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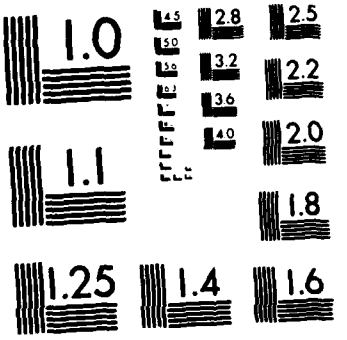

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OPTIMISATION OF THE THERMOELECTRIC FIGURE OF MERIT IN FINE GRAINED SEMICONDUCTOR MATERIALS BASED UPON LEAD TELLURIDE

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I. Work Undertaken

In our previous report the results were presented of our investigation into the effect of a reduction in the lattice thermal conductivity, due to phonon grain boundary scattering on the thermoelectric figure of merit of highly disordered alloys of lead telluride. The reduction was presented as a function of reduced Fermi energy (ξ) and at two temperatures, 300K and 800K. It was concluded that in a material moderately doped and with a mean grain size of $\sim$ 1um the figure of merit is significantly increased compared with "single crystals" or large grain size material.

In a material development programme carrier concentration values are more meaningful than reduced Fermi Energy and in this report we present the results of our calculations of the reduction in Z over the temperature range of operation of a device, and at three different carrier concentrations. Our results are embodied in the attached paper. The paper entitled "Temperature Dependence of the Figure of Merit of Improved Thermoelectric Materials based upon Lead Telluride" has been accepted for publication as a letter in J. Phys.D, Appl. Phys.

II. FUTURE PROGRAMME OF WORK

The objective of the investigation to date has been to obtain an estimate of the possible relative improvement in material performance due to phonon-grain boundary scattering. The theoretical model employed in our calculations is relatively insensitive to the choice of value taken for parameters such as effective mass and to the nature of the energy surfaces. As indicated in our previous report our immediate task is to develope a more realistic model and work is proceeding towards this objective.

TEMPERATURE DEPENDENCE OF THE THERMOELECTRIC FIGURE OF MERIT OF IMPROVED THERMOELECTRIC MATERIALS BASED UPON LEAD TELLURIDE

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Abstract:
The effect of a reduction in lattice thermal conductivity due to phonon-grain boundary scattering, on the thermoelectric figure of merit of highly disoredered alloys of lead telluride has been investigated as a function of temperature and for three different carrier concentrations. It is concluded that the figure of merit of material with a mean grain size of $\sim$1 μm is about 10% higher than equivalent 'single crystal' or large grain size material.

Thermocouples based upon lead telluride technology are employed in thermoelectric generators used in a number of US military applications (Guazzoni and Swaylik 1982). The conversion efficiency of a generator is dependent upon the figure of merit Z of the thermocouple material. One method of increasing Z and hence of improving the thermoelectric conversion efficiency is to reduce the thermal conductivity of the thermocouple material. This can be achieved by fabricating the thermocouples from small grain size material (Rowe and Bhandari 1983).

In a previous communication (Bhandari and Rowe 1983) the results were reported of an investigation into the effect of phonon-grain boundary scattering, doping and alloying, on the lattice thermal conductivity λ_L of lead telluride alloys. It was concluded that for moderately doped, highly disordered alloys possessing a mean grain size of $\sim$1 μm, the lattice thermal conductivity at room temperature was reduced by approximately 11-13% compared to comparable 'single crystal' or large grain size material. Thermoelectric generators employing thermocouples made from lead telluride alloys operate with a hot junction temperature of about 850 K and of interest is the behaviour of the thermoelectric figure of merit over the intended temperature range of operation of the device. In this note we report the results of our calculations of the effect of the reduction in lattice thermal conductivity on the thermoelectric figure of merit as a function of temperature.

Our objective is to estimate the improvement in the figure of merit rather than develop a rigorous theoretical model, and a number of simplifying assumptions have been made. A two band model with a parabolic multivalleyed structure is considered; acoustic lattice scattering is taken to be the dominant scattering mechanism; intervalley scattering is neglected and no distinction is made betweent he conductivity effective mass and density of states effective mass. Although the model adopted would be improved by considering non-parabolicity and including other scattering mechanisms such as polar optical; the results of preliminary calculations indicate that the predicted improvement in Z is relatively insensitive to the inclusion of these refinements in the model.

