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*New Equation of State
for Stainless Steel 347*

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by

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ABSTRACT

A new SESAME equation of state (EOS) for stainless steel 347 has been generated using the computer program GRIZZLY, and has been added to the SESAME EOS library as material number 4271. This new EOS is superior to its predecessor (material number 4270) in several respects.

I. INTRODUCTION

The SESAME equation of state (EOS) library has been an important tool for scientists throughout the world since its inception in 1971.¹ During this time, the numerical techniques used to calculate the phenomenological EOSs contained in SESAME have been significantly improved. Perhaps the single most important advance to date was the development of the computer program GRIZZLY as a general purpose code for generating SESAME EOSs.² Unlike previous codes, GRIZZLY includes a wide variety of models for calculating all of the necessary components of a SESAME EOS.³

Given the long history of the SESAME library, it is to be expected that some of the older EOSs in the library (particularly those developed prior to GRIZZLY) would 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 stainless steel; material number 4270. Unlike more recent additions to the SESAME library, there is no clear documentation of the methods used to generate material number 4270. In addition, the original EOS was subsequently partitioned into so-called two-temperature tables (individual ionic and electronic contributions) using approximations which are crude at best.

In this investigation, a new EOS has been constructed for stainless steel 347 using GRIZZLY.² This work is a direct response to requests by users of the SESAME library. The new EOS has thermodynamically consistent two-temperature EOS tables and includes vapor pressure and melting tables. The new EOS has been added to the SESAME library as material number 4271.

In the next section, the models and parameters used to generate the EOS for stainless steel are described in detail. This new SESAME EOS is then discussed and compared with experimental data in Section III.

II. METHODOLOGY

Most of the EOSs in the SESAME library are partitioned into three terms for the pressure P , the internal energy E , and the Helmholtz free energy A :

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

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

$$A(\rho, T) = A_s(\rho) + A_n(\rho, T) + A_e(\rho, T) \quad (3)$$

where ρ is the density and T is the temperature. (In the SESAME library, discrete values of ρ and T are chosen to form a mesh on which P , E , and A are stored.) The

subscripts s , n , and e denote the contributions from the static lattice (i.e., frozen nuclei) cold curve (zero temperature isotherm), the nuclear motion, and the thermal electronic excitations, respectively. It is thus possible to calculate (or update) each term independently using any desired model. This partitioning also allows users to perform two-temperature calculations; i.e., calculations in which the ions and the electrons are allowed to have different temperatures. Here, all three components of the EOS for stainless steel have been generated with GRIZZLY.²

In GRIZZLY, the only model currently available for calculating the thermal electronic contributions is the Thomas-Fermi-Dirac (TFD) model.³ First, thermal electronic contributions were generated for each individual type of atom in stainless steel 347. Those monatomic thermal electronic EOSs were then combined via additive volume mixing² to form the total electronic contribution to the EOS. This portion of the calculation requires an ambient density (ρ_0) for the total EOS and the weight fraction (W_i), atomic number (Z_i), and atomic mass (A_i) for each species of atom (i). Stainless steel 347 is a well-defined type of steel with an ambient density of about 7.91 gm/cc⁴ and is composed of Fe combined with 17% to 19% Cr, 9% to 13% Ni, less than 2% Mn, less than 1% Si, and traces of several other elements.⁵ For material number 4271, stainless steel 347 has been approximated by a mixture of 70% Fe, 19% Cr, and 11% Ni; the same composition as was used for material number 4270. The atomic masses used for Fe, Cr, and Ni were 55.85, 52.00, and 58.71, respectively.⁶

The thermal nuclear contributions for material number 4271 were obtained with the recently developed JDJNUC nuclear model⁷ in GRIZZLY. In this model, the

material is treated as a Debye solid at low temperatures and as an ideal gas at high temperatures. The JDJNUC model smoothly switches between these two limits for temperatures near the melt line, which is obtained from the Lindemann law. At the melting point on each isotherm, the JDJNUC model builds in a small two-phase region to simulate the melting transition. This part of the calculation requires an ambient value for the melt temperature (T_m) and some analytical form for the Gruneisen parameter as a function of density [$\gamma(\rho)$]. The Debye temperature (Θ_D) is then computed internally from T_m using an empirical relationship based on the behavior of pure elements. Here, the melt temperature of stainless steel 347 was approximated by that of elemental Fe; $T_m = 1808$ K.⁶

