Conf-940633--1

LA-UR- 94-1451

Title: THE SESAME DATABASE

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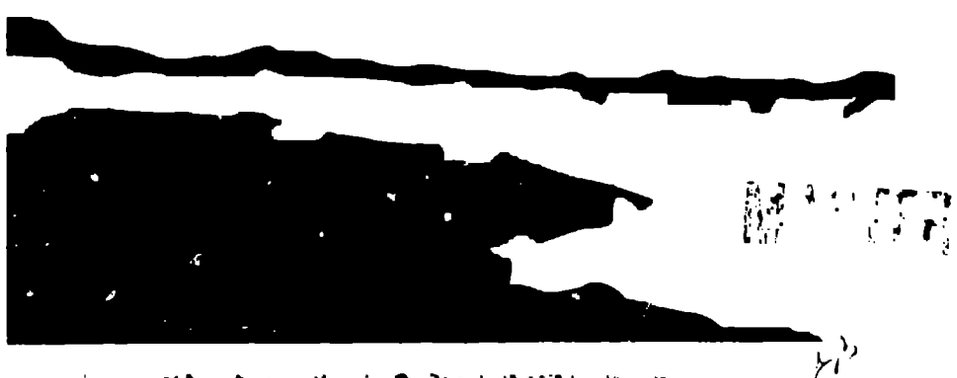
Submitted to: 12th Symposium on Thermophysical Properties
Boulder, CO
June 19-24, 1994



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The SESAME Database[1]

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[1] Paper presented at the Twelfth Symposium on Thermophysical Properties, June 19-24, 1994, Boulder, Colorado, U.S.A.

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ABSTRACT

The SESAME database has been in existence for over twenty years and has been provided to over three hundred users worldwide. Currently, we supply the following: equation of state and material properties data, including pressure, internal energy, and Helmholtz free energy as functions of density and temperature, shear modulus, melting curves, and vaporization information; electron transport properties, including electrical conductivity, thermal conductivity, thermoelectric coefficient, and electron conductive opacity; and opacity data, including mean ion charge, Rosseland mean opacity, and Planck mean opacity. The opacity and transport data are available for the elements. The equation of state and material properties are for a broad variety of materials from elements, to composites, to compounds, to rocks. The ranges of density and temperature that are covered are typically extreme; from zero density to 10^5 gm/cc, from zero Kelvin to 10^9 Kelvin.

We have supplied less general tables to users with their own specialized needs. We wish to continue such and to expand SESAME to SESAME++. This will be an enlarged database including more types of material data for an expanded group of users with more diverse interests.

KEY WORDS: equation of state, materials database, opacities, thermodynamic data, transport

1. INTRODUCTION

1.1 THE SESAME DATABASE

The SESAME Equation-of-State (EOS) Library is a standardized, computer-based library of tables for the thermodynamic properties of materials with FORTRAN subroutines for the use of the Library. All are developed and maintained by the Mechanics of Materials and Equation-of-State Group (T-1) of the Theoretical Division at Los Alamos National Laboratory.

The Library currently contains data for about 170 materials, including simple elements, compounds, metals, minerals, polymers, mixtures, etc. The EOS's for existing materials in the Library are upgraded when appropriate, and EOS's for new materials are added frequently. The Library is used by many researchers (a few hundred), both inside and outside the Laboratory; external users include scientists at various institutions in the United States and in other countries. The Library is presently being offered to all interested users free of charge.

The thermodynamic data stored in the Library include tables of pressure P and energy E (and also in many cases, of Helmholtz free energy A), each as a function of density ρ and temperature T. Besides total P, E, and A tables, often separate P, E, and A tables of thermal electronic and ion (including zero point) contributions are available. Some materials also have vaporization, melt and shear tables. The typical density and temperature ranges are from 10^{-6} to 10^{4} gm/cc and 0 to 10^{5} ev, respectively.

While there do exist SESAME Libraries for other properties, as outlined in the abstract, for the remainder of this paper we restrict our attention to the EOS library.

1.2 THEORETICAL MODELS AND METHODS

Because of the large ranges of density and temperature, and because of the very diverse kinds of phases and materials encountered in the Library, the global EOS's in the Library are formed using various combinations of different theoretical models in different regions with interpolation between, usually thermodynamically consistent. Thus SESAME is somewhat different from most data compilations in that it is not a collection of experimental data or the

results from some standard theory. A SESAME table is typically the product of fitting semi-empirical theories to experimental data for a given material. This normalized model is then used to calculate the full table.

Most often the models include a Thomas-Fermi-Dirac theory for thermal electronic contributions to the EOS. A few EOS's incorporate the INFERNO model for an atom embedded in an electron gas at finite temperature; electron-band structure models, including augmented plane-wave, LMTO, KKR, and Gaussian orbital approaches; or a Saha model for ionization equilibrium.

Other models include Einstein, Debye, Cowan, Chart-D and generalized Chart-D models for lattice vibrations in solids; hard-sphere perturbation approaches for fluids; and rigid-rotator and harmonic-oscillator methods for molecular rotational and vibrational terms, respectively.

