MATERIAL MODELS FOR AEROGEL DUST COLLECTORS. W. W. Anderson and F. J. Cherne, DE-9, MS P952, Los Alamos National Laboratory, Los Alamos, NM 87545.

Introduction: Interpretation of analysis data from interplanetary and cometary dust particles collected in space via impact into low-density media depends critically on knowing how the collection process affected the material being examined. Models currently in use are deficient in several respects. Most notably, the existing models are based on semianalytic one-dimensional propagation codes and use material models for the aerogels that are overly simplistic. We are developing a more detailed and accurate model that will be used to invert observables such as track morphology to obtain thermal histories of specific recovered samples. This will aid the analysis community in interpreting observed atomic arrangements and volatile element compositions and distributions. Such a model will also be useful in tailoring future collectors for specific mission profiles.

Collection Model: A major component of this project is developing an accurate material model for the aerogel. In the collection process, the aerogel state ranges from essentially unstrained aerogel to highly shocked, partially ionized atomic fluid. As part of our effort, we are developing a new broad-range material model, concentrating on the thermodynamic equation of state (EOS), thermal transport properties, and shear strength or viscosity, as appropriate.

Dynamic Model. The dynamic model we are developing is an explicitly three-dimensional Lagrangian with a finite element treatment of the material in regions where the effective shear strength is significant. The finite elements are converted to discrete particles similar to those in smooth particle hydrodynamics calculations. This treatment thus requires a material description that will be efficient in hydrocode calculations.

Material Model. The low-pressure, low-temperature behavior of shocked aerogel is based on data from the literature [1,2], which allow the plastic and elastic properties of the aerogel to be constrained. Thermal transport modeling is such a case is relatively straightforward and response to shear stress behavior has been measured. As the shock energy becomes sufficient to induce bond breakage, the data that exist specifically for aerogel are confined to measurements of the shock Hugoniot, including pyrometric measurements of the shock temperatures.

We have developed a model for the EOS that explicitly includes polymeric SiO_2 (glass) including distended material, and the species SiO, Si, O, Si^+, O^+, and e^-. Here, we present results for the Si-O atomic fluid. While there are some data for the gaseous atomic species at very low pressures, these results are of limited use for extrapolation to the higher density states relevant to the current project. We use published energies as reference state values, but the *P-V-T* equation of state and transport properties are based on molecular dynamic calculations.

At present, we assume that the system is in thermodynamic equilibrium. We have specifically avoided the tendency in most developments of model potentials in the Si-O system to develop a model that will cause bonding between the Si and O atoms. Instead, we develop the atomic potentials for the atoms as inert species and account for bonding by explicitly modeling SiO as a separate species, allowing minimization of the system Gibbs free energy to determine the relative abundance of the different species, with the constraint that

$$x_{O} = x_{SiO} + 2x_{Si}$$

We use pure species equations of state for SiO, Si, and O atomic fluids and account for excess quantities of mixing using the scaled particle theory of Boublik [3]. We are in the process of validating the excess quantities using a number of calculations of the mixed systems. Part of the problem is that the interatomic/intermolecular potentials of the mixed systems are more difficult to assess.

Interatomic potentials for the pure Si and O systems are based on the assumptions that the core overlap repulsion should be equivalent to that of the noble gas in the same period, while the attractive term is constrained by a combination of the functional form used and the estimated potential well depth. The potential well depth is scaled from the same-period noble gas, correcting for estimated atomic radius and mass, and the form of the potential used is

$$\varphi(r) = \varepsilon\left\{\exp\left[\frac{2n(\sigma - r)}{\sigma}\right] - 2\exp\left[\frac{n(\sigma - r)}{\sigma}\right]\right\}$$

where σ is the atomic separation corresponding to the potential minimum. This form is similar near the minimum to the familiar *n-2n* potentials such as the Lennard-Jones potential, but its shape is more realistic at larger and smaller separations. For Si, we use $\varepsilon = 1178$ J/mol, $n = 6.726$, and $\sigma = 4.289$ Å. For O, the appropriate values are $\varepsilon = 294.6$ J/mol, $n = 6.726$, and $\sigma = 3.158$ Å.

