B1-B2 Transition in Calcium Oxide from Shock-Wave and Diamond-Cell Experiments

Raymond Jeanloz, T. J. Ahrens, H. K. Mao, and P. M. Bell

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ABSTRACT. Volume and structural data obtained by shock-wave and diamond-cell techniques indicate that calcium oxide transforms from the B1 (sodium chloride type) to the B2 (cesium chloride type) structure at 80 to 70 gigapascals (6.6 to 5.7 Mbars) with a volume decrease of 1.1% per stage. The agreement between the shock-wave and diamond-cell results independently confirm the ruby-fluorescence pressure scale to about 65 gigapascals. The shock-wave data agree closely with ultrasonic measurements on the B1 phase and also agree satisfactorily with equations of state derived from ab initio calculations. The discovery of this B1-B2 transition is significant in that it allows considerable enrichment of calcium components in the earth's lower mantle, which is consistent with homogeneous accretion theories.

Calcium oxide, initially in the B1 (NaCl type) structure, is expected to transform to the B2 (CsCl type) structure at high pressure, by analogy with the B1-B2 transitions found in alkali halides (1, 2). There is considerable interest in such transitions both in theoretical studies of oxide structures (3-5) and because of their possible occurrence in the earth's lower mantle. We have carried out shock-wave experiments on CaO to determine its equation of state (Hugoniot) (6), as well as x-ray diffraction, under static high pressures, through a diamond cell (7); both techniques demonstrate a B1-B2 transition in CaO at 60 to 70 GPa (0.6 to 0.7 Mbars). To our knowledge this is the first documentation of the B2 structure in an oxide of direct geophysical interest.

Our new data are given in Table 1 and Fig. 1, along with previous results for CaO (8). For comparison, theoretical Hugonions based on finite strain theory and ab initio (modified electron gas) calculations for the B1 and B2 phases are also given (9). The shock data provide an accurate dynamic compression curve for CaO and the x-ray data from the diamond cell confirm the nature of the structural transition. The diamond-cell experiment indicates that the transition begins at 80 (±2) GPa on the ruby-fluorescence pressure scale (7) and at room temperature (295 K), whereas the shock-wave data indicate a slightly higher transition pressure: about 67 to 70 GPa, but at approximately 1150 K (10). A volume decrease of 1.9 ± 1 percent is found at the transition in both sets of experiments, which is in agreement with simple systematics among the data for B1-B2 transitions in halides (11) and provides additional support for applying such systematics to oxides. The consistency of the shock-wave and diamond-cell results for the transition pressure in CaO provides an approximate but independent confirmation of the ruby-fluorescence scale calibration ± about 65 (±5) GPa. Thus the B1-B2 transition in CaO may be a convenient and readily reversible pressure-calibration point for ultrahigh-pressure static experiments.

The shock-wave data corresponding to the B1 phase are in excellent agreement with previous static compression data (6) and theoretical Hugonions based on finite-strain (P30) and ab initio (modified electron gas) calculations (9). Also shown are two geological models for the lower mantle (13). Error bars for the shock-wave data are approximately the size of the symbol for smaller; the datum in parentheses is considerably less certain. The open symbol represents an alternative interpretation of the 70-GPa result (9).

Fig. 1. New shock-wave data for CaO compared with previous, static compression data (6) and theoretical Hugonions based on finite-strain (P30) and ab initio (modified electron gas) calculations (9). Also shown are two geological models for the lower mantle (13). Error bars for the shock-wave data are approximately the size of the symbol for smaller; the datum in parentheses is considerably less certain. The open symbol represents an alternative interpretation of the 70-GPa result (9).
Table 1. Calcium oxide diamond-cell results.

<table>
<thead>
<tr>
<th>Majer</th>
<th>Relative</th>
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<tbody>
<tr>
<td></td>
<td>Run</td>
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<tr>
<td></td>
<td>Pressure* (GPa)</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>4V1</td>
<td>60.6</td>
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<tr>
<td>4V2</td>
<td>63.2</td>
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<tr>
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<td>4V4</td>
<td>63.7</td>
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<tr>
<td>6V1</td>
<td>66.8</td>
</tr>
</tbody>
</table>

*The precision is ±2 GPa; the absolute accuracy of the calculation is about ±0.5 GPa. The intensity of 200 and 110 is 100 bins for B1 and B2 phases, respectively. The intensity of 100 is about 80% relative. Relative intensities of k lines are reported on visual estimates.

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References and Notes
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