Thermoelectric power sources have consistently demonstrated their extraordinary reliability and longevity for deep space missions as well as terrestrial applications where unattended operation in remote locations is required. They are static devices with a high degree of redundancy, no electromagnetic interferences, with well documented “graceful degradation” characteristics and a high level of scalability. They are also tolerant of extreme environments (temperature, pressure, shock and radiation). The development of new, more efficient materials and devices is the key to improving existing space power technology and expanding into efficient, cost-effective systems using high grade heat sources, generated through fossil fuel combustion or as a waste exhaust stream.

Proven state-of-practice Si0.8Ge0.2 alloys have a combined dimensionless figure of merit (ZT) value of only 0.55 when averaged over operating temperatures of 1275 K to 575 K. In addition, the significant Ge content of these materials precludes their use for large scale terrestrial applications due to cost considerations. We present an overview of NASA-funded collaborative research efforts to identify and characterize advanced bulk thermoelectric materials capable of quadrupling average ZT values while maintaining reliable operation for more than 15 years at temperatures up to 1300 K. Some of the materials being investigated may have good potential for larger scale terrestrial applications.

The research areas include structurally complex refractory rare earth compounds, electronic band-engineered advanced PbTe and bulk 3-D nanostructures that emulate results obtained on low dimensional superlattices through “force engineering” and “self-assembling” techniques.

The first research area concerns two families of very low lattice thermal conductivity refractory rare earth compounds which have demonstrated peak ZT values near 1.5 at 1273 K. We briefly discuss recent experimental results, guided by first principle electronic structure calculations, in tuning the properties of these rare earth compounds through suitable chemical substitutions and structural modifications. A second research area focuses on advanced PbTe materials and utilizing high degeneracy bands due to band convergence at high temperatures to generate large power factors. While not of practical interest for terrestrial applications, these compounds are good model systems that could be applied to more practical materials.

The last main research area, perhaps of most interest to terrestrial applications, focuses on engineering bulk homogenous and composite 3-D nanostructures that effectively decouple electrical and thermal transport effects to enable independent optimization strategies. Silicon and silicide nanostructured materials have been predicted to have the potential for large gains in ZT values through a combination of low lattice thermal conductivity brought by effective interface scattering and tuning of electrical transport through the introduction of suitable nanoscale inclusions. Strategies to achieve the necessary grain size, size distribution and nanoscale inclusion “seeding” in thermally stable bulk structures are presented.

Validation of the high ZT values of some of the more mature novel thermoelectric materials is carried out by fabricating and testing simple high temperature thermoelectric couple devices. A factor of more than two increase in average ZT values and up to 15% conversion efficiency has been achieved to date on devices tested in vacuum and inert gas environments at high operating temperatures.

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