Calculation of Transport Coefficients in Dense Plasma Mixtures

T. HAXHIMALI, W.H. CABOT, K.J. CASPERSEN, J. GREENOUGH, P.L. MILLER, R.E. RUDD, E.R. SCHWEGLER, Lawrence Livermore National Laboratory — We use classical molecular dynamics (MD) to estimate species diffusivity and viscosity in mixed dense plasmas. The Yukawa potential is used to describe the screened Coulomb interaction between the ions. This potential has been used widely, providing the basis for models of dense stellar materials, inertial confined plasmas, and colloidal particles in electrolytes. We calculate transport coefficients in equilibrium simulations using the Green-Kubo relation over a range of thermodynamic conditions including the viscosity and the self-diffusivity for each component of the mixture. The interdiffusivity (or mutual diffusivity) can then be related to the self-diffusivities by using a generalization of the Darken equation. We have also employed non-equilibrium MD to estimate interdiffusivity during the broadening of the interface between two regions each with a high concentration of either species. Here we present results for an asymmetric mixture between Ar and H. These can easily be extended to other plasma mixtures. A main motivation for this study is to develop accurate transport models that can be incorporated into the hydrodynamic codes to study hydrodynamic instabilities. *This work was performed under the auspices of the US Dept. of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344.

Tomorr Haxhimali
Lawrence Livermore National Laboratory

Date submitted: 26 Jul 2011