Phonon Drag in SiGe Thermoelectric Alloys

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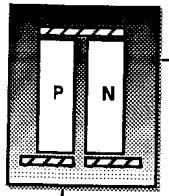
APS March Meeting
Kansas City
Tuesday March 18, 1997

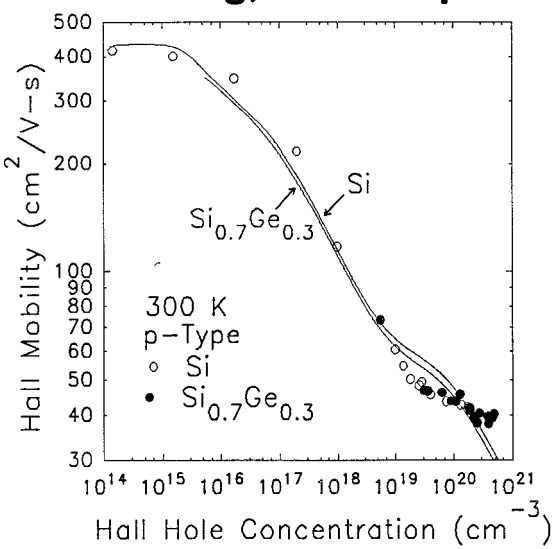


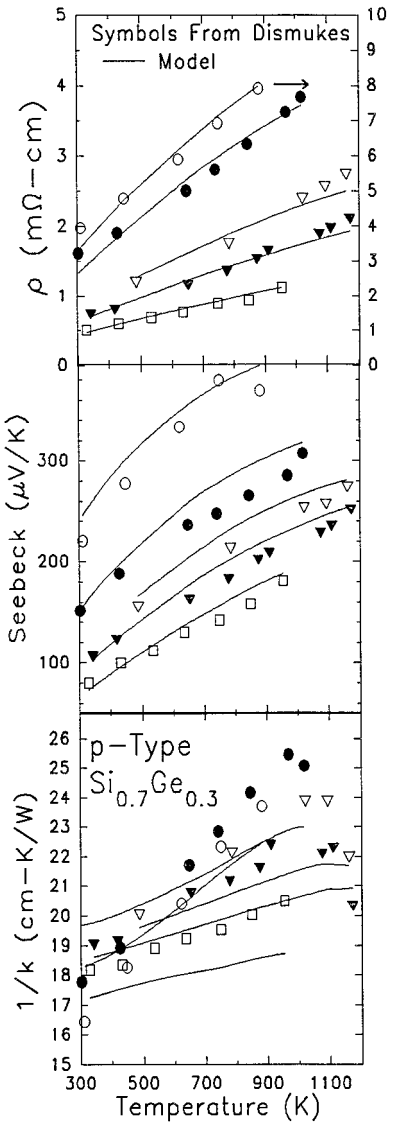
Introduction

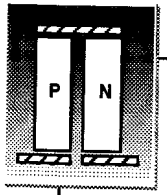
- Phonon-drag is routinely neglected and generally considered small in thermoelectric materials where
  - lattice thermal conductivity is small due to alloying
  - doping level and temperature are relatively high
- But Klemens recently estimated the phonon drag thermopower (S_g) as large as k/e (=86 μV/K) at 900 K
  - Klemens, Proc. XV Int.Conf. on Thermoelectrics, 1996, p. 206.
- Calculate S_g and effect on ZT using
  - simple expressions for S_g due to Klemens & Ziman
  - transport model previously developed for SiGe alloys
    - » *no new adjustable parameters*

Transport in SiGe

- **Previously modeled electrical and thermal transport in Si-Ge alloys over a range of composition, temperature and doping level.**
  - **n-type: Vining, J. Appl. Phys. 69, 331 (1991).**
  - **p-type: Vining, MRS Symp. Vol. 234, 95 (1991).**
- **Reproduces experiment with RMSD ~10%**
- **Neglected Phonon-drag, low Temperature S data.**







Phonon Drag Expressions

$$S_g = \frac{3k}{e}\frac{N}{n}\left(\frac{T}{\Theta}\right)^3 \int_0^{\Theta/T} \frac{x^4 e^x}{\left(e^x - 1\right)^2} \frac{\tau_{ep}^{-1}}{\tau_{total}^{-1}} dx$$

