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Optimization of the Thermoelectric Figure of Merit of Modified Silicon Germanium Alloys

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OPTIMISATION OF THE THERMOELECTRIC FIGURE OF MERIT OF MODIFIED SILICON GERMANIUM ALLOYS

1. **Introduction**

alpha Squared Sigma

In this report a working theoretical model for the power factor ($\alpha^2\sigma$) of silicon germanium alloys is presented and the dependence of this parameter on carrier concentration and number of valleys explored.

2. **Outline of theoretical model**

Although silicon-germanium alloys cannot be described as narrow band gap semiconductors, the high level of doping employed in thermoelectric applications necessitates the inclusion in the theoretical model of deviations from the usually assumed parabolic bands. Non-parabolicity of the bands is usually represented in terms of a parameter $\beta = k_\beta T/E_g$, where k_β is Boltzmann constant, T the absolute temperature and E_g the energy band cap. The electrical transport properties are expressed in terms of the generalised Fermi integrals defined by:-

$$ {}_{n}L^{m}_{\ell} = \int_0^\infty \left(-\frac{\partial f}{\partial \eta}\right) . \eta^{n}\left(\eta(1+\beta.\eta)^{\ell}\right).d\eta $$

where f is the usual Fermi distribution, $\eta = E/k_\beta T$ is the reduced carrier energy n, m and l are numbers which take different values for various parameters and scattering mechanisms. At room temperature and above, acoustic phonon scattering is the most important carrier scattering mechanism. In the initial model intervalley scattering (IVS) has been neglected. This is a reasonable approximation as IVS involves high energy phonons which are excited only at high temperatures.

The Seebeck coefficient is given by:

$$ \alpha = \frac{k_\beta}{e}(\delta - \xi) $$

where $\delta = {}^{1}L^{1}_{-2}/{}^{1}L^{0}_{-2}$

and the carrier concentration $n = N_v \frac{1}{3.\pi^2}\left(\frac{2m^*_{ds}\, k_\beta T}{h^2}\right)^{3/2} {}^{0}L^{3/2}_{0}$

where m_{ds}^{*} is the density of states effective mass for a single valley, and N_v, the number of valleys.

The reduced electrical conductivity defined by $\sigma' = \left(\frac{k_\beta}{e}\right)^2 \frac{T}{\lambda_L}\sigma$ is given by $\sigma' = \left[\frac{k_\beta{}^2 hC_{11}}{3\pi^2\epsilon_1{}^2}\right] N_V \; {}^{0}L^{1}_{-2} \; \frac{T}{(m_C{}^{*}\lambda_L)}$

Various terms have their usual meanings.

The electrical power factor is given by:

$$\alpha^2\sigma = \frac{k_\beta{}^2 hC_{11}}{3\pi^2\epsilon_1{}^2}\,\frac{N_V}{m_C{}^{*}}\;{}^{0}L^{1}_{-2}\;(\delta - \xi)$$

values for various parameters employed in the calculations are given in Table 1

Table 1

E_g(eV)	m_{ds}^{*}/m_0	m_C^{*}/m_0	c_{11} (Nm^{-2})	ϵ_1 (eV)	λ_L ($Wm^{-1}deg^{-1}$)
1.132	0.29	0.26	1.7×10^{11}	6.2	5.0

3 Results

The dependence of the Seebeck coefficient (α), electrical conductivity (σ) and the power factor ($\alpha^2\sigma$) on carrier concentration and number of valleys N_V are presented in figures 1-5.

4 Conclusions

Two main conclusions can be drawn from the reported results.

1. A large number of equi-energetic valleys give rise to a higher power factor at room temperature, when intervalley scattering can be considered negligibly small.
2. Higher doping levels are required in order to take advantage of the large number of valleys.

5 General Conclusion

A working theoretical model has been developed for silicon-germainium alloys and employed in investigating the dependence of the power factor on carrier concentration and number of valleys. The effect of intervalley scattering should be taken into account if N_v is large, even at room temperature. At higher temperatures, both intra- and intervalley scattering should be considered. The theoretical model will be refined to take these factors into consideration, and the analyses extended to explore the dependence of the power factor on alloy composition.

