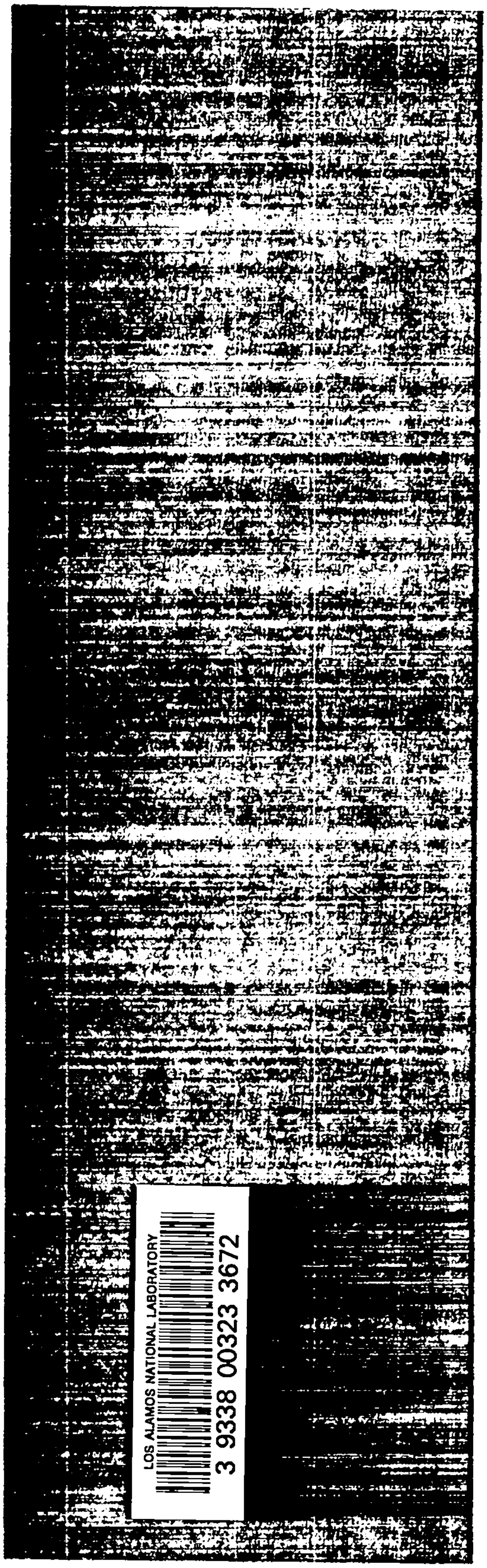
LA-11488-MS



SESAME Equation of State Number 7386, Fused Quartz

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.

LA-11488-MS

UC-700
Issued: January 1989

SESAME Equation of State Number 7386, Fused Quartz

J. C. Boettger

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

SESAME EQUATION OF STATE NUMBER 7386, FUSED QUARTZ

by

J. C. Boettger

ABSTRACT

A new equation of state (EOS) for fused quartz (SiO_2) has been constructed for the SESAME library as material number 7386. This new EOS provides a substantially better representation of the principal Hugoniot than has been achieved in previous EOS's for fused quartz included in the SESAME library.

During the last decade, considerable progress has been made in improving the techniques used to generate phenomenological EOS's for the SESAME library, culminating in the development of the computer program GRIZZLY, which is currently used to produce such EOS's.[1] It is to be expected that those EOS's in the SESAME library which were produced prior to the advent of the GRIZZLY code (1984) may not be of a quality consistent with the current state of the art and should be updated as the need arises. One such EOS is that for fused quartz (SESAME material number 7381),[2] a material which is of current interest to several users of the library. The author found that the principal Hugoniot for 7381 is in serious disagreement with existing experimental data.[3] To rectify this situation, a new EOS for fused quartz (SiO_2), which is in better agreement with experiment, has been generated with GRIZZLY and will be added to the SESAME library as material number 7386.

In the SESAME library, EOS's are partitioned into three terms for the pressure P and the internal energy E:

$$P(\rho,T) = P_c(\rho) + P_n(\rho,T) + P_e(\rho,T) \tag{1}$$

$$E(\rho,T) = E_c(\rho) + E_n(\rho,T) + E_e(\rho,T) \tag{2}$$

where ρ is the density and T is the temperature. The subscripts c, n, and e denote the contributions due to the cold curve (zero temperature isotherm), the nuclear motion, and the thermal electronic excitations. It is thus possible to treat each term independently using any desired model.