Other approaches include molecular-dynamics (MD) computer simulations of metals, of rigid diatomic and triatomic molecules, and of nonrigid diatomic molecules. Pseudopotentials and melting in metals have been studied by MD. The capacity also exists in the T-1 Group to study glasses and solid-solid transitions by MD.

Various somewhat empirical methods are also used: virial expansions; analytic fits of data to various intermolecular potentials, including Lennard Jones (6-12), Buckingham (exp-6), and modified Morse potentials; multi-parameter functional fits of data; Mie-Grüneisen equation of state; etc.

The aim of the SESAME Library is to have thermodynamically self-consistent EOS's that are made with the best possible physics and the best possible agreement with available experimental data-given realistic time constraints. Most EOS's in the SESAME Library have been generated by the T-1 Group, but the Library does include some EOS's originally constructed by researchers at other institutions (such as the National Bureau of Standard and Lawrence Livermore National Laboratory and adapted by the T-1 Group for the SESAME Library). The T-1 Group uses its own versions of some externally developed theoretical models to generate EOS's, but also develops its own new models and methods.

Other features of various EOS's in the SESAME Library include treatments of shock data, incorporation of various phase transitions (including Maxwell constructions or van der Waals loops for first-order phase transitions), modeling of foams or porous materials, and calculation of dilute gas mixtures.

Of recent interest is the inclusion of better theoretical models and methods for (1) melting and (2) nonideal mixtures in the mechanisms used to generate the global EOS's. Many of these improved models and methods have been developed by various T-1 Group members and can be used now for calculations of individual thermodynamic points or of small regions in phase space. Still other models and methods are being developed in these areas, as well as in many other areas of interest in the calculation of EOS's for a variety of diverse materials.

1.3 SESAME SOFTWARE

SESAME Subroutine Library

The SESAME subroutine library was developed to simplify use of tabular EOS data. SESAME tables are transmitted to users on magnetic tapes, e-mail, or other electronic means in a card image format that can be read and interpreted by the user's computing system. The user is also supplied with FORTRAN subroutines that preprocess the data into a compact binary file and update this file as needed. The user is supplied with subroutines that search this file for a given material, load data into a local array, and compute thermodynamic functions by search and interpolation. Linear and rational function interpolation schemes are available for one and two dimensions. Thus, the database is available for directly reading into computer codes.

Routines are available to compute P and E (and their first derivatives) as a function of ρ and T and also to compute P and T (and their first derivatives) as a function of ρ and E. Other EOS data that can be computed include isotherms, isochores, adiabats, Hugoniots (shock velocities and particle velocities), vapor-liquid coexistence curves, thermodynamic behavior of foams, phase transitions, and melt and shear modulus tables.

Display Codes

The T-1 Group has a number of in-house display codes that combine various subroutines mentioned in the preceding section to provide tabular and graphical representation of the EOS data. SES2D and SES3D are two- and three-dimensional graphics codes using DISSPLA graphics which plot tabulated data. SES2D plots isotherms, isochores, Hugoniots and adiabats. The SHIP code displays the Library data in tabular form and the DSPLX code is used to calculate Hugoniots, isentropes, and other quantities which it also displays in tabular form. Finally, SESLIST is used to generate a catalog of materials in a SESAME Library along with a description of methods used to calculate each table and its density-temperature range.

2. BASELINE EOS THEORY

Almost all of the equations of state being produced for SESAME are now being done with one method, one set of models. Also, over the years by far most of the EOS's have been created by similar modeling. In this section we will outline this baseline method. We will also mention a couple of more elaborate methods that are sometimes used, especially for metals. Finally, we have discontinued using a number of techniques that produced a few EOS's that are in the Library. Report LA-10160-MS should be consulted for these [1].

The standard thinking for SESAME is that an EOS is composed of three parts; the zero temperature isotherm (cold curve), the thermal ionic, and thermal electronic. We model each separately and construct the total EOS, the 301 table, by summing the three. Other tables, 304, 305, and 306, come from the individual parts. By convention we put the zero point motion of the ions in with the thermal ionic contribution.

The thermal electronic contribution is calculated using finite temperature Thomas-Fermi-Dirac (TFD) theory. Our current model for this is due to Liberman [2] and is the same as that of Cowan and Ashkin [3] but treats exchange and correlation with a local density approximation. The thermal part is produced by running TFD everywhere including zero temperature and then subtracting the TFD cold curve from the whole table. For a few materials the INFERNO model [4] for the finite temperature electronic structure has been used Here the Dirac equation is

solved for the single particle quantum levels in the self-consistent field of an atom in a constrained spherical cell. INFERNO obtains structure from the electron ionization while TFD smoothes through such.

Our ionic models have been very similar with the current one having more details of melting [5]. The solid region is treated with Debye theory. The location of melting is determined by the Lindemann formula. Above melting an interpolation is made, going smoothly to ideal gas at high temperatures. For these models it is necessary to know the Debye temperature as a function of density. This we obtain from simple analytic forms fit to data.