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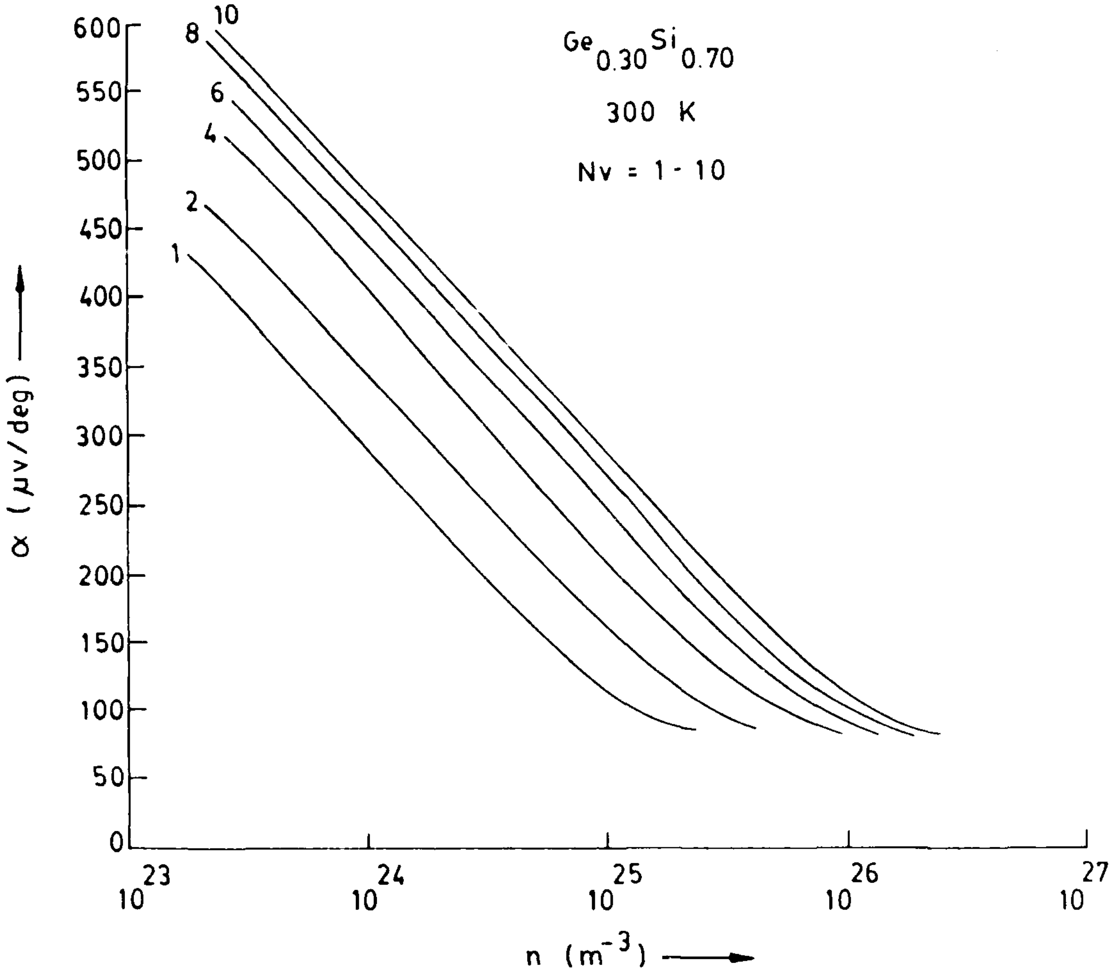

