Pressure Treated Glasses for Increased Thermal Conductivity

Project Summary for General Public

Crystals tend to conduct heat very well, with a diamond made out of carbon being the best conductor, and crystalline silicon, which is the base for microelectronic materials, also capable of moving heat very well, thus preventing microprocessor chips from overheating. The ability of crystal to conduct heat efficiently is associated with the collective motion of atoms, or ions, in the form of propagating thermo-mechanical waves enabled by an ordered array of atoms/ions forming the crystal. However, atoms in some materials have a difficult time falling in an ordered array during synthesis. Prominent examples include oxide-based glasses, such as silicon dioxide, i.e., silica glass, or the majority of polymers out of which plastics are made. These non-crystalline materials, i.e., glasses, exhibit very low thermal conductivity because there are few propagating thermal waves inside of them, and instead, most of the atomic vibrations are rather aimless and not capable of moving much heat around. Furthermore, in the case of oxide glasses, which due to their optical transparency have a number of important applications, thermal conductivity is not only low, but its range is also very narrow. This low conductivity can be an asset when thermal insulation is a goal, such as in the case of a silica-based protective space shuttle cover. In many cases, however, low thermal conductivity is a limitation. For example, during material synthesis low thermal conductivity leads to large temperature differences across the material, which tends to create thermal stresses, and can cause premature fracture and failure.

In our project, following clues from ours and other researcher work we will use computer models and simulations to explore a possibility that high pressure densified glasses might have much larger thermal conductivity than regular glasses. Computer simulations will determine thermal conductivity dependence on the details of the glasses' atomic-level structure, and to evaluate contributions to thermal transport from individual thermal waves. The simulation results provide guidance by which we will synthesize glasses in the laboratory under a range of pressure and temperature protocols. We will determine structural characteristic and thermo-mechanical properties of these glasses, most prominently thermal conductivity. The experimental results will feed back to the modeling effort by verifying the predictions of simulation, and, if needed, by guiding the design of more accurate models.

The major significance of the proposed work will be in substantially expanding the ability of glasses to move heat more efficiently. This work will also contribute to a better understanding of the thermal transport mechanism in glasses. From the application point of view, the development of synthesis-processing protocols to create glasses with significantly larger conductivity will be of a great interest to commercial glass companies, and it might expand the application of glasses to new products and devices that require efficient heat removal strategies.