Preface

Why Thermoelectrics?

In the last 10–20 years, thermoelectric materials have attracted renewed interest, as concerns with the efficient use of energy resources and the minimization of environmental damage have become important current issues. Thermoelectric devices can recycle some of the waste heat and transform it back into electrical energy, thereby reducing energy losses. However, applications are only one of the reasons for studying thermoelectricity. Thermoelectric phenomena [1, 2] have played an important role in the history of physics on several occasions and continue to do so today. In the middle of the nineteenth century, the explanation of the Seebeck and the Peltier effects required the unification of electrodynamics and thermodynamics [3]. A new phenomenon, the Thompson heat, emerged as a necessary condition for the internal consistency of the unified theory. Interestingly, the success of the "macroscopic" approach based on "measurable quantities", like the electrical field, the displacement currents, and the heat, was played against the "microscopic" approaches, based on "atoms", "molecules," or other constructs, considered to be "fictitious" at that time. The idea of the particle current, as opposed to the "displacement current" of the nineteenth century electrodynamics, was introduced by Drude some 40 years later. In the early twentieth century, the proof of the equivalence of the Seebeck and the Peltier coefficients was a breakthrough achievement in the theory of irreversible phenomena [4]. Immediately after World War II, the search for better thermoelectrics became a major driving force in the physics of heavily doped semiconductors which led to many specialized applications. However, the widespread use of thermoelectricity was inhibited by the low efficiency and the high cost of the devices.

Thermoelectric devices are heat engines that either convert heat into electricity or use electricity to pump heat from a cold to hot reservoir. The possibilities arising from the fact that electricity can be generated directly from heat, the Seebeck effect known since 1821 [1], are beginning to be more widely appreciated. Thermoelectric devices can reduce petrol consumption in motor vehicles by 5–10 %, reducing significantly the oil needs. They are also used for power generation in remote regions, where thermoelectricity ensures a continuous power supply for electronic equipment. This is an important, but only one type of application of a thermoelectric effect. The other thermoelectric effects, the Peltier effect [2] and Thompson effect [3], can be used for cooling without the use of environmentally hazardous compressing fluids, providing microcooling for the electronics industry and refrigeration without mechanically moving parts. All of these can play important roles in the development and efficient use of sustainable energy resources [5]. The scientific and technological advances in this field could have important implications for modern society.

Figure of Merit

The main problem in nearly all of these applications is the rather low efficiency of the processes of energy conversion. The important factors which determine the efficiency are the total thermal conductivity and the power factor of the thermoelectric material, which is given by the product of the electronic conductivity and the square of the Seebeck coefficient. The ratio of the power factor and the thermal conductivity defines the dimensionless figure of merit, ZT, which characterizes a given material in a simple way. The value of ZT of the order of 1 or higher is needed for the more widespread use of thermoelectric devices. A high figure of merit requires the use of a material with a large power factor and a low thermal conductivity. These tend to be incompatible requirements; for example, a good metal has a high electrical conductivity but also a high thermal conductivity. Materials which have high thermopower tend also to have low electrical conductivity.

Most current applications of thermoelectricity are based on heavily doped semiconductors, discovered in the late 1950s [6], with ZT less than 1. Several strategies for improving the figure of merit have recently been developed and new materials with $ZT \geq 1$ have been reported [7]. The aim of this research field is to find or fabricate materials with large ZT but that are at the same time cheep and abundant enough for a widespread application.

Reducing Heat Losses

One strategy for enhancing ZT is to reduce heat losses by increasing the phonon scattering, while keeping electron transport unchanged, which is known as the phonon glass–electron crystal strategy. The materials that fulfill these requirements are clathrates and skutterudites [8, 9] with large voids in the crystal structure. The voids are filled with atoms which are relatively free to rattle, and so reduce the thermal transport by the phonons. Another strategy along the same lines is to reduce the heat conduction by scattering the phonons on the interfaces or imperfections in nano-precipitates, nanostructured layered materials, or composites. A much improved high-temperature figure of merit has recently been reported for PbTe-SrTe nano-precipitates [10] and PbTe/PbSeTe superlattices [11]. An enhanced figure of merit is also expected in quantum dots, nano-wires, and molecular devices, due to their restricted dimensionality [12]. These artificial systems offer a completely new route to thermoelectricity that is yet to be explored. An increased efficiency can be achieved with segmented materials, where each part of the thermoelectric device operates in optimal conditions. A progress along any of these lines requires that the thermoelectric materials be engineered with nano-scale precision.

Increasing the Power Factor

The other strategy of enhancing ZT is to increase the power factor using materials with strongly correlated electrons which give rise to sharp variations in the density of states [13] and transport relaxation time [14]. We do not expect the strongly correlated electrons to compete with the semiconductors at high temperatures but they can be attractive for application in the temperature range in which the semiconductors cannot operate. The rare earth intermetallic compounds with heavy fermions or valence fluctuations, like $YbAl_3$ [15] or $CePb_3$ [16] have large power factors even below 100 K. The enhancement is due to the presence of a broad many-body resonance close to the Fermi energy. Some correlated materials, like iron silicides [17, 18], acquire a large power factor due to the proximity of the Fermi level to the hybridization gap and the formation of a narrow asymmetric density of states near the chemical potential. High-temperature superconductors [19] and some other oxides [20, 21] exhibit thermoelectric anomalies caused by the proximity of the chemical potential to the Mott-Hubbard gap. In heavily doped semiconductors, like lead telluride, the power factor is enhanced by the resonant enhancement of the of density of states due to the impurities [22, 23]. In all these cases, the quantum-mechanical approach is indispensable.

What Happened at the Workshop?

There have been important developments in the fabrication and design of new thermoelectric materials. They have considerable potential, due to the possibility of combining materials with quite different attributes to influence the various factors which contribute to the overall figure of merit. Modern thermoelectricity is a multidisciplinary field, requiring the expertise of material physicists, chemists, and metallurgists and the support of theory. There have also been important recent advances in theoretical methods and a deeper understanding of the parameters that affect the performance of materials in thermoelectric devices. These have brought the goal of producing materials with the required characteristics for commercial application a significant step closer. The aim of the workshop was to build on the success achieved so far.

The research workshop brought together the experts in the different field to exchange latest results and ideas, and to discuss directions for future work. The program focused on a particular issue each day, discussing the various strategies for increasing the figure of merit. There have also been several theoretical contributions using various approaches, some based on simplified models, others aiming at first principles calculations for particular materials, to get a deeper understanding of the interplay of the factors that influence thermoelectric properties.

What's in This Volume?

The contributions to this volume cover the broad range of issues discussed at the workshop, from the experimental work of fabricating and characterizing the properties of new materials to enhance ZT through to theoretical work on renormalized band structure calculations and model Hamiltonians to obtain a deeper understanding of the thermoelectric properties of these materials. They give a guide to the current activity in the field and show that real progress is being made. More work, however, will be needed. We hope the ideas presented here will encourage and stimulate further developments in the field to bring forward the day when the general production of high-efficiency thermoelectric devices can be realized.

Zagreb, London

Veljko Zlatić
Alex Hewson

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