Figure 1

Variation of α with carrier concentration and number of valleys

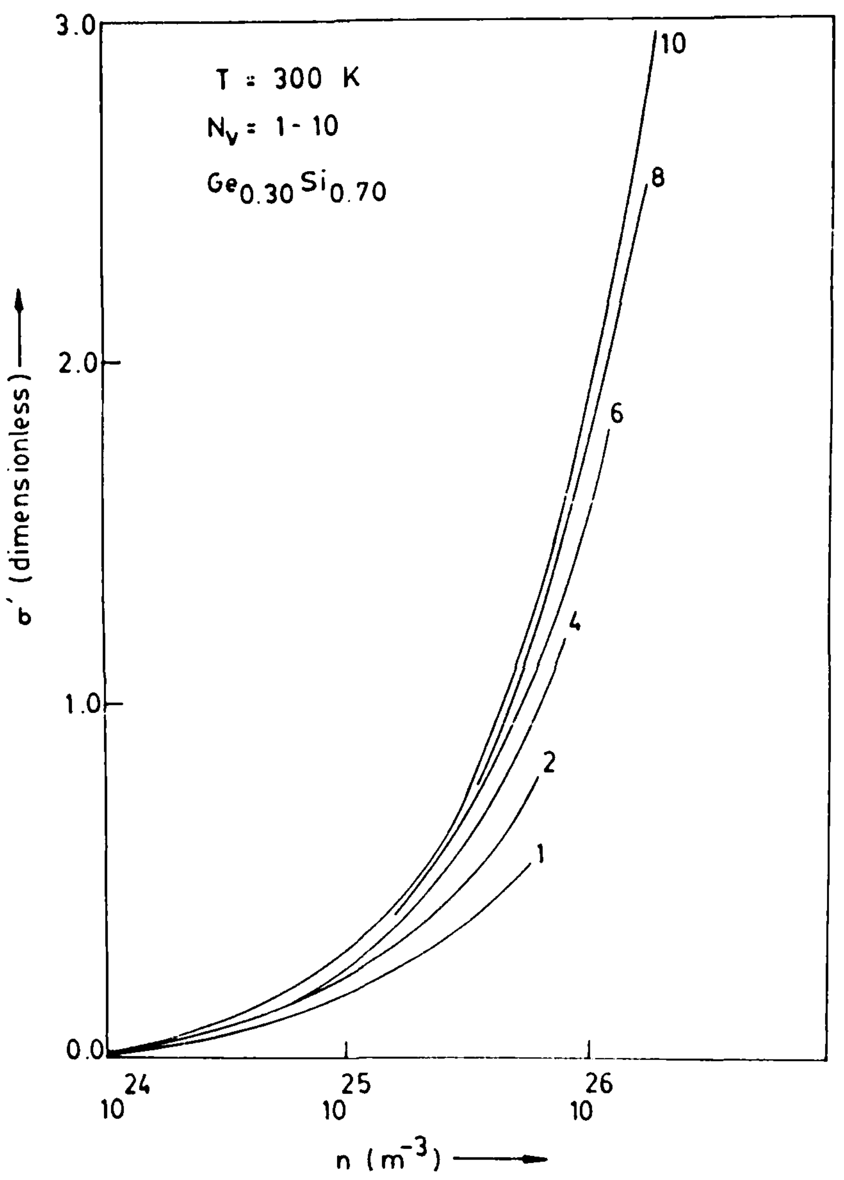

Figure 2

Variation of σ' with carrier concentration
