s2.m1.o5 **Electron density distribution in stishovite, SiO_2,: a high energy synchrotron radiation study.** A. Kirfel[1], T. Lippmann[2]. [1]*Mineralogisch-Petrologisches Institut, Universität Bonn, Poppelsdorfer Schloss, D-53115 Bonn,* [2]*GKSS, Max-Planck-Str., D-21502 Geesthacht*
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The electron density distribution of the high-pressure polymorph of SiO_2, stishovite (a = 4.1773, c = 2.6655 Å, S.G. $P4_2/mnm$, Z = 2), has been redetermined by single-crystal diffractometry using synchrotron radiation of 100.42 keV in order to obtain absorption and extinction free data. The room temperature diffraction experiments on a sample of irregular shape obtained from [1] were performed on the Triple-Crystal Diffractometer installed at beamline BW5 at HASY-LAB/DESY, Hamburg [2]. For a full sphere up to $\sin\Theta/\lambda = 1.35$ Å^{-1}, 3795 reflections were recorded resulting in a set of 269 unique reflections with an in-ternal agreement factor $R(F^2) = 0.0117$.

The structure refinements using the VALRAY programme package [3] converged at R(F) = 0.0111, wR(F) = 0.0131, GoF = 2.45 for the IAM and at R(F) = 0.0055, wR(F) = 0.0044, GoF = 0.90 for a multipole model featuring neutral atoms and multipole expansions up to hexadecapoles. For each atom, the radial expansion coefficients of the multipole orders (l>0) were constrained to a common value. Absence of extinction was indicated by a refined correction parameter equalling zero within error limit. The excellent quality of the data is also illustrated by a HO-refinement ($s > 0.7$ Å^{-1}) yielding R(F) = 0.0068, wR(F) = 0.0053, GoF = 0.85. Both static deformation densities and structure amplitudes compare well with corres-ponding results from LAPW calculations [4].

Ensuing topological analysis of the total model electron density distribution revealed bond critical point properties for the two unique Si-O bonds, $Si\text{-}O_{eq}$ (d = 1.757 Å, ρ_c = 0.74 eÅ^{-3}, $\nabla^2\rho_c$ = 11.0 eÅ^{-5}) and $Si\text{-}O_{ap}$ (d = 1.808 Å, ρ_c = 0.62 eÅ^{-3}, $\nabla^2\rho_c$ = 8.5 eÅ^{-5}). Calculations of the atomic basins and related properties [4] resulted in charges of +3.45 e and –1.72 e for Si and O, respectively. The volumina of the respective basins are 2.32 and 10.48 Å^3, corresponding to spheres with radii of 0.82 and 1.36 Å.

The comparison with the results derived from earlier X-ray tube data [5] combining single-crystal and powder intensities shows also reasonable agreement.

Notes

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