A generalized version of the standard CHART-D model⁸ has been used to describe $\gamma(\rho)$; the IGRUN=7 option in GRIZZLY.² In this formulation, the Gruneisen parameter is expressed as a quadratic function of ρ in the expanded region and as a quadratic function of $1/\rho$ in the compressed region. Four items of input are required to completely specify $\gamma(\rho)$; ambient values of γ and its derivative with respect to $\ln \rho$ (GAMREF and DGAMMA), and its asymptotic values $\gamma(0)$ and $\gamma(\infty)$. For $\gamma(0)$ and $\gamma(\infty)$ the default values of 1 and 2/3 were used. GAMREF was taken to be the ambient Gruneisen parameter for Fe; i.e., 1.66.⁹ Finally, DGAMMA was chosen to have a small negative value (-0.05) to ensure that the nuclear isotherms are smooth.

At modest compressions (≤ 2.0), the static lattice cold curve for material number 4271 was calculated by removing thermal contributions from an input Hugoniot expressed as a straight line fit to experimental shock velocity (U_s) vs. particle velocity

(U_p) data.^{4,10} The input Hugoniot used here was $U_s = 4.62 + 1.42 U_p$, in km/s.⁴ For high compressions, the cold curve was required to smoothly extrapolate to a mixed TFD cold curve. This method of calculation ensures that the compressed EOS will reproduce the experimental Hugoniot and also have the correct asymptotic behavior. In the expanded region ($\rho < \rho_0$), the cold curve was forced to have a generalized Lennard-Jones form² that was constrained to smoothly connect with the compressed portion of the cold curve and have the correct cohesive energy (E_c). The cohesive energy of stainless steel has been estimated by that of elemental Fe, 99.4 kcal/mole.⁹ The only remaining parameter needed for the calculation is a parameter (FACLJ) which controls the shape of the cold curve in the expanded region. Here, FACLJ has been used to adjust the output values of the critical temperature (T_c) and critical pressure (P_c). It was found that reasonable values for T_c and P_c could be obtained with FACLJ = 0.7; see below.

III. RESULTS

Figure 1 shows a selected group of P vs. ρ isotherms from the new SESAME EOS for stainless steel 347. In general, the isotherms for material number 4271 do not exhibit any questionable behavior. It is also apparent that the new EOS for stainless steel has a critical temperature of about 8700 K and a critical pressure of about 19 kbar. These values compare quite favorably with previous estimates which suggest $T_c \approx 9000 \rightarrow 10000$ K and $P_c \approx 10$ kbar.¹¹ It is not possible to get a very accurate estimate of the critical point for material number 4270, but simple inspection of that

EOS suggests a T_c in the range of $8000 \rightarrow 10000$ K and a P_c which is in the range of $20 \rightarrow 30$ kbar. While these values are comparable to those for 4271, the newer EOS should give a slightly better description of stainless steel near the critical point.

Figure 2 compares the theoretical Hugoniot for material numbers 4270 and 4271 with experimental Hugoniot data for stainless steel 347.⁴ While both of the theoretical Hugoniot are in basic agreement with the data, the Hugoniot for the newer EOS (4271) is in somewhat better agreement with experiment for U_p values greater than 2.0 km/s. It is also clear from Fig. 2 that the new SESAME EOS for stainless steel 347 should be reliable for all applications involving shock loading.

In general, although the total EOSs for 4270 and 4271 are similar, the newer EOS should be slightly more accurate both in the vapor dome region and along the principal Hugoniot. In addition, as was noted earlier, the two-temperature tables for the older EOS are very noisy and were generated from the total EOS using very crude approximations; whereas, for material 4271, the total EOS was obtained directly from the two-temperature tables. For these reasons, material number 4271 should be preferred over 4270 for virtually all applications.

Figure 1. Selected isotherms from the new SESAME EOS for stainless steel 347. In order, the isotherms shown are for $T = 0$ K, 1160 K, 2900 K, 5800 K, 8700 K, 11600 K, 29000 K, and 58000 K.

Figure 2. The theoretical Hugoniots for material numbers 4271 (solid line) and 4270 (dashed line) are compared with Hugoniot data for stainless steel 347.

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