and number of valleys

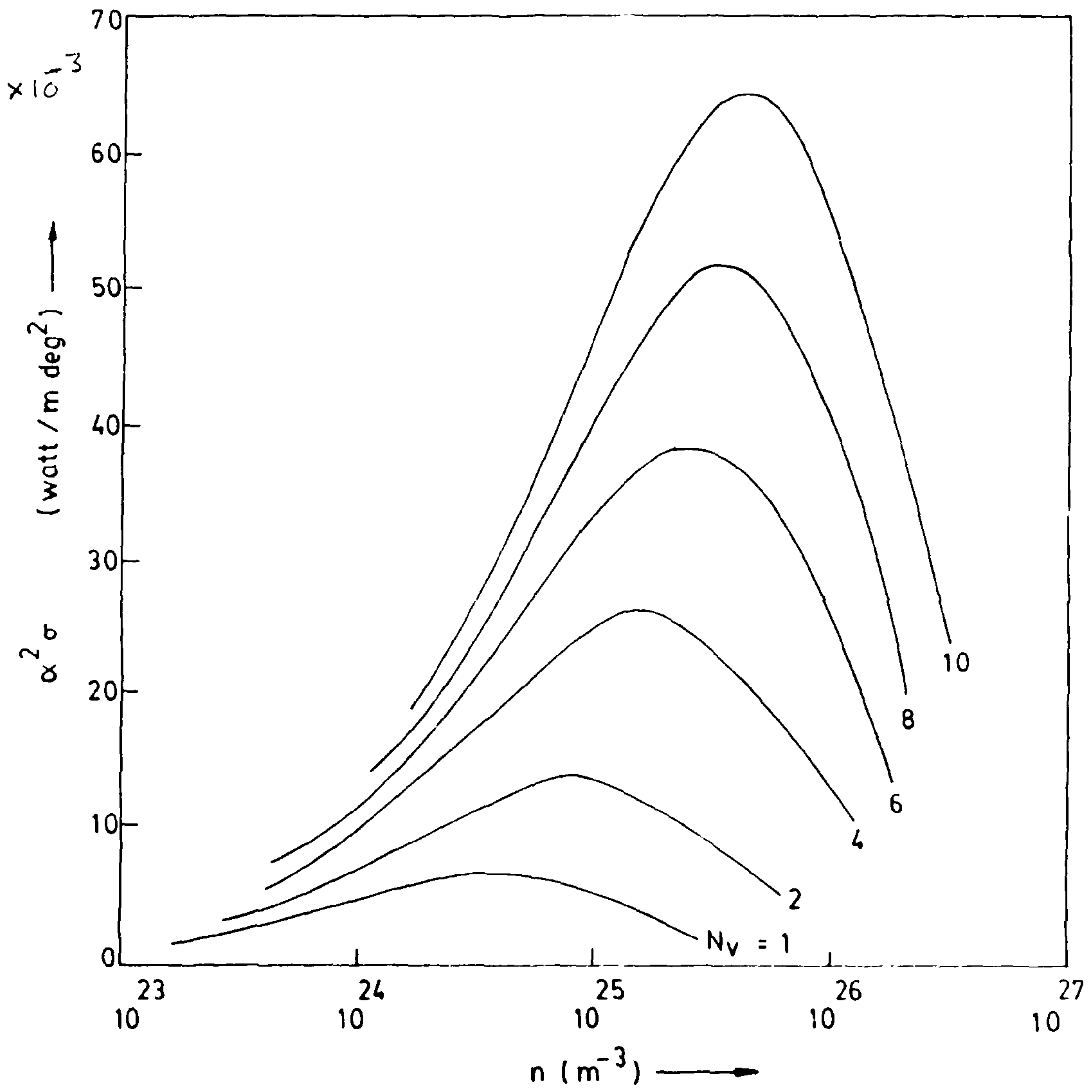

Figure 3

Variation of $\alpha^2\sigma$ with carrier concentration
and number of valleys

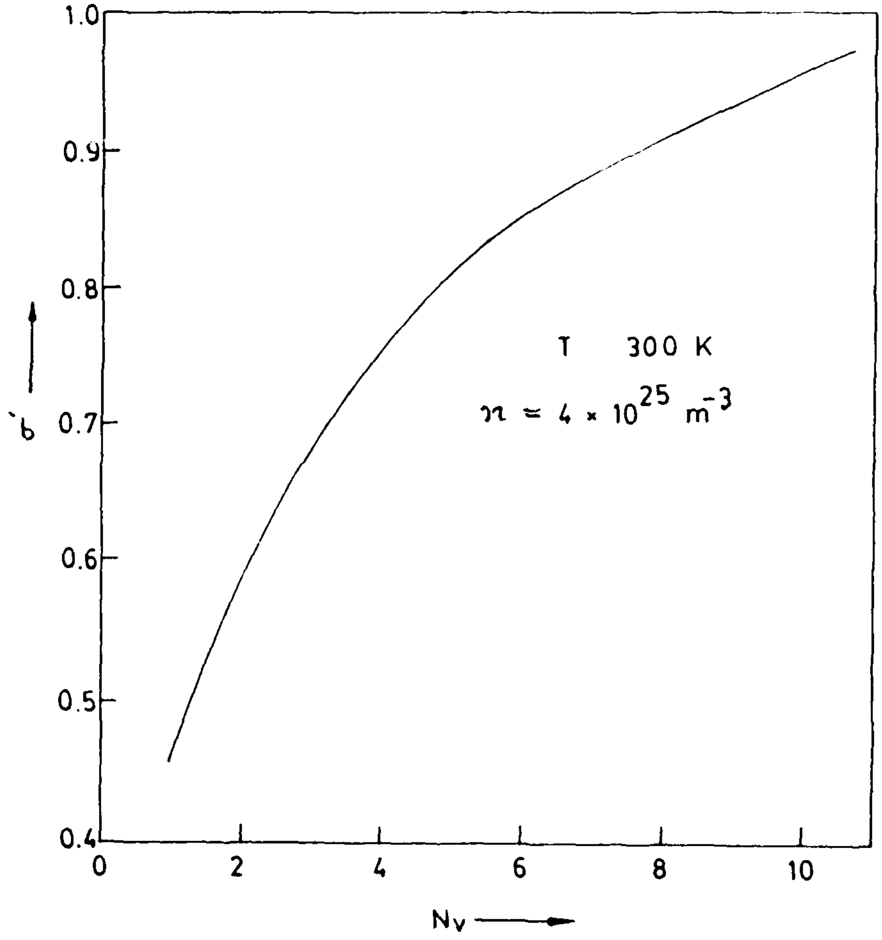

