disordering occurs in 20-30 minutes at 858 K and in a few minutes at temperatures ≥ 999 K. The order parameter decreases with increasing temperature and XFe. Complete disorder is attained in dolomite at ~ 1240 K, 100-220 K lower than previously thought, and in an ankeritic-dolomites.s. with an XFe of 0.43 at temperatures as low as ~ 900 K. The temperature-composition dependence of the disorder process was fitted with a phenomenological approach intermediate between the Landau theory and the Bragg-Williams model and predicts complete disorder in pure ankerite to occur already at ~470 K.

The relatively low temperature experiments of this study also constrain the breakdown of dolomite to aragonite+Fe-bearing magnesite at 3 GPa to temperature lower than 500 °C favoring an almost straight Clapeyron-slope for this disputed reaction.

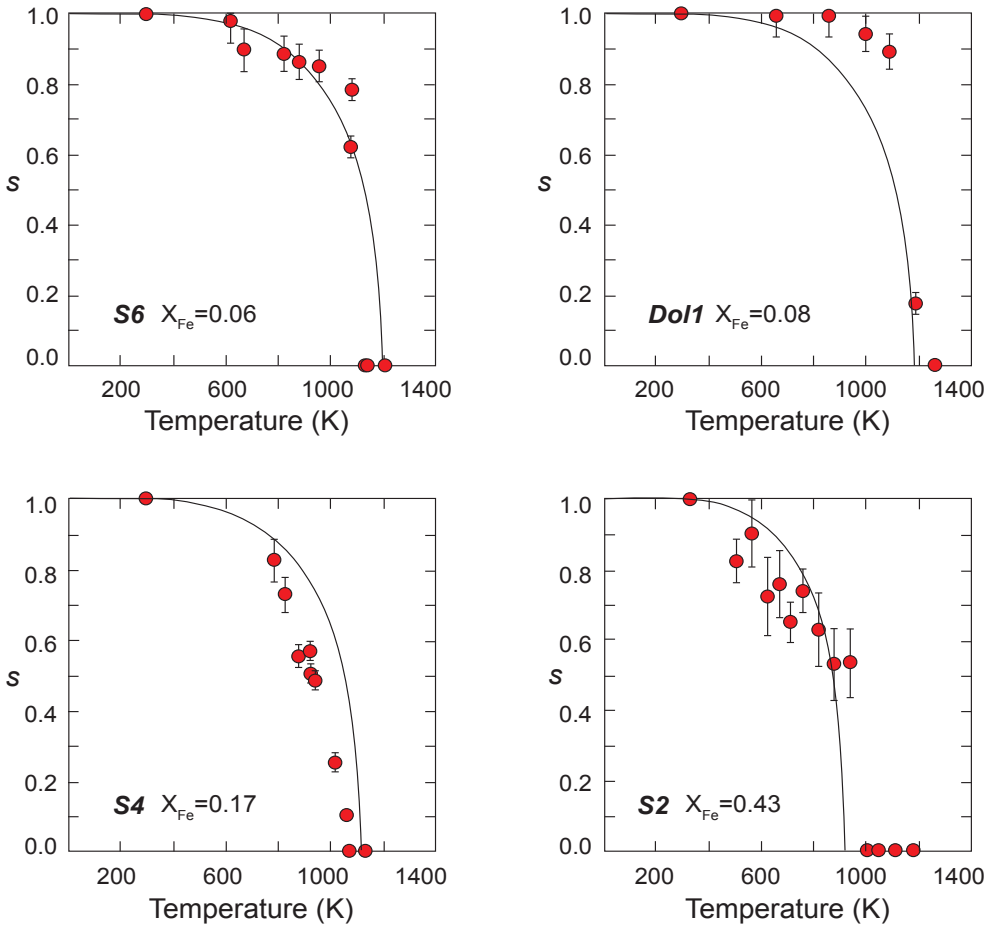

Fig. 1 - Plots of the ordering parameter ***s***, expressed as the normalized peak area ratio I_{101}/I_{110} , vs. temperature. The solid lines are the best fit to the experimental data of the model

Ref.

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