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SESAME Equation of State Number 7740: Polycarbonate

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ABSTRACT

An equation of state (EOS) for polycarbonate (a widely used polymer) has been generated with the computer code GRIZZLY and will be added to the SESAME library as material number 7740. Although a number of the input parameters used in the calculations are based on rough estimates, 7740 provides a good match to experimental Hugoniot data and should be reliable on or near the principal Hugoniot.

Polymers form a class of materials which are of great technological importance and it is not surprising that there are frequent requests by users of the SESAME library for equation(s) of state (EOS) for specific polymers. In response to one such request, I have used the computer code GRIZZLY[1] to generate an EOS for the polymer polycarbonate which will be added to the SESAME library as material number 7740. Unfortunately, in spite of their importance, polymers are generally poorly characterized experimentally, in part because of difficulties in producing uniform samples with reproducible compositions and properties. Polycarbonate is no exception and, as a result, 7740 is somewhat speculative due to a scarcity of exerimental data to be used as input to GRIZZLY. [Even the chemical composition used here $(C_{16}H_{14}O_3)$[2] is based on an idealized picture of polycarbonate and cannot be expected to accurately represent any real lab sample.] In spite of this difficulty, 7740 should be quite reliable in applications which only require the EOS of polycarbonate on or near the principal Hugoniot, which has been matched to experimental data.[2]

In the SESAME library, the EOS are partitioned into three terms for the pressure P and the

internal energy E:

$$P(\rho,T) = P_c(\rho) + P_n(\rho,T) + P_e(\rho,T) \quad (1)$$

$$E(\rho,T) = E_c(\rho) + E_n(\rho,T) + E_e(\rho,T) \quad (2)$$

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 7740 was calculated with GRIZZLY by first using the TFD model[1,3] to generate the electronic EOS of each constituent (C, H, and O) separately and then obtaining the electronic EOS for polycarbonate via additive volume mixing.[1] The nuclear contribution was calculated using the CHART-JD nuclear model,[4] with a Gruneissen parameter of the CHART-D form.[5] These two components of the EOS require several items of empirical data: the chemical composition ($C_{16}H_{14}O_3$),[2] the atomic masses of each constituent (C - 12.01, H - 1.008, O - 15.999),[6] the reference density (1.196 gm/cc),[2] the Debye temperature (136 K), the reference Gruneisen parameter (1.33), the cohesive energy (120 kcal/mole), and the melting temperature (600 K). (The latter 4 input parameters simply represent reasonable estimates.)

The cold curve for 7740 was obtained in the compressed region by removing thermal contributions from the experimental Hugoniot data[2] for compressions up to 2.3 and then extrapolating to a mixed TFD cold curve at large compressions. This part of the calculation requires the experimental Hugoniot in the form of shock velocity (U_s) vs. particle velocity (U_p). Here, the U_s vs. U_p data have been represented by three straight-line segments defined by four (U_p, U_s) points; (0.0, 2.33), (2.7, 6.569), (3.7, 7.15), and (5.2, 9.4), all in km/s. In the expanded region, the cold curve has been fitted to a Lennard-Jones form which is required to reproduce the input cohesive energy and smoothly connect with the compressed portion of the cold curve. Generating this expanded part of the cold curve requires an input parameter FACLJ (here 3.0).[1]

In Figure 1, the theoretical principal Hugoniot of material number 7740 is compared with the

existing experimental data for polycarbonate. The agreement between experiment and theory is quite good, as is to be expected given the empirical nature of 7740. Thus, 7740 should be very reliable for applications which only require the EOS of polycarbonate near the principal Hugoniot. For portions of the EOS which lie far from the Hugoniot, 7740 will be more speculative.

