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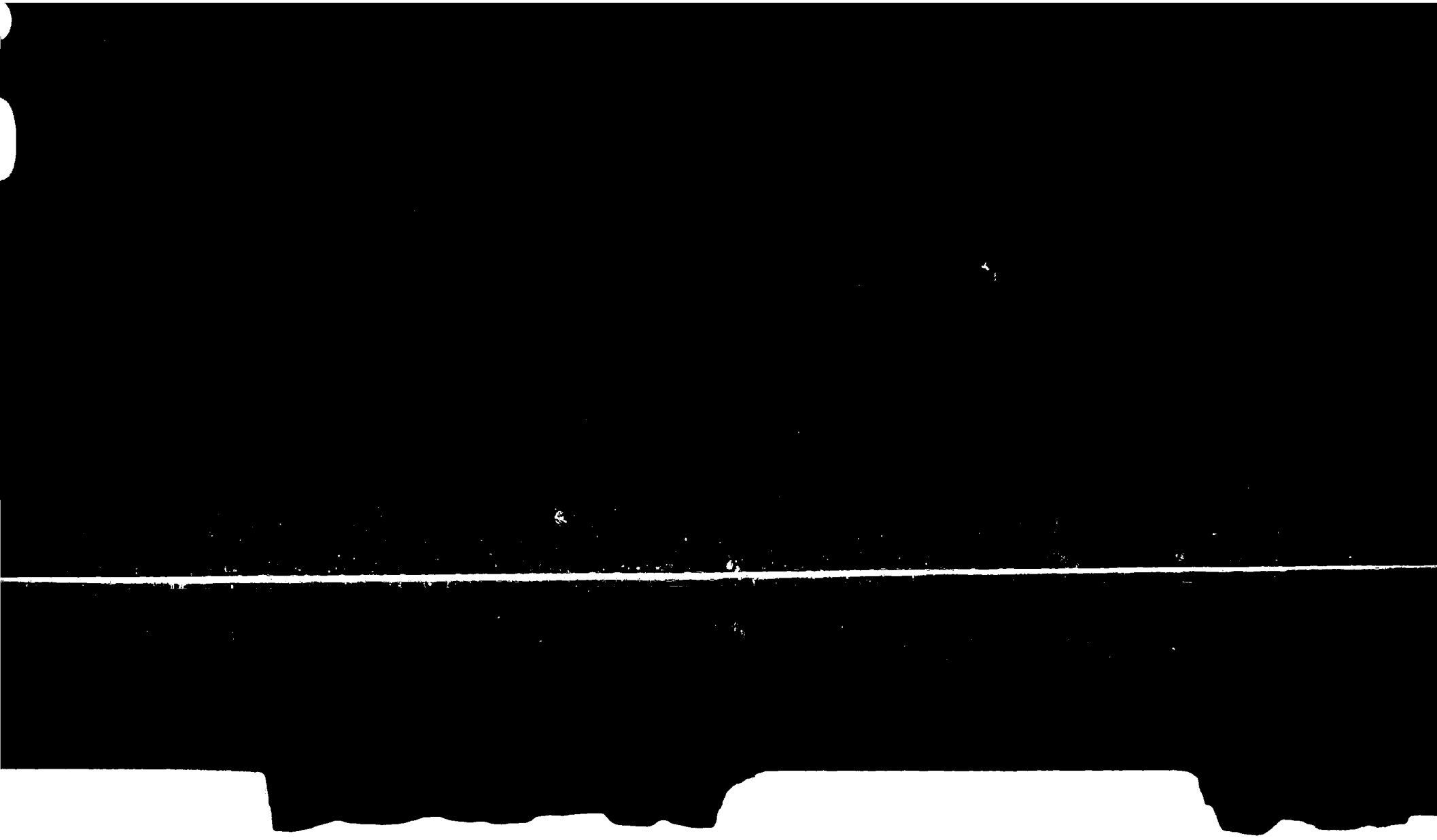

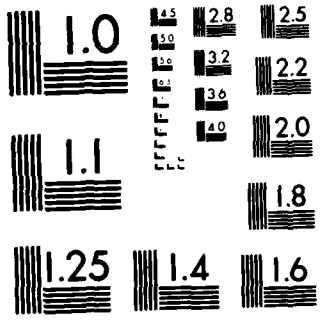

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OPTIMISATION OF THE THERMOELECTRIC FIGURE OF MERIT IN FINE GRAINED SEMICONDUCTOR MATERIALS BASED UPON LEAD TELLURIDE

