Crystal structure of solid oxygen at high pressure and low temperature

A careful sample preparation and annealing around 240 K allowed very good diffraction patterns in the orthorhombic δ phase to be obtained. This phase is stable at low temperatures, in contrast to some recent data[1], and transforms with decreasing pressure into a monoclinic phase, which is identified as the low-pressure α phase. The discontinuous change of the lattice parameters, and the observed metastability of the α phase increasing pressure suggest that the transition is of first order. The results have been published by **Gorelli et al. in Phys. Rev B 65, 172106 (2002)**

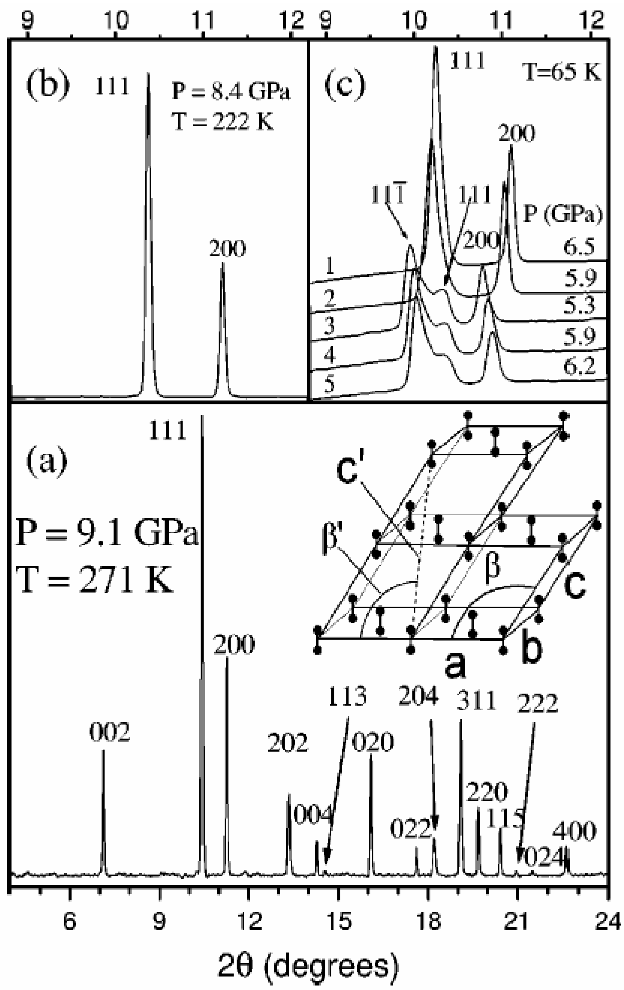

FIG. 1. (a) Angle dispersive diffraction pattern of oxygen at 9.1 GPa and 271 K (λ=0.4171 Å). The indexing corresponds to the enlarged cell abc' (see inset). (b) The orthorhombic structure persists with cooling of the sample, as demonstrated by the detail of the 111 and 200 reflections at 222 K and 8.4 GPa. (c) Diffraction patterns obtained during decompression from 6.5 to 5.3 GPa and subsequent compression from 5.3 up to 6.2 GPa at 65 K. The numbering on the left indicates the time sequence of the measurements, while on the right the pressure is indicated.