The equations used in calculating the thermoelectric figure of merit are cited in the literature (Ure 1972, Bhandari and Rowe 1980). The temperature dependences of effective mass m* and energy gap ε_g are taken into account (Ravich et al 1970) using

$$\frac{1}{m^*}\frac{dm^*}{dT} \quad \frac{1}{\varepsilon_g}\frac{d\varepsilon_g}{dT}$$

$$\varepsilon_g(T) = \varepsilon_g(T_o) + \frac{d\varepsilon_g}{dT}(T - 300)$$

with T_o = 300K, $d\varepsilon_g/dT = 4 \times 10^{-4}$, $m^* = 0.2m_o$ at 300K, λ_L at 300 K is 1.70 $Wm^{-1}K^{-1}$ and is assumed to vary inversely with temperature.

The variation of carrier concentration n with temperature is obtained by relating the variation of Seebeck coefficient with reduced Fermi potential (Gaur et al 1966) to the temperature dependence of the Seebeck coefficient for various carrier concentrations (Efimova et al 1971).

The results of our calculations are displayed in figure 1, where the thermoelectric figure of merit Z is plotted as a function of temperature and for three different carrier concentrations. Comparison is drawn between small grain size and 'single crystal' material.

It is concluded that the thermoelectric figure of merit of highly disordered lead telluride type material with a mean grain size of $\sim$1 μm is about 10% larger than equivalent 'single crystal' or large grain size material.

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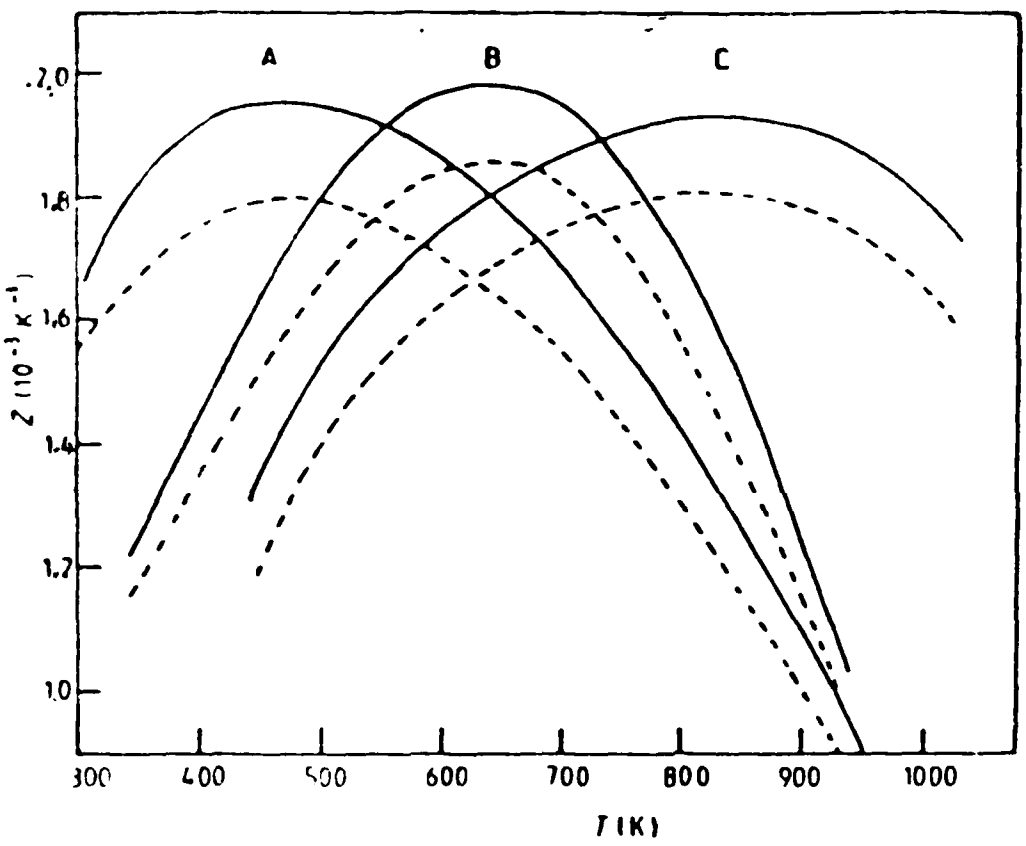

Figure 1. Plots of the thermoelectric figure of merit Z for a highly disordered alloy of lead telluride with three different carrier concentrations n, as a function of temperature: A, $n = 5 \times 10^{24}$ m^{-3}; B, $n = 10^{25}$ m^{-3}; C, $n = 2 \times 10^{25}$ m^{-3}. Curves: —— λ_t corresponds to material with a mean grain size ~ 1 μm; — — — — λ_t corresponds to 'single crystal' or large grain size material.

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