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

1. Work Undertaken

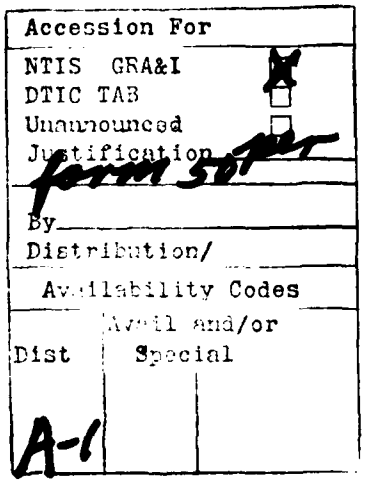
In the previous report (No.3) we presented the results of our investigation of the relative improvement in the thermoelectric figure of merit Z of alloys based upon lead telluride which accompanied the use of fine grain size material. The improvement in Z was calculated over the temperature range of operation of a device employing lead telluride technology and at three different carrier concentrations. It was concluded that the thermoelectric figure of merit of highly disordered lead telluride type material with a mean grain size of ~1μm was about 10 percent larger than equivalent "single crystal" or large grain size material.

As pointed out previously, the theoretical model employed, although adequate for use in obtaining estimates of the relative improvements in Z, the improvement in Z is rather insensitive to the values taken for parameters such as effective mass and to the nature of the energy serfaces, The next stage of our investigation i.e. identification of potentially good thermoelectric materials based upon lead telluride will require the development of a theorectical model which provides a realistic value for the absolute magnitude of Z. Such a model must include (1) The effect of a multivalley energy band structure (2) Non-parabolicity of the energy surface, (3) Combinations of scattering mechanisms.

In this report we present the results of our calculations of the effect of a multivalley energy band structure on the thermoelectric figure of merit. (Submitted to Physica Status Solidi). It is concluded that intervalley scattering significantly reduces the beneficial effect of a multivalley energy band structure. At optimum doping ($-1<\xi<0$) intervalley scattering reduces the ratio $(ZT)_{multivalley}/(ZT)_{single\ valley}$ by approximately 25%.

II. FUTURE PROGRAMME OF WORK

The theoretical model will be further refined by including non-parabolic energy surfaces.



THE EFFECT OF A MULTIVALLEY ENERGY BAND STRUCTURE ON THE THERMOELECTRIC FIGURE OF MERIT

It has been generally accepted for some considerable time that a semiconductor which possesses a multivalley energy band structure should exhibit a higher value of the thermoelectric figure of merit Z than a similar material which has only a single valley. A comparison of the measured Z values for thermoelectric semiconductors supports this view. Multivallied semiconductors such as bismuth telluride, lead telluride and silicon germanium alloys are the best materials over their temperature rangesof operation [1]. Previous analyses have shown that in the non-degenerate limit and neglecting intervalley scattering, the figure of merit increases monotonically with the number of valleys N_v [2,3]. In practicethermoelectric semiconductors are doped to relatively high carrier concentrations in order to optimise the materials thermoelectric properties. In the region of optimum doping, a multivalley energy band structure and intervalley scattering may have a significant effect on the figure of merit compared to that in the non-degenerate limit.

In this note we report the results of our calculations into the effect of intervalley scattering on the figure of merit of a multivallied semiconductor, as a function of carrier concentration (expressed in terms of reduced Fermi energy ξ).

The dimensionless figure of merit $(ZT)_{mv}$ for a multivalley energy band semiconductor can be expressed as:

$$(ZT)_{mv} = \frac{(\alpha'_e)^2 (\sigma_e')_{mv}}{1 + (\sigma_e' \Psi_e)_{mv}} \qquad (1)$$

where the symbols have the same meaning as in reference [1,4].Assuming that σ_e' is independent of the number of valleys and that the effect of intervalley scattering manifests itself primarily through the carrier mobility and electrical conductivity the effect of a multivalley energy band structure in ZT can conveniently be discussed in terms of the ratio:-

$$\frac{(ZT)_{mv}}{(ZT)_{sv}} = \frac{(\sigma_e')_{mv} \left\{1 + (\sigma_e' \Psi_e)_{sv}\right\}}{(\sigma_e')_{sv} \left\{1 + (\sigma_e' \Psi_e)_{mv}\right\}} \qquad (2)$$

In evaluating equation 2 as a function of ξ we have neglected optical phonon scattering. Intervalley scattering has been included following the method developed by Herring [5] who obtained an expression for the temperature dependence of carrier mobility as a function of W_2/W_1, W_2 and W_1

are measures of the strength of coupling of the charge carriers to intervalley and intravelley modes respectively. Although the model formulated is a general one we are specifically interested in thermoelectric alloys based upon lead telluride and the parameters taken are appropriate to that material.

