1. *Thermophysical Properties of Gases Used in Semiconductor Processing*

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Objective: To provide industry with high-accuracy data for modeling CVD (chemical vapor deposition) processes and for calibration of MFCs (mass flow controllers) used in semiconductor processing.

Problem: Many process gases are toxic, and/or corrosive, and/or pyrophoric. The thermophysical property data for such gases are sparse and rarely accurate. Accurate thermophysical property data are required to model the gas streams that are used in CVD processes. (For example, models are needed for the velocity, temperature, and concentration profiles in the vicinity of a hot susceptor.) Accurate thermophysical property data are also needed to calibrate the MFCs used to meter process gases. These MFCs are calibrationed with benign "surrogate" gases (*e.g.* N_2, CF_4, SF_6, or C_2F_6) but are used to deliver process gases (*e.g.* Cl_2, HBr, BCl_3, WF_6) for CVD, plasma etching, and other processes. Accurate calibrations are required to scale processes up from prototype to pilot plant and to production. Since MFC operation depends upon heat transfer, converting a surrogate gas calibration to a process gas use requires the heat capacity, thermal conductivity, density, and viscosity of both gases as functions of the temperature and the pressure.

Approach: The Fluid Science Group is using acoustic techniques to measure the thermophysical properties of three classes of gases: (1) binary mixtures of CVD carrier gases with process gases, (2) pure process gases, and (3) surrogate gases. The Group is developing a comprehensive, reliable database for these gases that provides the heat capacity, thermal conductivity, viscosity, and the pressure-density-temperature relation. The data base will include diffusion coefficients for mixtures of the gases. Values for diffusion coefficients will be obtained from models for the intermolecular potentials between carrier gases and process gases.

Results and Future Plans: We developed a facility for safely measuring the properties of these hard-to-handle gases. During FY00, we measured the speed of sound in $(CH_3)_3Ga$ (a pyrophoric organo-metallic) and NF_3 (an aggressive oxidizer), two gases given high priority by the SEMATECH MFC Working Group. Figure 1 displays speed-of-sound data for $(CH_3)_3Ga$. Typically, the data range from below the boiling temperature to 200 °C and from 25 kPa to 1500 kPa or 80% of the vapor pressure.

The acoustic data are analyzed to determine the ideal-gas heat capacity and the equation of state with uncertainties of approximately ±0.1%. Model pair potentials are also derived from the data. These models are used to reliably extrapolate the equations of state to temperatures above 1000 K and to estimate the transport properties.

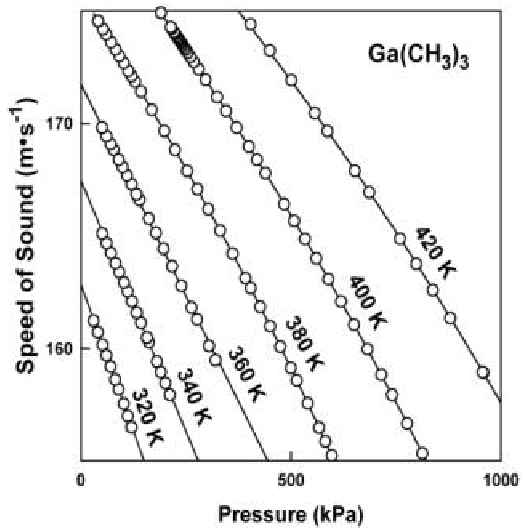

Figure 1 Speed-of-sound measurements in tri-methylgallium.

The NIST results are being disseminated through the internet in a user-friendly database at *http://properties.nist.gov/semiprop/* and also in review publications and peer-reviewed articles in archival journals.

We plan to measure the speed of sound in other poorly characterized process gases. Acoustic measurements of the transport properties have begun, starting with the viscosity of the calibration gases CF_4, C_2F_6, and SF_6. These will be extended to process gases and the Prandtl number will be measured. As data are acquired, the on-line data base will be updated.

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J.J. Hurly, ***"Thermophysical Properties of Gaseous HBr and BCl_3 from Speed-of-Sound Measurements,"*** Int. J. Thermophysics. (in press).

M.R. Moldover, K.A. Gillis, J.J. Hurly, J.B. Mehl, and J. Wilhelm, ***"Acoustic Measurements in Gases: Applications to Thermodynamic Properties, Transport Properties, and the Temperature Scale,"*** Vol. IV, Chap. 12 in Handbook of Elastic Properties of Solids, Fluids, and Gases, edited by R. Raspet and M. Levy, Academic Press (in press).