The thermal electronic part of 7386 was calculated with GRIZZLY by first using the TFD model[1,4] to generate the electronic EOS's of each constituent (Si and O) separately and then obtaining the electronic EOS for SiO_2 via additive volume mixing.[1] (This is the same procedure as was used in constructing 7381.) The nuclear contribution to 7386 was calculated using the CHART-JD model[5] (7381 used the Cowan[6] model). These two components of the EOS require six items of empirical data: the atomic masses of the two constituents (Si - 28.086, O - 15.999),[7] the reference density (2.204 gm/cc),[3] the Debye temperature (950 K),[8] the reference Gruneisen constant (0.65),[8] the cohesive energy (146 kcal/mole),[8] and the melting temperature (1900 K).[9] The cold curves for 7386 and 7381 were both obtained in the compressed region by removing thermal contributions from experimental Hugoniot data[3] for compressions up to about 2.1 and then extrapolating to a mixed TFD cold curve at large compressions.[1]

In addition to the data already described above, construction of the cold curve requires experimental Hugoniot data as input (in the form of u_s vs u_p). For fused quartz, the existing Hugoniot data are somewhat complicated (see Fig. 1) and cannot be represented by a single straight line as is possible for many other materials. The data for fused quartz in Fig. 1 clearly exhibit a region of u_p (1.0 km/s - 2.25 km/s) for which u_s is virtually constant. This flat portion of u_s vs u_p represents a two phase region connecting a low pressure phase and a high pressure phase. It is difficult to determine what the correct form of the Hugoniot should be for the low pressure phase because the elastic-plastic transition for the Hugoniot occurs at a u_p of about 0.85 km/s.[10] Thus, the only well determined point for the low pressure phase is the intercept (either 4.071 km/s[3] or 4.09 km/s[11]). The high pressure phase of fused quartz is well characterized by the experimental data but exhibits a pronounced curvature just above the two phase region. For 7381, the Hugoniot data were fitted by three straight lines which can be defined by four points (u_p, u_s); (0.000, 4.075), (0.708, 5.212), (2.610, 5.212), and (4.500, 8.406), in km/s.[2] For 7386, the same data were fitted by four straight lines which can be defined by five points; (0.000, 4.09), (0.85, 5.1), (2.25, 5.10), (3.022, 5.950), and (4.494, 8.461), in km/s. The three line and four line fits are both displayed in Fig. 1.

On the basis of the differences in modeling between 7381 and 7386 discussed above, 7386 could be expected to be somewhat superior to 7381 along the principal Hugoniot, but the differences should not be large. However, whereas the current programming used in GRIZZLY ensures that the calculated EOS will reproduce the input Hugoniot data to a high degree of precision, earlier programs used did not necessarily achieve such self-consistency between the input and output Hugoniots.[12] The Hugoniot for 7386 is shown in Figure 1 together with the experimental data, the three line fit used as input to 7381, and the calculated Hugoniot for 7381 (recall that the calculated Hugoniot for 7386 is essentially identical to the input Hugoniot). It is obvious from Fig. 1 that 7381 is in very poor agreement with both the experimental data and the three line fit that was used in its construction. In contrast, the new EOS (7386) gives good agreement with all of the experimental data above the elastic-plastic transition (u_p = 0.85 km/s).

To summarize, the new EOS for fused quartz described here (7386) represents a substantial improvement over the old EOS (7381). Thus, 7386 should be preferred for all calculations involving fused quartz. (For polycrystalline or crystalline quartz, the appropriate EOS is material number 7383.)[8]

REFERENCES

1. Joseph Abdallah, Jr., "User's Manual for GRIZZLY", Los Alamos National Laboratory report LA-10244-M (September 1984).
2. K. S. Holian, editor, *T–4 Handbook of Material Properties Data Bases*, Vol. 1c, Los Alamos National Laboratory report LA-10160-MS (November 1984).
3. S. P. Marsh, editor, *LASL Shock Hugoniot Data* (U. C. Press, 1980).
4. See for example, R. D. Cowan and J. Ashkin, Phys. Rev. 105, 144 (1957)
5. The CHART-JD nuclear model was developed by J. D. Johnson at Los Alamos during 1986-1987.
6. The Cowan nuclear model was developed by R. D. Cowan at Los Alamos about 1957.
7. N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Holt, Rinehart, and Winston, 1976).
8. J. D. Johnson, "EOS for Polycrystalline Quartz", Los Alamos National Laboratory report LA-10391-MS (May 1985), and references therein.
9. Rough estimate based on various values listed in *CRC Handbook of Chemistry* and *Physics*, 69th Edition, R. C. Weast, editor (CRC Press, Inc. 1988).
10. J. Wackerle, J. Appl. Phys. 33, 922 (1962).
11. M. van Thiel, editor, "Compendium of Shock Wave Data", Lawrence Livermore Laboratory report UCRL-50108 (June 1977).

