NIST Metallurgy Division
Computational Thermodynamics
Projects and Databases

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SGTE Meeting
December 4, 2000
MPI-MF Stuttgart

Metallurgy Division Staff Involved in Phase Diagram Research

William J. Boettinger: process modeling
Carelyn E. Campbell: diffusion modeling
Albert V. Davydov: semiconductor systems
Ursula R. Kattner: databases and software
Kil-Won Moon: experimental studies
Current Projects

- Solder alloys
  - equilibrium diagrams and solidification path
- Superalloys
  - solidification modeling
  - homogenization modeling
- Compound-semiconductor - metal contacts
  - p-T-x phase diagrams
  - metallization path evaluation
- Compilation of public domain databases

Solder Database under Development

**Sn, Ag, Bi, Cu, In, Pb, Sb, Ga, Zn, Al, Au, Ge, Si**

- 7 component database adequate for most solder alloys
- 9 component database - intermediate goal
- 13 component database - long term goal
- assessments from literature or NIST

<table>
<thead>
<tr>
<th>Elements in Database</th>
<th>Binary Subsystems</th>
<th>Ternary Subsystems</th>
<th>Sn-base Ternary Subsystems</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>21 (21 done)</td>
<td>36 (11 done)</td>
<td>15 (7 done)</td>
</tr>
<tr>
<td>9</td>
<td>36 (34 done)</td>
<td>94 (12 done)</td>
<td>28 (8 done)</td>
</tr>
<tr>
<td>13</td>
<td>78 (72 done*)</td>
<td>286 (21 done)</td>
<td>66 (10 done)</td>
</tr>
</tbody>
</table>

* 22 of the 72 may need readjustment
Current State of the Solder Database

- **Ag, Bi, Cu, Pb, Sn**
  - all binary descriptions evaluated
  - state of ternary descriptions
    - Ag-Bi-Cu  extrapolated
    - Ag-Bi-Pb  extrapolated
    - Ag-Bi-Sn  extrapolated
    - Ag-Cu-Pb  assessed
    - Ag-Cu-Sn  partially assessed
    - Ag-Pb-Sn  extrapolated
    - Bi-Cu-Pb  extrapolated
    - Bi-Cu-Sn  extrapolated
    - Bi-Pb-Sn  assessed
    - Cu-Pb-Sn  extrapolated

  * data indicate that ternary excess parameter may not be needed
  † Hayes *et al.*, *Z. Metallkde.*, 77 (1986) 749
  ‡ Yoon and Lee, *Calphad* 22 (1998) 167

Experimental Work on Solder Systems

- **Sn-Ag-Cu**: verification of composition and temperature of Sn-rich ternary eutectic
  - Sn-rich equilibrium diagram

- **Sn-Bi-Pb**: examination of effects of Pb contamination of Sn-Bi solders
  - solidification path
  - non-equilibrium solidification (Scheil)
Superalloy Database under Development

**Ni, Al, Co, Cr, Hf, Mo, Re, Ta, Ti, W, Fe, Nb, Zr, B, C**
- 10 component database is the minimum needed
- 15 component database - long term goal
- Assessments from literature or NIST

<table>
<thead>
<tr>
<th>Elements in Database</th>
<th>Binary Subsystems</th>
<th>Ternary Subsystems</th>
<th>Ni-base Ternary Subsystems</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>45 (39 done)</td>
<td>120 (18 done)</td>
<td>36 (14 done)</td>
</tr>
<tr>
<td>15</td>
<td>105 (87 done*)</td>
<td>455 (48 done)</td>
<td>91 (26 done)</td>
</tr>
</tbody>
</table>

*14 of the 87 may need readjustment

Current State of the Superalloy Database

- **Ni, Al, Co, Cr, Hf, Mo, Re, Ta, Ti, W**
- Most phases included
- Emphasis on liquid, $\gamma$ and $\gamma'$
- Verification by comparison with experimental literature data in progress
Diffusion Mobility Database for Ni-Based Superalloys

Constituents: Ni-Al-Co-Cr-Hf-Ta-Ti-Mo-Re-W-B
Evaluation of the diffusion mobilities in the FCC phase

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Constituent Binary Systems</th>
<th>Constituent Ternary Systems</th>
<th>Completed Binary Systems</th>
<th>Completed Ternary Systems</th>
</tr>
</thead>
<tbody>
<tr>
<td>Current</td>
<td>55</td>
<td>165</td>
<td>12 (Ni-based)</td>
<td>3 (Ni-Al-Cr; Ni-Al-Ti; Ni-Al-B)</td>
</tr>
<tr>
<td>2000-2001</td>
<td></td>
<td>9 (Co-based)</td>
<td>2 (Ni-Al-Co; Ni-Co-Cr)</td>
<td></td>
</tr>
</tbody>
</table>

Database constructed using thermodynamic factors from the thermodynamic database compiled by NIST/Metallurgy Division.

1 Ni-Al-Cr system assessed by Engström and Ågren, Z. Metallkd. 87 (1996) 92.
2 Ni-Al-Ti system assessed by Matan et al., Acta mater. 46 (1998) 4567

Current State of the Semiconductor Database

- **Ga-N** p-T-x phase diagram assessed:
  - Pressure dependence for gas phase is used (up to 6 GPa)

- **Al-N** thermochemical and phase diagram data under evaluation

- **Ti-Ga-N** and **Ni-Ga-N** experiments in progress:
  - Phase diagrams (isothermal sections)
  - Interfacial reactions and diffusion path of Ti/GaN layers

- Database goals (intermediate and long term)
  - Al, Ga, N, Ti, Ni, In, Mg, Au, Pt
Other Topics of Interest

- Data of interest to NIST
  - Pressure dependence
  - Possible revision of SGTE lattice stabilities
- North-American effort to coordinate activities in computational thermodynamics
- Public versus proprietary databases

NIST-Interest in Pressure Dependence for Compound-Semiconductors

- Description of pressure dependence necessary because of pressure range covered (0.1 MPa - 6 GPa)
- Gas phase: Data in literature are given in different forms of equations of state (Van der Waals, virial, etc.)
  ⇒ Recommendation for equation and form needed
- Condensed phases
  - Guidelines for implementation needed
  - Database with unary data needed
  - Concentration dependence?