τ_{ep}^{-1} = rate that phonons are scattered by electrons

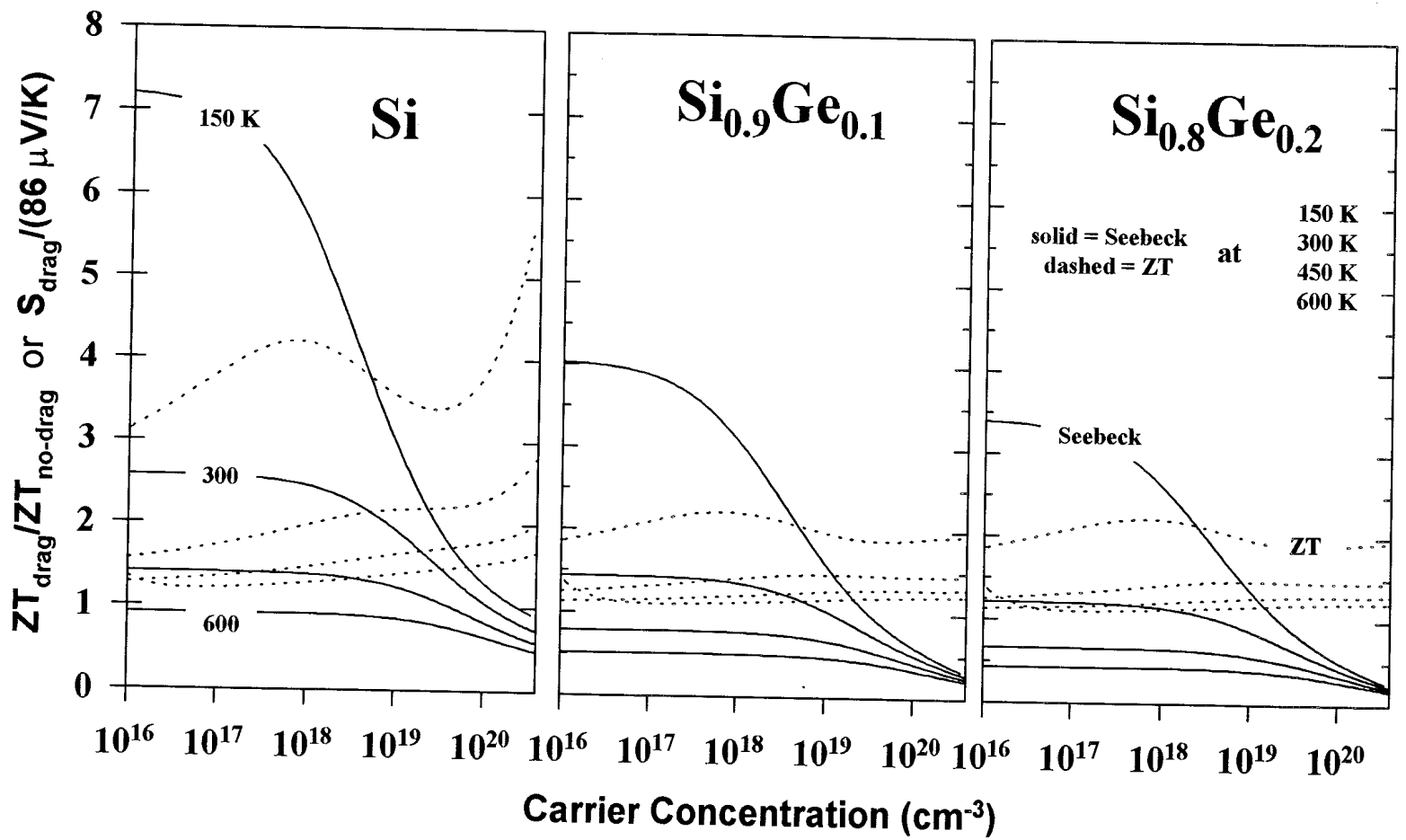
$\tau_{total}^{-1} = \tau_{ep}^{-1} + \tau_{pp}^{-1} + \text{etc.}$

