SESAME Equation of State
Number 7530, Basalt

CIC-14 REPORT COLLECTION
REPRODUCTION COPY

Los Alamos
Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36.
Prepared by Jo Ann Brown, Group T-1

An Affirmative Action/Equal Opportunity Employer

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.
SESAME Equation of State
Number 7530, Basalt

J. F. Barnes
S. P. Lyon
ABSTRACT

A full-range equation of state (EOS) for dry, nonporous basalt with a grain density of 2.868 g/cm³ has been constructed and placed on the SESAME library as material number 7530.

As with most rocks, basalt is found with varying composition. It is an igneous rock, composed largely of complex minerals of the plagioclase feldspar and pyroxene groups; typically it contains very little identifiable quartz. In oxide abundance it is fairly similar to the diabases and gabbros, other igneous rocks of about the same density but different texture. The particular molecular composition represented by equation-of-state (EOS) 7530 is given in Table I, where data are taken from Clark¹; corresponding atomic abundance is shown in Table II. For this mixture the average atom, as used in the GRIZZLY² code, is calculated to have an atomic number \( \bar{Z} = 10.665 \) and an atomic weight \( \bar{A} = 21.574 \). The EOS is constructed to have a reference density \( \rho_o = 2.868 \) g/cm³, the assumed dry grain density of basalt. The EOS can be mixed with a suitable SESAME EOS for water if desired, and through the hydrocode setup the user can allow for the desired degree of porosity.

High pressure shock Hugoniot data on basalt are somewhat sparse, and since in fact the composition of the samples used in the existing
experiments was not as given in Table I anyway, we chose to use the more complete set of shock data on diabase given by McQueen, Marsh, and Fritz. Ahrens and Gregson showed that at the lower pressures where data exist the Hugoniots for gabbro, diabase, and basalt are in good agreement when account is taken of their differing initial density. We would expect the Hugoniots to agree also at higher pressures where the mineral makeup is "forgotten." Because the diabase samples had a density of 2.99 g/cm³, we constructed the EOS at that density and then scaled it to the basalt density given above. We assumed that the breaks in the experimental shock data reported in Reference 3 are due to a single phase change and approximated the $U_s - U_p$ Hugoniot by three straight lines.

A new version of the "CHART JD" ion thermal (nuclear) model that incorporates an improved treatment of the melting transition was used, along with the CHART-D prescription for the variation of the Grüneisen parameter, gamma, with compression. Reference gamma, Debye temperature, cohesive energy, and melt temperature were simply computed as the number-weighted average of the major constituents, as shown in Table III. Although this is a crude procedure, better treatment for these quantities isn't warranted when one considers 1) the other approximations used in constructing equations of state for mixtures (such as the average atom approximation) and 2) the uncertainties of some of the entries in Table III. Note that, for example, since sound speeds and other data for calculation of $\gamma_0$ and $\Theta_D$ seem to be unavailable for ferrous oxide we used the calculated values for Fe₂O₃. It should also be noted that, as used here, cohesive energy is the energy required per mole of average atoms to separate a substance into its separate atoms at
0 K. The last line of Table III gives the calculated number-weighted averages of the quantities that we used as input to GRIZZLY. In construction of the cold curve, the Lennard-Jones factor was taken to be 0.185, which resulted in a critical temperature of about 6675 K.

Results are shown in Figures 1 through 4. Figure 1 shows selected pressure isotherms over the entire temperature range of the SESAME library table. Below the calculated critical isotherm van der Waal loops are obtained, and the 301 table in SESAME contains these loops. Figure 2 shows the corresponding isotherms with Maxwell equal-area construction. Data for effecting this replacement are stored in the 401 table of the library. Figure 3 shows the energy isotherms and Figure 4 the principal Hugoniot.

<table>
<thead>
<tr>
<th>Chemical Composition of Basalt as Used in EOS 7530 (Ref. 1)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>SiO₂</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>CaO</td>
</tr>
<tr>
<td>MgO</td>
</tr>
<tr>
<td>Al₂O₃</td>
</tr>
<tr>
<td>FeO</td>
</tr>
<tr>
<td>H₂O</td>
</tr>
<tr>
<td>Na₂O</td>
</tr>
<tr>
<td>TiO₂</td>
</tr>
<tr>
<td>Fe₂O₃</td>
</tr>
<tr>
<td>K₂O</td>
</tr>
<tr>
<td>MnO</td>
</tr>
<tr>
<td>P₂O₅</td>
</tr>
</tbody>
</table>
TABLE II
Atomic Abundance as Used in EOS 7530

<table>
<thead>
<tr>
<th>Element</th>
<th>Abundance (By Number)</th>
</tr>
</thead>
<tbody>
<tr>
<td>O</td>
<td>60.11 %</td>
</tr>
<tr>
<td>Si</td>
<td>18.26</td>
</tr>
<tr>
<td>Al</td>
<td>5.96</td>
</tr>
<tr>
<td>Ca</td>
<td>4.01</td>
</tr>
<tr>
<td>Fe</td>
<td>3.48</td>
</tr>
<tr>
<td>Mg</td>
<td>3.39</td>
</tr>
<tr>
<td>H</td>
<td>2.18</td>
</tr>
<tr>
<td>Na</td>
<td>1.56</td>
</tr>
<tr>
<td>Ti</td>
<td>0.55</td>
</tr>
<tr>
<td>K</td>
<td>0.38</td>
</tr>
<tr>
<td>P</td>
<td>0.07</td>
</tr>
<tr>
<td>Mn</td>
<td>0.06</td>
</tr>
</tbody>
</table>
TABLE III
Estimates of the Grüneisen Parameter, Debye Temperature, Cohesive Energy, and Melt Temperature for the Major Constituents of Basalt and Their Resulting Weighted Averages

<table>
<thead>
<tr>
<th></th>
<th>$\gamma_0$</th>
<th>$\Theta_D$</th>
<th>$E_{coh}$</th>
<th>$T_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SiO$_2$</td>
<td>0.653</td>
<td>950 K</td>
<td>146 kcal/mol</td>
<td>1883 K</td>
</tr>
<tr>
<td>CaO</td>
<td>2.40</td>
<td>640</td>
<td>127</td>
<td>2853</td>
</tr>
<tr>
<td>MgO</td>
<td>1.72</td>
<td>630</td>
<td>118</td>
<td>3125</td>
</tr>
<tr>
<td>Al$_2$O$_3$</td>
<td>1.595</td>
<td>1034</td>
<td>145</td>
<td>2288</td>
</tr>
<tr>
<td>FeO</td>
<td>(1.64)</td>
<td>(610)</td>
<td>110</td>
<td>1642</td>
</tr>
<tr>
<td>Fe$_2$O$_3$</td>
<td>1.64</td>
<td>610</td>
<td>114</td>
<td>1838</td>
</tr>
<tr>
<td>Basalt</td>
<td>1.17</td>
<td>851</td>
<td>137</td>
<td>2158</td>
</tr>
</tbody>
</table>
REFERENCES


Selected pressure isotherms, containing van der Waal loops, for EOS 7530.
Selected pressure isotherms for EOS 7530 with van der Waal loops replaced by calculated equilibrium vapor pressures.
Fig. 3.

Selected energy isotherms for EOS 7530.
Fig. 4.

Shock velocity versus particle velocity on principal Hugoniot for EOS 7530.