Supporting Information for

**Stability and Thermoelasticity of Diaspore by Synchrotron X-ray Diffraction and Raman Spectroscopy**

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TABLE S1 The chemical composition of diaspore (wt. %)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Na2O | FeO | P2O5 | SiO2 | Cr2O3 | K2O | MgO | MnO | CaO | Al2O3 | NiO | TiO2 | Total |
| diaspore | 0.01 | 0.511 | - | - | 0.027 | - | - | - | 0.001 | 85.81 | 0.005 | 0.055 | 86.419 |
| - | 0.562 | 0.009 | - | 0.066 | - | 0.021 | 0.052 | 0.02 | 86.745 | 0.002 | - | 87.477 |
| 0.028 | 0.56 | - | - | - | - | - | 0.015 | - | 86.078 | - | 0.062 | 86.743 |
| - | 0.501 | 0.037 | 0.036 | 0.067 | 0.008 | - | - | - | 86.727 | - | 0.051 | 87.427 |

-: none

TABLE S2 The unit-cell parameters of diaspore at high pressures

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Pressure (GPa) | *a* (Å) | *b* (Å) | *c* (Å) | *V* (Å3) |
| 0.26 (1) | 4.3968 (7) | 9.418 (2) | 2.8458 (12) | 117.85 (3) |
| 0.59 (2) | 4.3929 (7) | 9.413 (2) | 2.8433 (12) | 117.57 (3) |
| 1.23 (5) | 4.3872 (7) | 9.398 (2) | 2.8403 (12) | 117.11 (3) |
| 3.77 (15) | 4.3589 (7) | 9.351 (1) | 2.8279 (6) | 115.27 (3) |
| 4.57 (18) | 4.3511 (7) | 9.342 (1) | 2.8233 (6) | 114.76 (3) |
| 5.53 (22) | 4.3390 (7) | 9.321 (1) | 2.8195 (6) | 114.03 (3) |
| 6.67 (27) | 4.3294 (7) | 9.298 (1) | 2.8138 (6) | 113.27 (3) |
| 7.64 (31) | 4.3202 (6) | 9.280 (1) | 2.8088 (6) | 112.60 (3) |
| 8.56 (34) | 4.3105 (6) | 9.264 (1) | 2.8045 (6) | 111.99 (3) |
| 9.88 (39) | 4.2963 (7) | 9.249 (1) | 2.7965 (6) | 111.12 (3) |
| 11.23 (45) | 4.2866 (7) | 9.225 (1) | 2.7896 (6) | 110.31 (3) |
| 13.42 (51) | 4.2681 (7) | 9.191 (1) | 2.7794 (6) | 109.02 (3) |

The numbers in parentheses represent the error, for example, 0.26 (1) means 0.26 ± 0.01

TABLE S3 The unit-cell parameters of diaspore at high temperature and room pressure

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Temperature (K) | *a* (Å) | *b* (Å) | *c* (Å) | *V* (Å3) |
| 297 | 4.3981 (1) | 9.4137 (4) | 2.84137 (7) | 117.640 (7) |
| 323 | 4.3982 (1) | 9.4151 (4) | 2.84175 (6) | 117.675 (6) |
| 353 | 4.3984 (1) | 9.4164 (4) | 2.84210 (6) | 117.713 (6) |
| 383 | 4.39918 (9) | 9.4177 (3) | 2.84252 (5) | 117.766 (5) |
| 413 | 4.3997 (1) | 9.4191 (4) | 2.84276 (5) | 117.808 (6) |
| 443 | 4.4005 (1) | 9.4208 (4) | 2.84319 (5) | 117.869 (5) |
| 473 | 4.40151 (9) | 9.4228 (3) | 2.84379 (5) | 117.946 (5) |
| 503 | 4.4024 (1) | 9.4237 (2) | 2.84426 (5) | 117.998 (4) |
| 533 | 4.4034 (1) | 9.4263 (3) | 2.84492 (5) | 118.088 (5) |
| 563 | 4.40437 (9) | 9.4275 (3) | 2.84539 (5) | 118.146 (5) |
| 593 | 4.4054 (1) | 9.4299 (4) | 2.84610 (5) | 118.235 (6) |
| 623 | 4.4064 (1) | 9.4315 (4) | 2.84673 (5) | 118.307 (6) |
| 653 | 4.40850 (9) | 9.4347 (3) | 2.84766 (5) | 118.442 (5) |
| 683 | 4.4093 (1) | 9.4354 (4) | 2.84804 (6) | 118.488 (6) |
| 713 | 4.4105 (1) | 9.4378 (4) | 2.84844 (5) | 118.568 (6) |

|  |  |
| --- | --- |
| (a) | (b) |
|  |  |

FIGURE S1. Single crystal X-ray diffraction patterns of diaspore at 0.26 GPa (a) and 13.42 GPa (b).

|  |  |
| --- | --- |
|  |  |
|  |  |

FIGURE S2. The representative Le Bail profile fitting patterns of diaspore at 298 K (a), 413 K (b), 533 K (c), and 713 K (d). Observed spectra (black lines), fitted spectra (red solid lines), difference plots (blue solid lines), and Bragg peak positions (tick marks) are shown.