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OPTIMISATION OF THE THERMOELECTRIC FIGURE OF MERIT IN FINE GRAINED SEMICONDUCTOR MATERIALS BASED UPON LEAD TELLURIDE.

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I. Introduction

It has been reported that grain boundary scattering has a significant effect in reducing the lattice thermal conductivity of silicon germanium alloys[1-3]. This phenomenon does not appear to be accompanied by a deterioration in the other parameters which occur in the thermoelectric figure of merit. Consequently, small grain size silicon germanium alloys exhibit a higher figure of merit than comparable "single crystal" or large grain size material. Although grain boundary scattering of phonons is particularly favoured in silicon germanium alloys because the large difference in atomic masses of the constituent atoms give rise to substantial alloy disorder scattering, this phenomenon will also be present in other thermoelectric semiconductor alloys.

Fossil fueled thermoelectric generators employing modules based upon lead telluride technology have found military applications[4]. Clearly any improvement in the thermoelectric conversion efficiency of the generator would lead to a saving in fuel; an important consideration when the device is used in a tactical situation.

Materials of the lead telluride family (tellurides, selenides and sulphides of heavy metals) possess in general comparatively large figures of merit at room temperatures. However their upper temperature of operation is restricted by their relatively small energy band gap and the consequent adverse minority carrier effects. On the other hand materials such as the tellurides and selenides of cadmium while possessing a large energy gap,unfortunately possess a low figure of merit. Evidently substantial improvements in thermoelectric performance may be achieved through a suitable alloy combination of a high energy gap telluride or selenide with a telluride or selenide of high figure of merit. In addition small grain size alloys of members of the lead telluride family whose constituents have large difference in molecular weights will exhibit an improved figure of merit. These considerations lead us to approach the project in a number of stages and consider systems of increasing complexity as follows:

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II. Programme of Work

1. A study of the reduction in lattice thermal conductivity with decrease in grain size for (a) undoped, (b) doped lead telluride.

2. Ascertain which alloy combination based on the lead telluride family gives the most suitable energy gap over the intended temperature range of operation.

3. Investigation of alloy combinations which in addition to satisfying (2), also exhibit significant grain boundary scattering.

4. Development of the theoretical framework for the computation of lattice thermal conductivity as a function of grain size - an anticipated difficulty is the aquisition of the phonon dispersion relations for these alloys.

5. Computation and optimisation of the thermoelectric figure of merit as a function of the Fermi level and grain size over the intended temperature range of operation.

6. An estimation of the improvement in figure of merit over that of existing materials over a similar temperature range of operation and the likelihood of achieving this improvement in practice.

III. References

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