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Electrical and thermal conducticity of metallic liquids at high pressure from ab-initio computations

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Electrical and thermal conducticity of metallic liquids at high pressure from ab-initio computations

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The electronic transport properties of liquid metals at high pressures are critical to understanding processes associated with the thermal evolution of planets and magnetic field generation in the liquid portion of their cores. Terrestrial planets, such as the Earth, contain iron as the primary core elements, the giant gas planets hydrogen in the metallic state. Unfortunately, the understanding of electronic (σ) and thermal conductivity (κ) from experiments relies on extrapolations both in temperature and pressure and a number of scaling relations, such as the validity of the Wiedemann-Franz law. Ab-initio simulations combining molecular dynamics simulations with linear response computations of the Onsager kinetic coefficients for uncorrelated snapshots of the MD trajectories provide an alternative route both electrical and thermal conductivity values of liquid metals at high pressure and temperatures. In recent work we have explored these electric transport properties of liquid Al [1] and Fe and some of its alloys in the Fe-O and Fe-Si system [2] at high temperature and pressure.

Al was chosen because of its free-electron like behavior at ambient conditions with low dispersion of electronic states and the small number of valence electrons. Also, previous computations using the same approach showed good agreement in electronic transport properties with experiments. We find that a Drude model does indeed describe the frequency dependent conductivity values well, and that the number of effective electrons (Neff) computed from the zero frequency limit of σ and the relaxation time yields a value of 2.8±0.2, close to the fully free-electron picture with Neff =3. As expected, electrical conductivity decreases with temperature, reflecting the temperature broadening of the Fermi function $\partial f/\partial \varepsilon'$. Charge delocalization under pressure leads to higher $\partial f/\partial \varepsilon'$ and consequently increasing σ; thermal conductivity shows the opposite trends to the extent that the Wiedemann-Franz law holds approximately.

For Fe and its alloys we found that values in σ decrease much more slowly than previously assumed, and our results help to resolve a long-standing controversy of the appropriate high pressure - high temperature values that have arisen from vastly different data measurements in two sets of shock wave experiments [3,4]. For the Fe-O alloys the Wiedemann-Franz law breaks down, with much smaller values of the Lorenz number than the one established in the Sommerfeld theory of metals. This indicates that electron scattering in the Fe-O liquids is strongly anelastic, resulting in a breakdown of the simple relaxation time picture of electronic migration.

[1] V. Vlček, N. de Koker and G. Steinle-Neumann, Phys. Rev. B 85, 184201 (2012).
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[3] R. N. Keeler, in Physics of High Energy Density (Academic Press), pp. 106-147 (1971).
[4] Y. Bi, H. Tan and F. Jing, J. Phys. Cond. Matter 14, 10849 (2002).