Figure 4

Variation of σ' with number of valleys

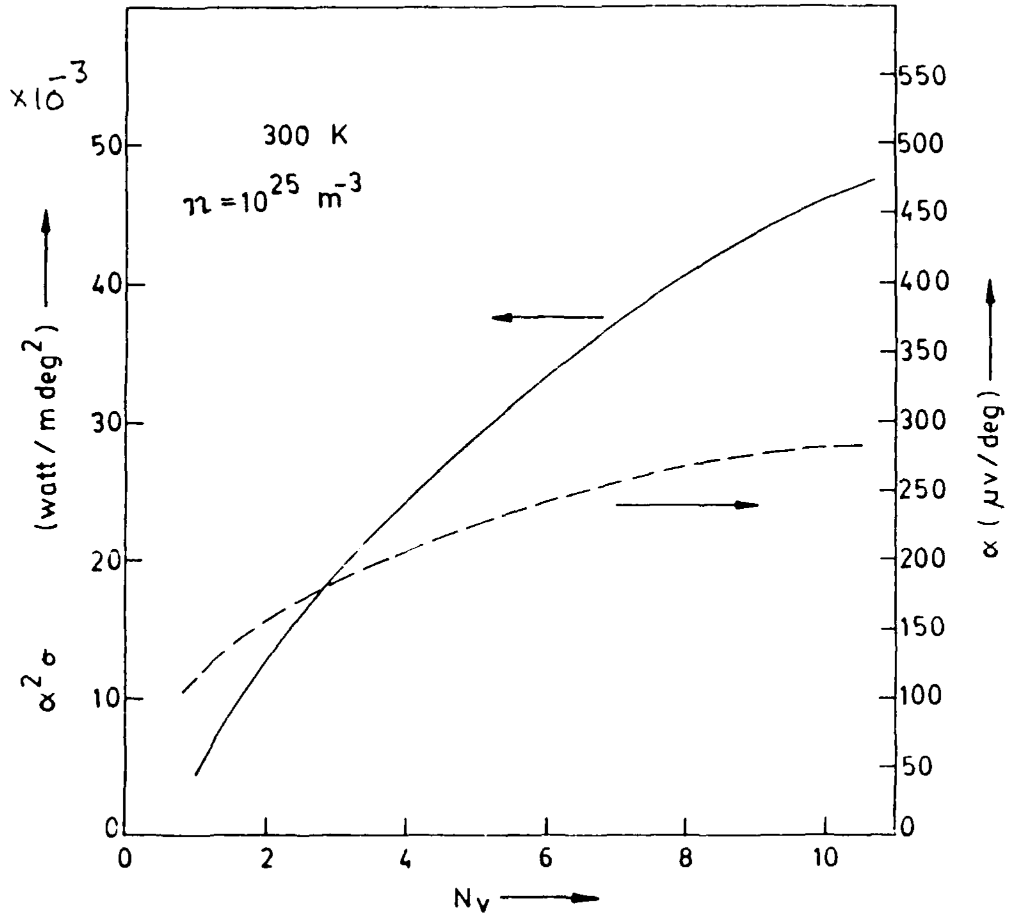

Figure 5

Variation of $\alpha^2\sigma$ and α with number of valleys