SUBJECT: APPROXIMATE THERMOELECTRIC PROPERTIES OF SILICON GERMANIUM AS A FUNCTION OF DOPANT CONCENTRATION, PARTICLE SIZE AND TEMPERATURE

FROM: CRONIN VINING

TO: WALT KUGLER

DATE: 4/1/87

The attached pages describe a technique for calculating the thermoelectric properties of 80% Si- 20% Ge as a function of dopant level (parameterized by N), temperature (parameterized by T) and particle size (parameterized by f) for both n-type and p-type material. The primary purpose of this exercise was to provide sufficient information to the design of the SP-100 TEM pump to allow for the approximate optimization of the dopant level for that application. While I have tried to take into account most of the major physical effects, obviously these results are not complete. In particular, these results neglect dopant precipitation effects, the effect of dopant concentration on the lattice contribution to the thermal conductivity and the effect of dopant concentration on the carrier mobilities. I have tried to pay particular attention to the relationship between the electrical resistivity and the Seebeck coefficient and believe that relationship is reasonably well represented here.

These data should not be used for final design purposes. If, for example, device design tradeoffs based upon these data indicate a much lower carrier concentration, or a lower thermal conductivity/higher electrical resistivity combination (as determined by the particle size parameter, f) is significantly more desirable for the TEM pump application than materials optimized for electrical power generation applications, then considerable materials development activities will be required to provide a verified materials properties database. These data are primarily intended as an initial estimate of the possible tradeoffs in order to determine whether the materials development activities are warranted. Design studies based upon other data should not be compared to design studies based upon these data in any absolute sense, since absolute values are not expected to be quantitatively reliable. Trends based upon these data, however, are expected to be reliable and realizable in practice.

A. Proceedure For Estimating Seebeck and Resistivity for $Si_{0.8}Ge_{0.2}$ As a Function of Dopant Concentration and Temperature

1. Select Temperature (T) and Dopant Concentration ($N > 0$ means p-Type; $N < 0$ means n-Type)

2. Calculate electron mobility using 1 + 2

3. Calculate hole mobility using 3 + 4

4. Calculate intrinsic carrier concentration using 5

5. Calculate minimum conductivity using 6

6 Calculate electrical conductivity using 7 and 8

7. Calculate the seebeck coefficient using 9

Notes: - Different carrier concentrations may be used in n-leg and p-leg.

- These results should reasonably reproduce the effect of varying the carrier concentration but should not be expected to be quantitatively reliable.

Estimate of Carrier Mobility

holes; Use data from ITM-131A, p-Type

$n = 1.64 \times 10^{20}\ \mathrm{cm}^{-3}$

(1)
$$\begin{aligned}\rho_+ = \ & 1.09216 \\ & + 1.88363 \times 10^{-3}\, T \\ & - 2.10473 \times 10^{-6}\, T^2 \\ & + 1.33956 \times 10^{-8}\, T^3 \\ & - 3.00512 \times 10^{-11}\, T^4 \\ & + 3.18578 \times 10^{-14}\, T^5 \\ & - 1.28058 \times 10^{-17}\, T^6\end{aligned}$$

T in °C

milliohm-cm

(2)
$$\mu_+ = \frac{1}{n e \rho_+} = \frac{\overset{38.11}{\cancel{3.811 \times 10^{-2}}}}{\rho_+}$$

$\mathrm{cm}^2/\mathrm{V\text{-}s}$

electrons; use data from ITM-16, n-Type

$n = 1.38 \times 10^{20}$

(3)
$$\begin{aligned}\rho_- = \ & 0.8698 \\ & - 1.155 \times 10^{-4}\, T \\ & + 2.157 \times 10^{-5}\, T^2 \\ & - 9.145 \times 10^{-8}\, T^3 \\ & + 1.864 \times 10^{-10}\, T^4 \\ & - 1.736 \times 10^{-13}\, T^5 \\ & + 5.927 \times 10^{-17}\, T^6\end{aligned}$$

T in °C

milliohm-cm

(4)
$$\mu_- = \frac{1}{n e \rho_-} = \frac{\overset{45.29}{\cancel{4.529 \times 10^{-2}}}}{\rho}$$

$\mathrm{cm}^2/\mathrm{V\text{-}s}$

Estimate of Band Gap and Minimum Electrical Conductivity From 10/86 ITM Monthly

Use acoustic mode scattering

$$\frac{E_g}{kT} + A_+ + A_- = \frac{E_g}{kT} + 2A = 11.01$$

$$\frac{E_g}{k} = 8412 \ K^{-1}$$

$$n_i = B\,T^{3/2} e^{-E_g/2k_BT}$$

$$\sigma_{min} = 2 n_i e (\mu_+ \mu_-)^{1/2}$$

$$= 61.7 \ \text{ohm}^{-1}\text{cm}^{-1} \ \text{at} \ 1200\,K$$

From ① through ④

$$\mu_+(1200\,K) = 11.93 \ cm^2/V\text{-}s$$

$$\mu_-(1200\,K) = 15.76 \ cm^2/V\text{-}s$$

⑤ $$\boxed{n_i = 1.1246 \times 10^{16}\, T^{3/2} e^{-4206/T} \ cm^{-3}, \ T \text{ in Kelvin}}$$

