Polarization Caloritronics

Joseph Heremans

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This proposal is to establish a new subfield in the physics of transport properties, *polarization caloritronics*, the study of the mixed transport of heat and polarization currents in ferroelectric materials. It will investigate the nature of polarization currents, a theoretical concept proposed by Bauer et al. in 2021 (*Phys. Rev. Lett.* **126**, 187603, 2021) for which the PI's group provided the first experimental evidence (Wooten et al., *Science Advances* **9**, eadd7194, 2023). Spin currents exist in ferromagnetic and antiferromagnetic materials; in electrically insulating ferromagnets they are carried by magnons, the thermal perturbations of the magnetization. Spin currents can be driven by temperature and magnetic field gradients; thus spin-Onsager relations can be written with spin conductivity, spin-Seebeck, spin-Peltier and magnon thermal conductivity as transport coefficients. The study of these is known as spin caloritronics. The proposal is to quantify the analog concepts for ferroelectric solids. By analogy, polarization currents in ferroelectric materials must be carried by the thermal perturbations of the ferroelectric order, labeled *ferrons* by Bauer et al. In displacive ferroelectrics, ferrons are a subset of phonons, namely those that involve the motion of ions that carry the charges responsible for the formation of dipole moments. Wooten et al. show that in displacement ferroelectrics ferrons are highly anharmonic phonons, including propagating acoustic phonons that are strain-coupled to the optical phonons more conventionally associated with the polarization. These propagating phonons are expected to carry a polarization current (like magnons carry a spin current) and can thus be driven by temperature and electric field gradients. By analogy again, we write polarization-Onsager relations, defining four transport coefficients: polarization conductivity, polarization-Seebeck, polarization-Peltier and ferron (phonon) thermal conductivity. The proposed research is to study these and develop the fundamental concepts for their applications. Two more experimental observations justify this approach. The first is a new polarization-drag experiment (the analog of the magnon-drag thermopower) for which preliminary are data shown in the proposal. The second is the very existence of a non-zero pyroelectric coefficient: since polarization is an extensive thermodynamic quantity, a change in polarization under temperature can formally be represented by a polarization flux in the Onsager relations. The work will have four objectives:

- The development of experiments that put in evidence the polarization currents and measure their transport coefficients. Unlike charge currents, which cannot be sustained in insulating ferroelectrics, polarization currents must be detected indirectly like spin currents. This effort transposes techniques used in spin caloritronics.
- The development of a theoretical framework for the polarization transport coefficients, based on density functional theory and molecular dynamics
- A materials characterization and optimization effort to find and/or synthesize materials with optimal polarization transport properties
- The development of the fundamental concepts for possible applications of polarization currents in electrically-driven heat switches, new thermoelectric concepts such as polarization-drag and polarization-Peltier effects, and ferronic logic and memories, by analogy with magnonics.

Prospective DoD applications include heat management, power generation and refrigeration, and logic circuits with THz capability. Ferrons are driven by an electric rather than magnetic field and are voltage rather than current controlled. Ferronic/phononic devices could operate above the frequency limitation of the ferromagnetic resonance, be more robust than magnonic devices against electromagnetic interference, and be potentially integrated with piezoacoustic devices.