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Editorial

As both the world's energy demand and the destructive environmental impact from the combustion of fossil fuels is constantly rising, it is a timely issue to sustain our electricity base via exploitation of waste heat converting it with thermoelectric generators.

Thermoelectrics has been defined as the Science and Technology associated with thermoelectric power generation and refrigeration. A thermoelectric convertor is formed by connecting two semiconducting materials (thermoelements) at a junction to form a thermocouple. When the junction is maintained at a temperature, which differs from the ambient, a voltage is established across the open ends of the thermocouple (Seebeck effect) and, if the circuit is closed with a resistance load, an electric current flows in the circuit. The device operates as a generator converting the flow of heat into electrical power. Conversely when a current is supplied to the thermocouple, heat is pumped from one junction to the other, depending on the direction of current flow (Peltier effect), and the device operates as a refrigerator. In practice, a large number of thermocouples are connected electrically in series and thermally in parallel to form a module. The module is the active component of a thermoelectric generator or refrigerator.

Although the efficiency of most of these devices has long been too inefficient, new ideas for enhancement of thermoelectric efficiencies via nanostructural engineering in combination with an increasing demand in modern refrigeration (*particularly spot cooling of electronic equipment*), as well as in electric power generation (*in hybrid automobile applications, etc.*), have spurred renewed interest in thermoelectrics within the last decade. Moreover, thermoelectric power generators are the irreplaceable power source for space and marine autonomous apparatus, for cathodic protection devices of pipelines, etc. In all these cases, simplicity and reliability of the devices, the complete absence of moving parts and the environment-friendliness (no fluorinated toxic coolants) outweigh their relatively high cost and low efficiency (typically less than 10%). It is important to note that thermoelectric power generation can run on waste-energy at zero-cost input energy. Industrial processes, home heating and automotive exhaust are currently the major producers of an enormous amount of unused waste heat to be tapped by thermoelectric energy converters.

Hitherto, the most important thermoelectric materials are (a) ‘‘skutterudites’’, (b) ‘‘clathrates’’, and (c) Zintl phases all showing a complex crystal structure and multicomponent composition. Besides, new techniques of synthesis, such as chemical/physical vapor deposition of thin/thick films, melt spinning and preparation of nano-structured materials have provided enhanced thermoelectric efficiencies. Design of thermoelectric materials (multi-component and multi-phase materials) requires a multidisciplinary approach comprising expertise in materials chemistry, physics, metallurgy, ceramics, in experiment and theory, electrical and device engineering etc. Accordingly, there is an increasing demand of reliable phase diagrams and phase stabilities. Thermochemical calculations using the CALPHAD approach in conjunction with key experiments have shown their strengths to provide these data in reasonable time even for multicomponent materials. As a complementary tool, ab initio techniques i.e. density functional theory calculations (DFT) nowadays are capable of providing not only enthalpy data with high accuracy and with moderate computational efforts, but also phonon dispersion, elastic constants, electronic structure, Fermi-surfaces, magnetic ground states, etc., defining relative phase stabilities and physico-chemical properties. The new computational tools are an indication of the importance of modeling and simulations. More challenging are ab initio calculations of phonon dispersions and phonon scattering in order to model thermal conductivity.

It is my belief that such a combined and balanced approach comprising experimental and computational techniques will ensure a sound physico-chemical basis for successful development and design of advanced engineered (thermoelectric) materials.

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