Si-Ge Nano-structured with Tungsten Silicide Inclusions

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NASA Cooperative Agreement: NNX08AB43A
### Objectives

- Investigate composite strategies with proven Si/Ge thermoelectrics.
- Validate theoretical modeling for silicide inclusion in Si/Ge, requires 10nm inclusions.
- Develop reliable uncertainty analysis for thermoelectric transport properties.
- Study thermal stability of composites.

### Material ZT

\[
ZT = \frac{\alpha^2 \sigma}{\lambda} T
\]

\[
\lambda = \lambda_{Elec.} + \lambda_{Lattice}
\]

### Test Matrix

<table>
<thead>
<tr>
<th>Si/Ge at% Ratio</th>
<th>2% Dopant</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>P-Type, B</td>
</tr>
<tr>
<td>70/30</td>
<td>0%</td>
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**Tungsten Silicide Volume Fraction**

- 0%
- 1%
- 2%
- 5%
Objectives

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• Validate theoretical modeling for silicide inclusion in Si/Ge, requires 10nm inclusions.
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Si-Ge with Tungsten Silicide Inclusions
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Powder Processing

- Planetary Milling
  - 8 Hours @ 300-580 rpm
  - Ball to powder ratio 3-5
- Spark Plasma Sintering (AFRL)
  - 800-1100°C @ 70-90 MPa
  - 5-10 min Hold

SEM

XRD

1” Diameter
Sources of Error

<table>
<thead>
<tr>
<th>Source</th>
<th>Magnitude</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermocouple radius</td>
<td>0.25 mm</td>
</tr>
<tr>
<td>Sample uniformity</td>
<td>±0.1 mm</td>
</tr>
<tr>
<td>Thermocouple separation</td>
<td>±0.1 mm</td>
</tr>
<tr>
<td>Caliper resolution</td>
<td>0.01 mm</td>
</tr>
<tr>
<td>Statistical variation</td>
<td>Calculated</td>
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<tr>
<td>DAQ voltage uncertainty</td>
<td>50ppm+1.2µV</td>
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<tr>
<td>DAQ current uncertainty</td>
<td>0.2%+0.3mA</td>
</tr>
<tr>
<td>Cold-finger effect</td>
<td>Calculated</td>
</tr>
<tr>
<td>Wire Seebeck variation</td>
<td>±3 %</td>
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<tr>
<td>Absolute temperature</td>
<td>±2 K</td>
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- 80/20
- 90/10

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2% Doped
- P-type, B
- N-type, P

Error Bars

Typical
Si-Ge with Tungsten Silicide Inclusions

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Si/Ge at% Ratio
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Tungsten Silicide Volume Fraction
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Oxygen (at%)
- Melt P-Type
- SPS P-Type
- SPS N-Type

RTG P-Type
- RTG N-Type

Temperature (Celsius)

Results
Si-Ge with Tungsten Silicide Inclusions

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Figure of Merit (ZT)
Si-Ge with Tungsten Silicide Inclusions

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**Introduction**

**Processing**

**Uncert.**

**Results**

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**Carrier Concentration (cm^-3)**

**N-Type**

- Start
- End
- Reset

**P-Type**

- Start
- End
- Reset

- Never fully recovers

- Dopant Segregated
- Dopant Re-distributed

**Resistivity (Ohm-cm)**

**Temperature (Celsius)**

- Cooling
- Heating

**Doped**

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Conclusion

• Silicide phase successfully reduces lattice thermal conductivity.
• Increased ZT for silicide composites as compared to baseline Si/Ge.
  • Need to control oxygen contamination to match baseline Si/Ge to RTG.
• Tungsten silicide phase offers tuning of carrier concentration.
• Silicide phase does not hinder thermal stability.

Acknowledgements

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AFRL Wright Patterson Air Force Base

Dr. Sabah Bux, Dr. Jean-Pierre Fleurial
JPL

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