

## New Materials for High Temperature Thermoelectric Power Generation

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## ABSTRACT

Thermoelectric devices convert thermal energy directly into electrical energy, require minimal maintenance, and can be operated over a large temperature range (room temperature to 1000 °C). Thermoelectric materials are described by a figure of merit, ZT, which measures how well a material converts heat flow to electricity – and is directly related to the efficiency, the higher the ZT the greater the efficiency. New ideas for overcoming intrinsic limitations in bulk materials have led to materials with significantly better performance. For example, thin-films of PbSe0.98Te0.02/PbTe where PbSe nanoparticles are embedded in a PbTe matrix show a ZT550 K ~ 2.5; this achievement is mainly due to a large reduction in the lattice thermal conductivity while maintaining relatively high carrier mobilities. In addition to reducing thermal conductivity in existing high ZT materials, the electronic properties of intrinsically low thermal conductivity materials may also be manipulated. Reaching 20% efficiency requires an average ZT value of 1.7 for a 1273 - 473 K temperature differential (typical of RTGs), and reaching 30% efficiency requires an average ZT value of 2.8 for a 1273 - 373 K temperature differential (a lower rejection temperature through improved efficiency). However, the number of materials with high ZT that can operate at 1273 K are limited.

We propose to develop nanostructured composites and new materials based on n- and p-type nanostructured Si1-xGex (ZT1273K  $\sim$  1) and the recently discovered p-type high temperature Zintl phase material, Yb14MnSb11 (ZT1273K ~1). The Zintl compound, Yb14MnSb11, doubles the ZT of the current state-of-the-art p-type high temperature material p-Si0.80Ge0.20 (SiGe) alloy, ZT ~0.5 at 1275 K, making Yb14MnSb11 an efficient p-type thermoelectric material for high-temperature applications. Electronic manipulation of Yb14MnSb11 has boosted the ZT to 1.4 (Yb14Mn1-xAlxSb11). Pairing Yb14MnSb11 in a segmented thermoelectric converter with CeFe4Sb12 allows for nearly a 4-fold efficiency improvement over that of Si1-xGex in CeFe4Sb12/SiGe, not only because of the significantly enhanced thermoelectric figure of merit, but also because of increased similarity in thermoelectric property compatibility factors. This proposal focuses on the development of the n- and p-legs of a thermoelectric device with the synthesis of new n-type SiGe/nanoparticle composites and electronic manipulation of p-type Yb14MnSb11. With the SiGe the challenge is synthesizing the small inclusions and dispersing them in the matrix; with Yb14MnSb11 the challenge is to tune the band structure and carrier concentration. Both parent phases have demonstrated high ZT at high temperatures and have melting points approaching 1700 K. The high performance properties will be validated at the Jet Propulsion Laboratory (JPL) and a couple fabrications will be demonstrated.

This research will place our students at the leading edge of development of advanced materials for thermoelectric devices that can offer a higher degree of efficiency and will provide an efficient feedback loop between the University and National Laboratory Partner.