The MD calculations are used to constrain initial analytic EOS parameters based on the expressions for internal energy per atom and pressure for a system represented by pair potentials:

$$E = \tfrac{3}{2}kT + 2\pi\rho\int_0^\infty g(r)\varphi(r)r^2 dr$$

$$P = \rho kT - \frac{2\pi\rho^2}{3}\int_0^\infty g(r)\frac{d\varphi}{dr}r^3 dr$$

where the densities in this case are atomic number densities. We write these expressions as

$$E = \frac{3RT}{2\mu} + 2\pi\rho I_1$$

$$P = \frac{\rho RT}{\mu} - \frac{2\pi\rho^2}{3}I_2$$

The integrals I_1 and I_2 are calculated by assuming that the radial distribution function is approximated by

$$g(r) = 1 + r^{-3}f(r)$$

where $f(r)$ is a series of alternating positive and negative boxcar functions with amplitude proportional to the equivalent hard sphere packing fraction, while the potential is approximated by the Lennard-Jones potential. The boundaries between adjacent boxcar functions are written as fractions of the equivalent hard sphere diameter of the atoms. In that case, the integrals become

$$I_1 = a_1\left(1+\sqrt{\frac{3kT}{2\varepsilon}}\right)^{3/2} + a_2\left(1+\sqrt{\frac{3kT}{2\varepsilon}}\right)^{1/2}$$
$$+ a_3\rho\left(1+\sqrt{\frac{3kT}{2\varepsilon}}\right) + a_4\rho$$

$$I_2 = 12I_1 - 6\left[a_2\left(1+\sqrt{\frac{3kT}{2\varepsilon}}\right)^{1/2} + a_4\rho\right]$$

and parameters a_i are fit to the MD simulation results for energy and pressure. In practice, the fits are scaled to fit shock Hugoniot and temperature data for aerogel [5-8], taking the bond breakage energies into account.

For O, the parameters are $a_1 = 7.311\times10^{-4}$ Jm^{3}kg^{-2}, $a_2 = 0.3532$ Jm^{3}kg^{-2}, $a_3 = 1.039\times10^{-5}$ Jm^{6}kg^{-3}, and $a_4 = 4.503\times10^{-2}$ Jm^{6}kg^{-3}. The EOS fit resulting from these

parameters agrees with the MD results to ~1%. For Si, the equivalent parameter values are $a_1 = 1.667\times10^{-3}$ Jm^{3}kg^{-2}, $a_2 = -1.548$ Jm^{3}kg^{-2}, $a_3 = 5.393\times10^{-5}$ Jm^{6}kg^{-3}, and $a_4 = 0.1287$ Jm^{6}kg^{-3}, but agreement with the MD results is in some cases only 20%, suggesting that a more realistic approximation for $g(r)$ is needed. Typically, the agreement with the MD results is better at higher temperatures, where the atomic fluid model is more relevant.

Fluid mixture model. The excess entropy of mixing of the different fluid species is based on the scaled particle theory of Boublik [3]. We specifically assume that Si and O are spherical and that SiO is nonspherical.

Transport properties. We find that, at low densities, thermal transport is dominated by kinetic transport, but that as mean free paths decrease, radiative transport becomes substantially more important. In particular, at energies where a significant fraction of photons can cause electronic transitions in the atoms, radiative transport is dominant. Radiative transport certainly dominates the deposition of energy in the rinteriors of monolithic dust grains. Fourier conduction in such cases is mitigated somewhat by ablation of the particle.

Conclusions: The model we are developing is much more suitable for assessing the capture process than existing models. Much of the new model requires numerical simulations because of the lack of suitable data, but hte integrated model can be tested against experimental data. Some aspects of the existing model, particularly the EOS of the atomic Si fluid, are still not entirely satisfactory, but the current state of the model is a substantial improvement over previous material descriptions.

References: [1] Gibiat V. et al. (1995) *J. Non-Cryst. Solids* 186, 244-255. [2] Scherer G. W. et al. (1995) *J. Non-Cryst. Solids* 186, 316-320. [3] Boublik, T., (1983), *Coll. Czech. Chem. Comm.* 48, 192-198. [4] Holmes N. C. et al. (1984) *Appl. Phys. Lett.* 45, 625-628. [5] Holmes N. C. and See E. F. (1992) *Shock Compression of Condensed Matter 1991*, 91-94. [6] Nikolaev D. N. et al. (2000) *Shock Compression of Condensed Matter—1999*, 121-124. [7] Fortov V. E. et al. (2003) *Mod. Phys. Lett. A* 45, 1835-1840. [8] Knudson M. D. et al. (2005) *J. Appl. Phys.* 97, 1-14.