The results of our calculations are presented in figure 1 where we have plotted the ratio $(ZT)_m/(ZT)_s$ at 300K as a function of ξ, with and without the inclusion of intervalley scattering. It is evident that in both cases the figure of merit is substantially increased in a multivallied structure. Although the effect of intervalley scattering on the figure of merit has been included in our calculations in an approximate manner we conclude that intervalley scattering significantly reduces the beneficial effect of a multi-valley energy band structure. At optimum doping ($-1<\xi<0$) intervalley scatterin reduces the ratio $(ZT)_m/(ZT)_s$ by approximately 25%.

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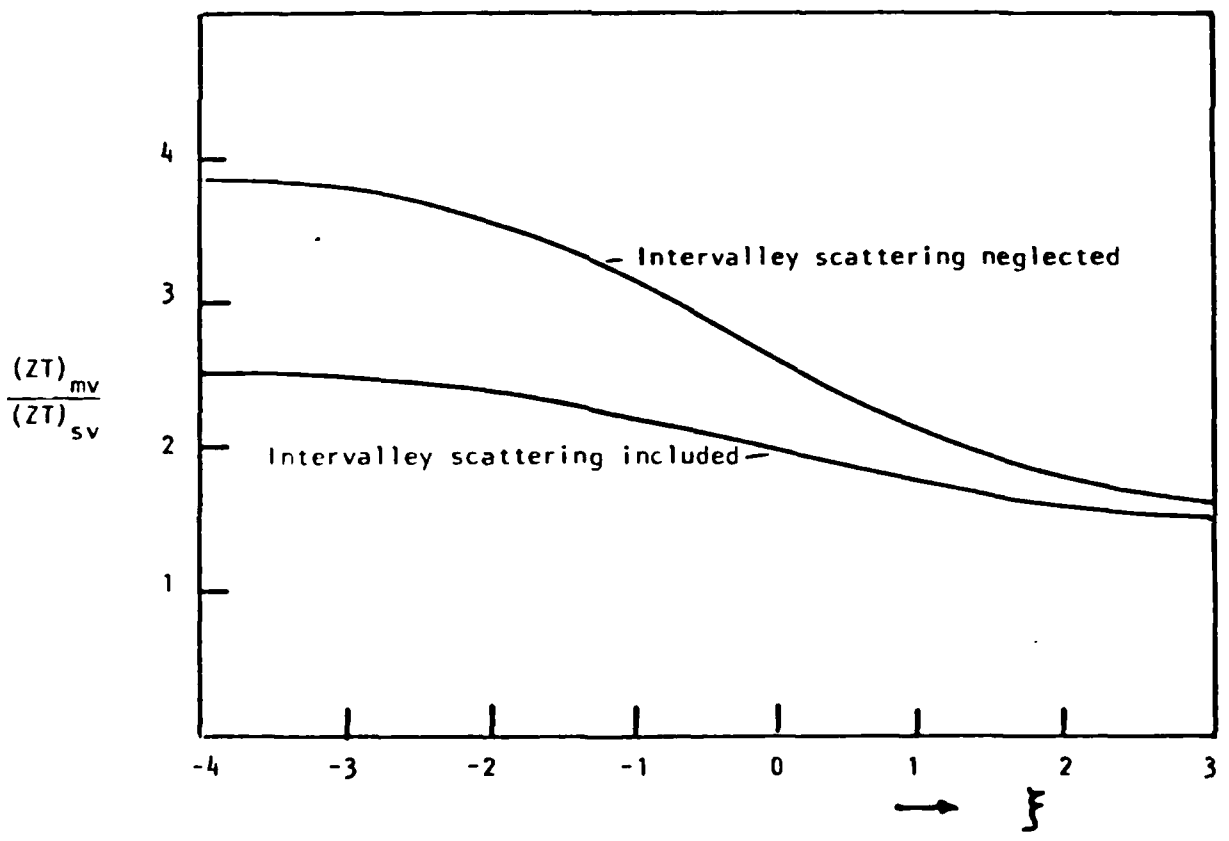
FIG 1. $(ZT)_{mv}/(ZT)_{sv}$ AS A FUNCTION OF REDUCED FERMI ENERGY ξ.



T = 300K; $N_v = 4$; $W_2/W_1 = 0.5$ is considered appropriate for disordered lead telluride

References:

1. D M Rowe and C M Bhandari, "Modern Thermoelectrics" , Holt, Rinehart and Winston, London (1983).

2. H J Goldsmid, A R Sheard and D A Wright, Brit. Journ. Appl. Phys. 9, 365, (1958).

3. R W Ure Jr. and R R Heikes, "Thermoelectricity; Science and Engineering (Ed. R P Heikes and R W Ure Jr.) Interscience, New York, (1961).

4. R W Ure, Jr., Energy Conversion, 12, 45 (1972).

5. C Herring, Bell Systems, Tech. J., 34, 237, (1955).

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