⑥ $$\boxed{\sigma_{min} = 3.204 \times 10^{-19}\, n_i (\mu_+ \mu_-)^{1/2} \ \text{ohm}^{-1}\text{cm}^{-1}}$$

OK

Estimate of Electrical Conductivity as a Function of Dopant Concentration and Temperature

(7) $$\boxed{\sigma_0(N,T) = n_i e \left(a\mu_+ + \frac{1}{a}\mu_-\right)}$$ in $ohm^{-1} cm^{-1}$

$e = 1.602 \times 10^{-19}$ coulomb

(8) $$\boxed{a \equiv \frac{1}{2} n_i^{-1} \left[\left(N^2 + 4n_i^2\right)^{1/2} + N \right]}$$ unit less

$N > 0 \Rightarrow$ p-Type sample

$N < 0 \Rightarrow$ n-Type sample

N may vary from about

$+3 \times 10^{20}$ to -2×10^{20}

Estimate of the Seebeck Coefficient as a Function of Dopant Concentration and Temperature

$$S = \pm \frac{k}{2e}\left(\frac{E_g}{kT} + A_+ + A_-\right)\left(1 - \frac{\sigma_{min}^2}{\sigma_0^2}\right)^{1/2} - \frac{k}{e}\ln\left[\frac{\sigma_0}{\sigma_{min}}\left(1 \pm \left(1 - \frac{\sigma_{min}^2}{\sigma_0^2}\right)^{1/2}\right)\right] + \frac{k}{2e}\ln\left[\frac{N_+ e^{A_+} \mu_+}{N_- e^{A_-} \mu_-}\right]$$

Use $\dfrac{N_+ e^{A_+} \mu_+}{N_- e^{A_-} \mu_-} = 0.59$

use upper sign for p-Type materials $(N > 0)$

use lower sign for n-Type materials $(N < 0)$

9

$$\boxed{S = \cancel{8}\,86.19\left[\pm\left(\frac{4206}{T} + 2\right)\left(1 - \frac{\sigma_{min}^2}{\sigma_0^2}\right)^{1/2} - \ln\left[\frac{\sigma_0}{\sigma_{min}}\left(1 \pm \left(1 - \frac{\sigma_{min}^2}{\sigma_0^2}\right)^{1/2}\right)\right] - 0.264\right] \ \mu V/K}$$

T in Kelvin

B. Proceedure for Estimating the Thermal Conductivity for $Si_{0.8}Ge_{0.2}$ As A Function of Temperature and Dopant Concentration

1. Calculate the electrical conductivity, σ_0, as in A

2. Calculate the electronic contribution to k_0 using 10

3. Calculate the lattice contribution using 11

4. Calculate the total using 12

Estimate of the Electronic Contribution to the Thermal Conductivity.

$$k_{el} = \left(\frac{k}{e}\right)^2 \sigma_o T \left\{ \frac{A_+ \sigma_+ + A_- \sigma_-}{\sigma_o} + \frac{n_i^2 e^2 \mu_+ \mu_-}{\sigma_o^2} \left[A_+ + A_- + \frac{E_g}{k_B T} \right]^2 \right\}$$

Take $A_+ = A_- = 2$, acoustic mode scattering

$$2.053 \times 10^{-37}$$

10 $$\boxed{k_{el} = 1.486 \times 10^{-\cancel{6}\,5} \sigma_o T \left\{ 1 + \cancel{5.133 \times 10^{-38}} \frac{\mu_+ \mu_- n_i^2}{\sigma_o^2} \left[1 + \frac{2103}{T} \right]^2 \right\}}$$

mW/cm-K

T in Kelvin

Estimate of the Lattice Contribution to The Thermal Conductivity

The lattice portion of the thermal conductivity of Sample ITM-93 has been calculated from the measured total thermal conductivity, the measured electrical resistivity and equation 10.

(11) $$\boxed{\begin{aligned} k_\ell = {} & 50.893 \\ & - 0.04115\, T \\ & + 2.0169\times10^{-5}\, T^2 \end{aligned} \qquad \begin{aligned} &T \text{ in Kelvin} \\ &\text{mW/cm-K} \end{aligned}}$$

(12) $$\boxed{k_0 = k_\ell + k_{el}}$$

Since the effect of doping on the lattice thermal conductivity has been ignored, 12 will underestimate k_0 for low dopant levels. This effect is small at 1300K, but may be 25% at 800K.

C. Particle Size Effects on the thermoelectric properties of $Si_{0.8}Ge_{0.2}$.

1. Select the Dopant concentration (N), and Temperature (T)

2. Calculate seebeck, Electrical Conductivity and Thermal Conductivity as in A and B

3. Select a particle size scaling factor f such that $0.5 \leq f \leq 1.1$

4. Calculate the final electrical conductivity as

$$\boxed{\sigma = f\,\sigma_0}$$

5. Calculate the final thermal conductivity as

$$\boxed{k = f\,k_0}$$

Note: $f = 0.5$ corresponds to a very fine particle size while $f = 1.1$ corresponds to zone-leveled materials. The Seebeck is unaffected by particle size.