Anomalous PVT behaviour of periclase – an ultra-sonic and Raman study between -200° and +100° C

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Periclase is an important geo-material; it is of NaCl-type structure, and is characterised by a remarkable P-T stability. We studied the ultrasonic (us) behaviour of MgO in dependence of temperature and pressure in the range of -200° to $+100^{\circ}$ C at 20 and 200 MPa. The us-results were compared with Raman data obtained from microcrystalline material over the same temperature range (0,1 MPa). The us-data reveal marked changes at -170° , -110° , $-30^{\circ}(?)$, and 15° C at either pressures. The same temperatures hold true for the Raman data. The selected band at 1100 cm^{-1} which is caused by polarisability of surface modes [1] shows discontinuous wave shift and significant change in the full width at half maximum (FWHM) at the same temperature of -170° , -110° , -30° (?) and 15° C.

Taking into account that no structural change occurs, we interpret the ultra-sonic phenomena as PVT-anomalies originating from MgO lattice vibrations. This interpretation is supported by our Raman data and by detailed analysis of Cp and thermal expansion data reported in the literature (e.g. [1] [2]) as well, furthermore, by a previous us-study at ambient pressure [3]. Generally, our observations indicate that homogenous crystal phases may show anomalous changes in their lattice vibrations in dependence of temperature and pressure.

[1] Schlecht & Böckelmann (1973) *Phys. Rev. Lett.*, **21**, 930-932.
[2] Barron et al. (1959) *Proc. Roy. Soc. London*, Ser. A, **250**, 70-83.
[3] White & Anderson (1966) *J. Appl. Phys.*, **37**, 430-432.