NIST Metallurgy Division Computational Thermodynamics Projects and Databases

Ursula R. Kattner
Metallurgy Division, NIST
Gaithersburg, MD 20899

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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

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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

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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

Elements in Database	Binary Subsystems	Ternary Subsystems	Sn-base Ternary Subsystems
7	21 (21 done)	36 (11 done)	15 (7 done)
9	36 (34 done)	94 (12 done)	28 (8 done)
13	78 (72 done*)	286 (21 done)	66 (10 done)

* 22 of the 72 may need readjustment

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Current State of the Solder Database

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

Ag-Bi-Cu	extrapolated	Ag-Pb-Sn	extrapolated
Ag-Bi-Pb	extrapolated*	Bi-Cu-Pb	extrapolated
Ag-Bi-Sn	extrapolated*	Bi-Cu-Sn	extrapolated
Ag-Cu-Pb	assessed[†]	Bi-Pb-Sn	assessed[‡]
Ag-Cu-Sn	partially 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

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Experimental Work on Solder Systems

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

  (Moon *et al*., *J. Electron. Mater*. 29 (2000) 1122-1136)
- **Sn-Bi-Pb:** examination of effects of Pb contamination of Sn-Bi solders
  - solidification path
  - non-equilibrium solidification (Scheil)

  (Moon *et al*., *J. Electron. Mater*., 30 (2001) 45-52)

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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

Elements in Database	Binary Subsystems	Ternary Subsystems	Ni-base Ternary Subsystems
10	45 (39 done)	120 (18 done)	36 (14 done)
15	105 (87 done*)	455 (48 done)	91 (26 done)

* 14 of the 87 may need readjustment

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Current State of the Superalloy Database

- **Ni, Al, Co, Cr, Hf, Mo, Re, Ta, Ti, W**
- Most phases included
- Emphasis on liquid, γ and γ'
- Verification by comparison with experimental literature data in progress

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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

	Constituent Binary Systems	Constituent Ternary Systems	Completed Binary systems	Completed Ternary Systems
Current	55	165	12 (Ni-based)	3 (Ni-Al-Cr†; Ni-Al-Ti‡; Ni-Al-B)
2000-2001			9 (Co-based)	2 (Ni-Al-Co; Ni-Co-Cr)

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

†Ni-Al-Cr system assessed by Engström and Ågren, *Z. Metallkd.* 87 (1996) 92.
‡ Ni-Al-Ti system assessed by Matan *et al.*, *Acta mater.* 46 (1998) 4587

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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)

  (Davydov and Anderson, in *"III-V Nitride materials and Processes"*, ECS Boston, 1998)
- **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

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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

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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.)

  $\Rightarrow$ Recommendation for equation and form needed
- Condensed phases
  - Guidelines for implementation needed
  - Database with unary data needed
  - Concentration dependence ?

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