12. J. D. Johnson, Los Alamos National Laboratory, personal communication, August 1988.

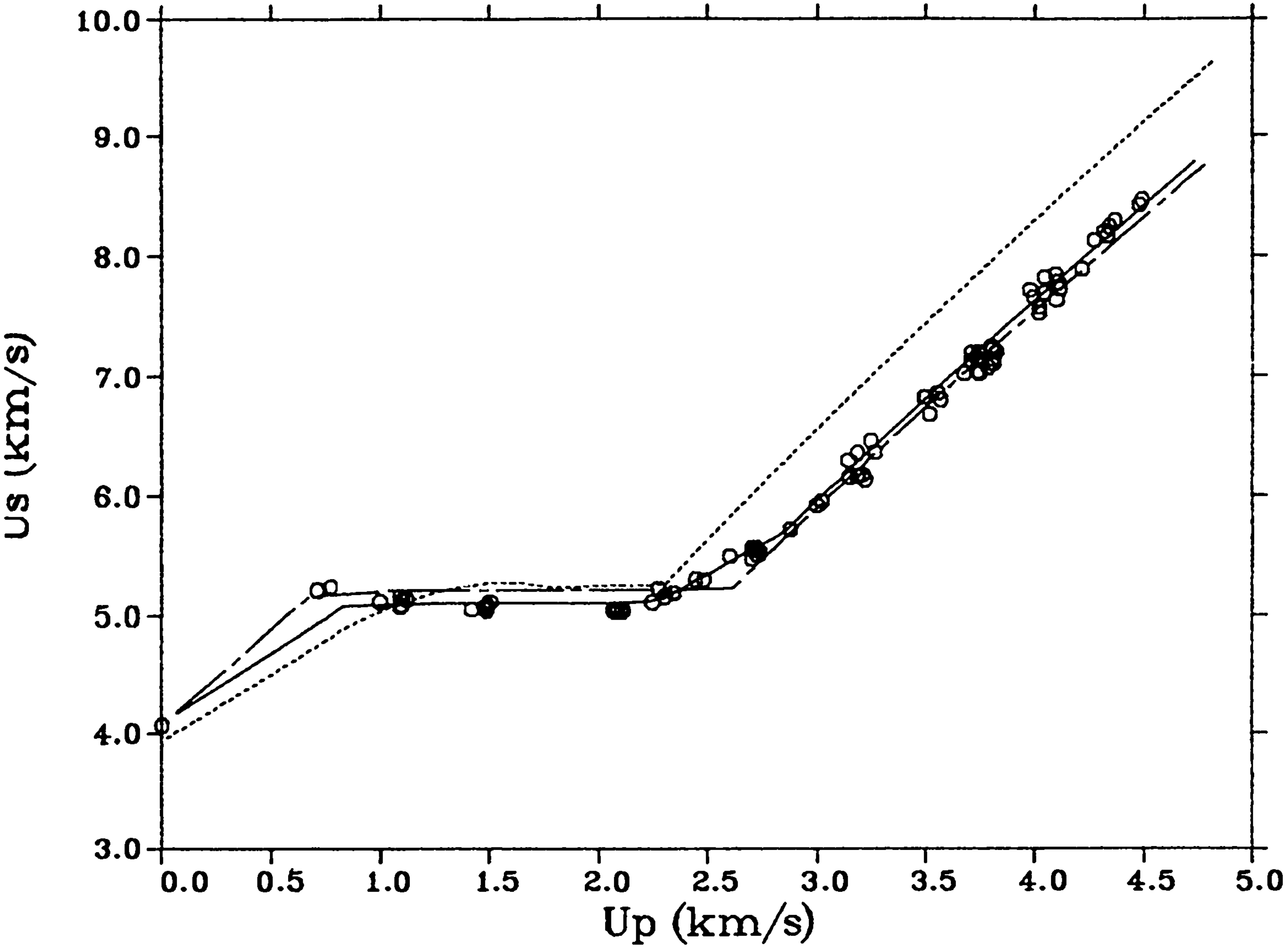


Fig. 1. Calculated Hugoniots for material numbers 7386 (solid line) and 7381 (dashed line) compared with experimental data from Ref. 3 and the three line fit used in generating 7381 (chain dash line).

Printed in the United States of America
Available from
National Technical Information Service
US Department of Commerce
5285 Port Royal Road
Springfield, VA 22161

Microfiche (A01)

Page Range	NTIS Price Code	Page Range	NTIS Price Code	Page Range	NTIS Price Code	Page Range	NTIS Price Code
001-025	A02	151-175	A08	301-325	A14	451-475	A20
026-050	A03	176-200	A09	326-350	A15	476-500	A21
051-075	A04	201-225	A10	351-375	A16	501-525	A22
076-100	A05	226-250	A11	376-400	A17	526-550	A23
101-125	A06	251-275	A12	401-425	A18	551-575	A24
126-150	A07	276-300	A13	426-450	A19	576-600	A25
						601-up*	A99

*Contact NTIS for a price quote.