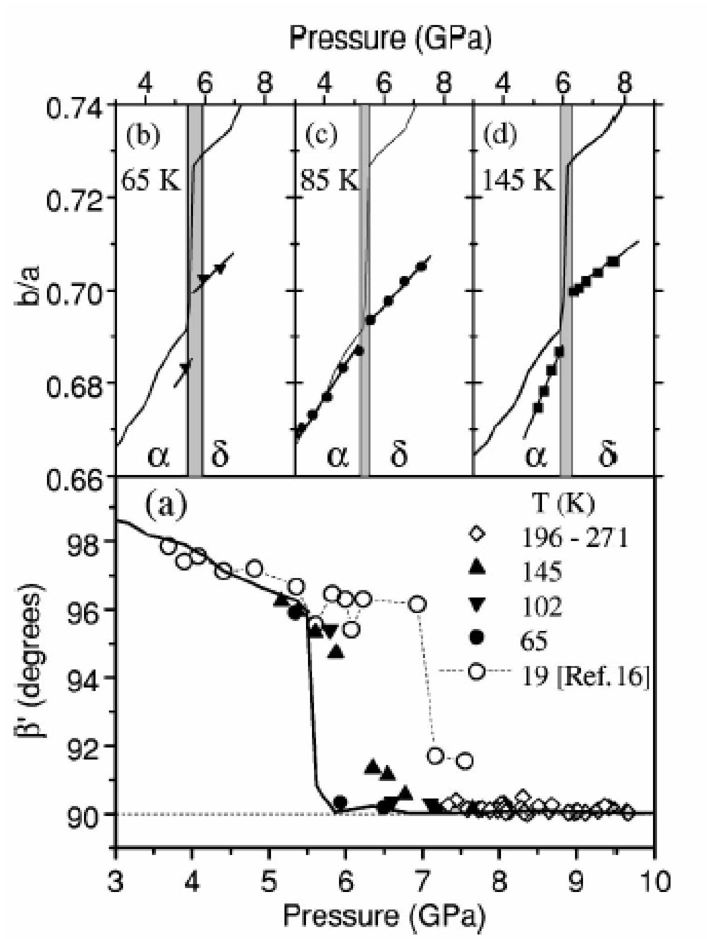

FIG. 2. (a) Evolution of the β' angle at different temperatures. Empty diamonds and all solid symbols are our results taken along decompression runs, while empty circles are data from Ref. 1. Errors on our data range from 0.02 to 0.3 degrees. (b–d) Evolution with pressure of the b/a ratio, at different temperatures, across the α-δ phase transition (solid symbols). Error bars for this quantity are smaller or of the order of the symbols size. The solid lines in both figures represent the values from lattice dynamic calculation[2], plotted versus rescaled pressure.

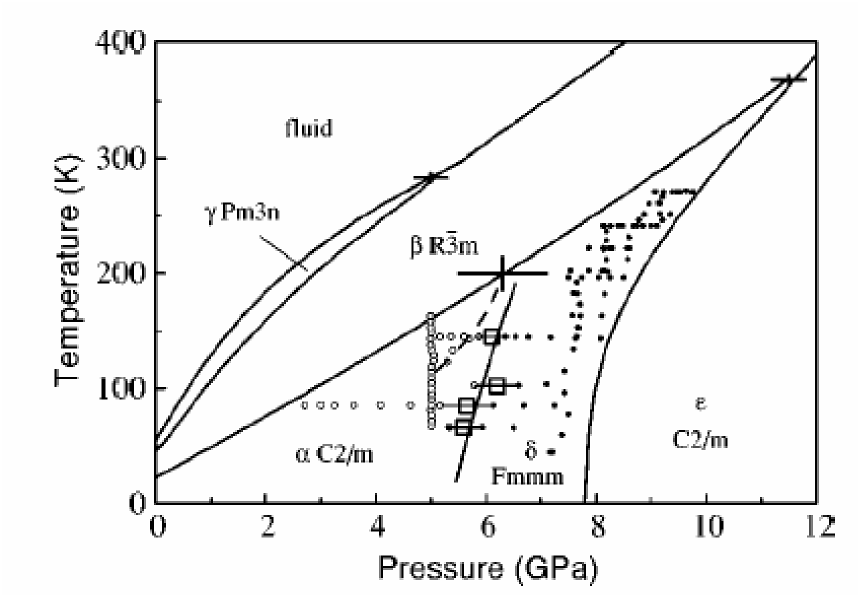

FIG. 3. Phase diagram of solid oxygen from Ref. 3, after removal of some low-pressure phase boundaries. Solids dots and empty circles represent values of P and T where an orthorhombic or monoclinic structure, respectively, has been measured. The empty squares show the observed δ-α transition, and the solid line is the possible α-δ phase boundary. The dashed line represents a phase boundary proposed by Yen and Nicol, Ref. 4.

---

[1] Y. Akahama et al., Phys. Rev. B **64**, 054105 (2001)
[2] R.D. Etters, K. Kobashi, and J. Belak Phys. Rev. B **32**, 4097 (1985)
[3] S. Desgreniers, Y.K. Vohra, and A.L. Ruoff, J. Phys. Chem. **94**, 1117 (1990)
[4] J. Yen and M. Nicol, J. Phys. Chem. **91**, 3336 (1987)