For the cold curve we look at three different density regions. We usually have shock wave data from the ambient density of the solid to some high density. Over this range we use the shock data and the above fit for the Debye temperature to calculate the cold curve from Mie-Grüneisen theory [6]. For higher densities an interpolation is made to TFD theory with a smooth connection to the Mie-Grüneisen region. For low densities a simple analytic form is again smoothly merged into the Mie-Grüneisen region. The other parameters for expansion are selected to obtain the correct cohesive energy and gas-liquid critical point. In a few special cases the Mie-Grüneisen procedure has been replaced by *ab initio* band-structure calculations.

The above method gives us our basic EOS tables. We also pull out the details of melting and vaporization and place those in special tables, 401, 411, and 412, for these phase transitions. Most recently we have included a zero temperature shear modulus table. It is sometimes appropriate to create an EOS that is a mixture. We use simple mixing rules such as additive volume and partial pressure [7].

While the above is our standard procedure and does account, by far, for most of our data-base, we have and still attempt to serve the users' special needs. This includes using models and limited regions with increased accuracies as well as going to material data other than equation of state. We hope to continue this expansion of what is treated in the SESAME Library.

3. STRUCTURE OF THE SESAME LIBRARY

The SESAME Library is a fileset consisting of a directory file and one or more material files. (We typically do not send the whole Library but only a subset of interest to the user.) Each material file corresponds to a specific material and consists of an index record followed by a variable number of data records or tables. The various types of SESAME data records and their structure are shown below.

The SESAME Library may be constructed with either a sequential or random I/O format. The sequential version has a one-word record mark at the end of each record, a one-word file mark at the end of each file and two end of file marks at the end of the Library. The random version has an address array in the second record of the directory file with address that can be used to locate the beginning of each material file and an address array in the index record of each material file containing the addresses of the data records for that material. The random and sequential versions may be read by the subroutines found in the SESAME subroutine package.

The SESAME libraries maintained by T-1 on the CRAY machines at LANL have random I/O format.

TYPES OF SESAME DATA RECORDS

Table 101	Comments
Table 102	Comments
Table 201	Atomic Number, Atomic Mass, Normal Density
Table 301	Total EOS (304 + 305 + 306)
Table 303	Ion EOS Plus Cold Curve (305 + 306)
Table 304	Electron EOS
Table 305	Ion EOS (Including Zero Point)
Table 306	Cold Curve (No Zero Point)

Table 401	Vaporization Table
Table 411	Solid Melt Table
Table 412	Liquid Melt Table
Table 431	Shear Modulus Table
Table 501	Opacity Grid Boundary, Calculated vs. Interpolated
Table 502	Rosseland Mean Opacity ($cm^2\ g^{-1}$)
Table 503	Electron Conductive Opacity[1] ($cm^2\ g^{-1}$)
Table 504	Mean Ion Charge[1] (free electrons per atom)
Table 505	Planck Mean Opacity ($cm^2\ g^{-1}$)
Table 601	Mean Ion Charge[2] (free electrons per atom)
Table 602	Electrical Conductivity (sec^{-1})
Table 603	Thermal Conductivity ($cm^{-1}\ sec^{-1}$)
Table 604	Thermoelectric Coefficient ($cm^{-1}\ sec^{-1}$)
Table 605	Electron Conductive Opacity[2] ($cm^2\ g^{-1}$)

[1]Opacity Model (Hubbard-Lampe)

[2]Conductivity Model (Ziman)

4. USE OF THE SESAME LIBRARY

In addition to the SESAME Equation of State Database, the user will also receive the subroutine library SESPACK. SESPACK consists of two distinct subroutine packages. The first is composed of the basic subprograms needed to implement SESAME tables in a computer program which uses equation of state data. The second is the HYDSES subroutine package for use in hydrodynamic codes. This package is described in "HYDSES: A subroutine package for using SESAME in hydrodynamic codes" [8].

There is no standard density-temperature grid for SESAME EOS tables. Each grid can be constructed to give the best representation of the EOS with as few points as possible. Consequently, storage requirements vary from material to material. At the present time, no table requires more than 15000 words. In most cases, a SESAME EOS table covers a much larger density and temperature range than is needed for a particular application. We provide a routine which reduces the size of the EOS tables by deleting data outside of specified density and temperature limits, thus decreasing storage requirements.

The routines in the basic subroutine package are classified into several types, as listed next. These routines are written in ANS FORTRAN so that users should not have to adapt them to their local compilers. However, there may be certain exceptions to this rule, in particular, input and output may be system dependent.

The classes of routines are: (1) generalized input/output; (2) library preprocessor; (3) packaged EOS routines for hydrocodes; (4) auxiliary packaged routines for Hugoniots and adiabats; (5) search and interpolation; (6) library manipulation; and (7) a test problem.

OBTAINING THE SESAME LIBRARY

To obtain the SESAME EOS data and subroutine library either mail or FAX your request to

SESAME Library, T-1, MS-B221

Los Alamos National Laboratory

Los Alamos, NM 87545

Fax No: 505-665-5757. Please include your choice of storage media and format. For a standard 2400 ft. magnetic tape specify either ASCII or EBCDIC character set and either 1600 or 6250 BPI. Electronic means are now our most common form of transmission, requiring details of how to ship the files to you.

Users interested in opacity data should contact

Group T-4, MS B212

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