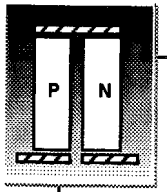
= total phonon scattering rate

$S_g \propto \frac{N}{n}$

$S_g \propto \frac{\lambda_{lattice}}{\mu}$

Phonon Drag


Si
$Si_{0.9}Ge_{0.1}$
$Si_{0.8}Ge_{0.2}$
150 K
300
600
Seebeck
ZT
solid = Seebeck
dashed = ZT
at
150 K
300 K
450 K
600 K
$ZT_{drag}/ZT_{no\text{-}drag}$ or $S_{drag}/(86\ \mu V/K)$
0
1
2
3
4
5
6
7
8
10^{16} 10^{17} 10^{18} 10^{19} 10^{20}
Carrier Concentration (cm^{-3})



Conclusions

- Phonon drag can represent a significant contribution to ZT
  - even at high temperatures
  - even at high doping levels
  - even in alloys
- Quantitative evaluation of ZT requires consideration of drag effect
- A unified, quantitative model for the thermoelectric/transport properties of Si is not presently available

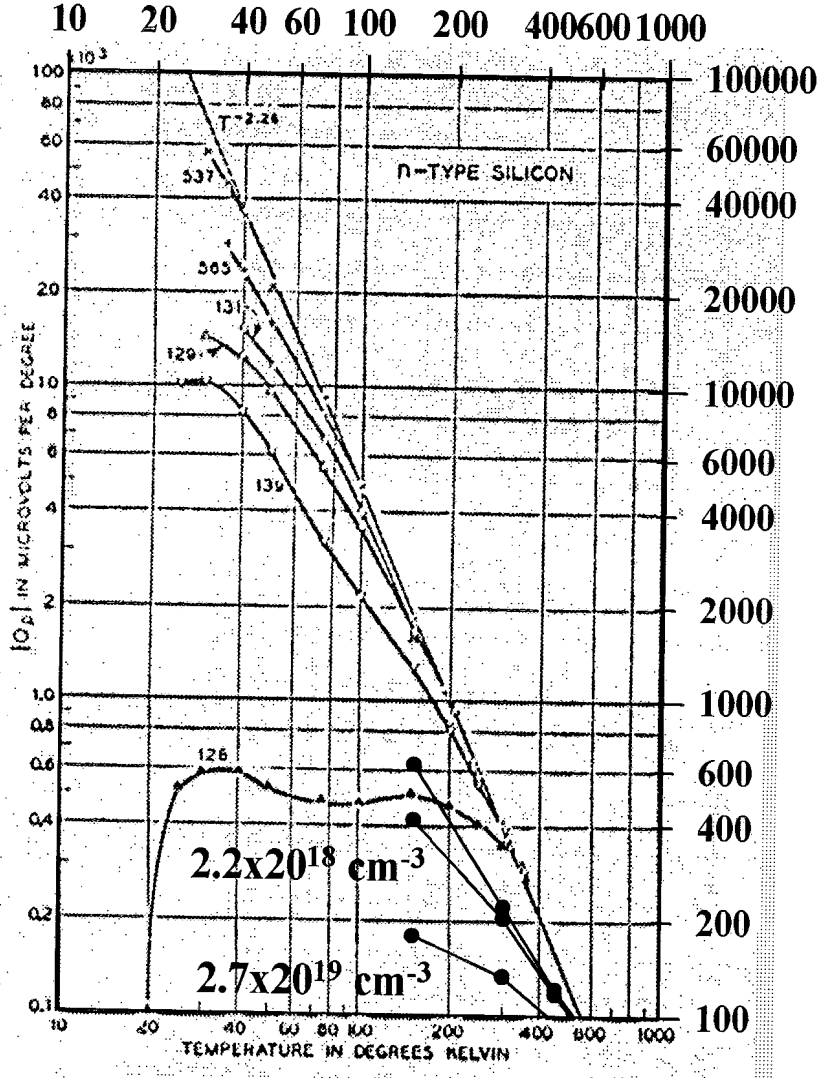


FIG. 3. Dependence of Q_p upon temperature for n-type samples which differ in size or donor concentration.

S_g in Si

From Geballe and Hull, Phys Rev. 98(4), 940 (1955)