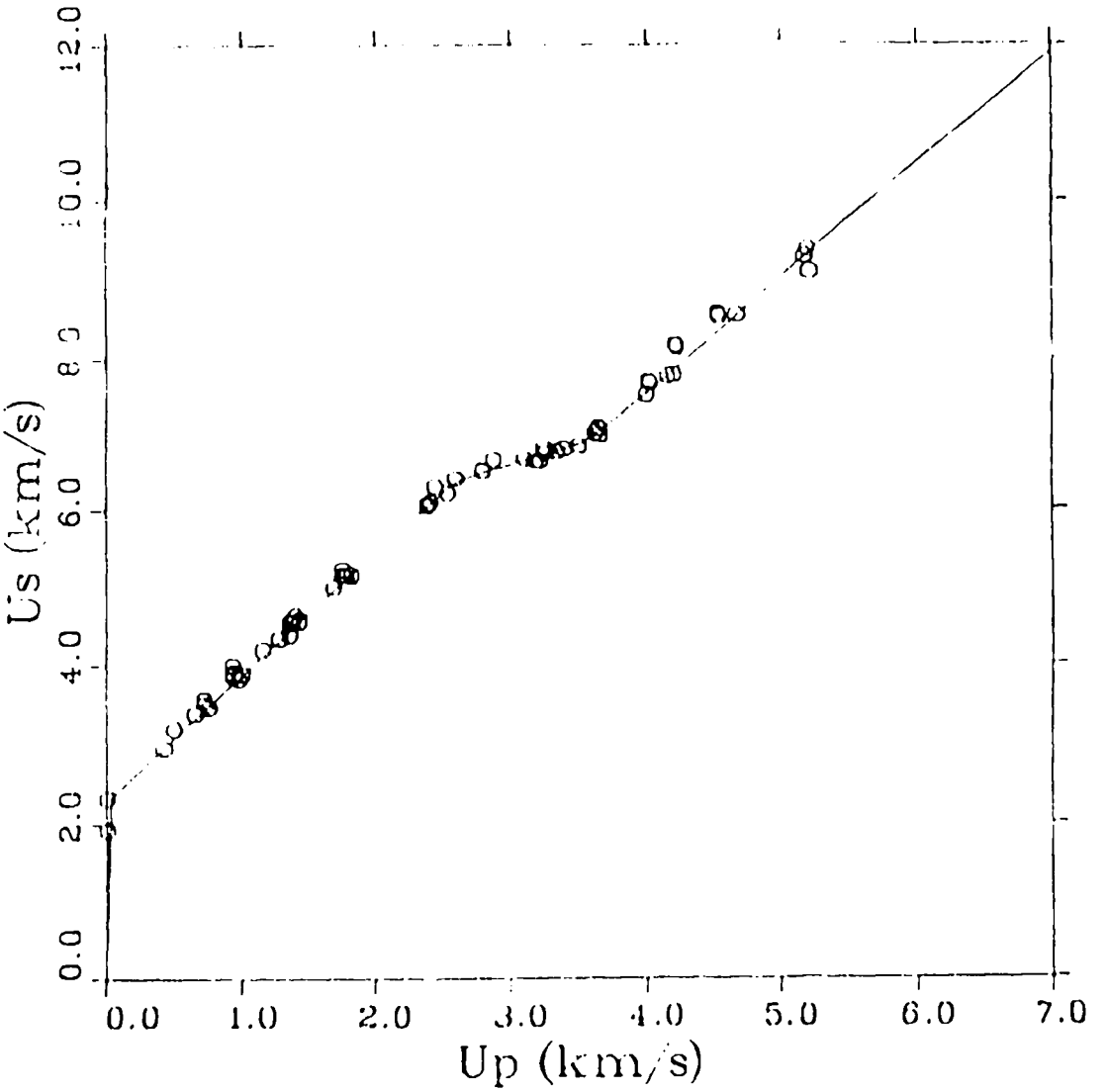

Figure 1 - The calculated principal Hugoniot for polycarbonate (solid line) is compared to the experimental data of Ref. 2.

REFERENCES

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