Fachbereich 11
Institut für Werkstofftechnik
Lehrstuhl für Materialkunde und Werkstoffprüfung
Prof. Dr.-Ing. H.-J. Christ

UNIVERSITÄT SIEGEN

An Extension of the Data-file for the System Co-Re-Cr-C-O: Sources and Restrictions of the Applicability

B. Gorr and H.-J. Christ

Content

- ✓ Introduction/Motivation
- ✓ Theoretical Background
- ✓ Development of the database
- ✓ Perspectives/Conclusions

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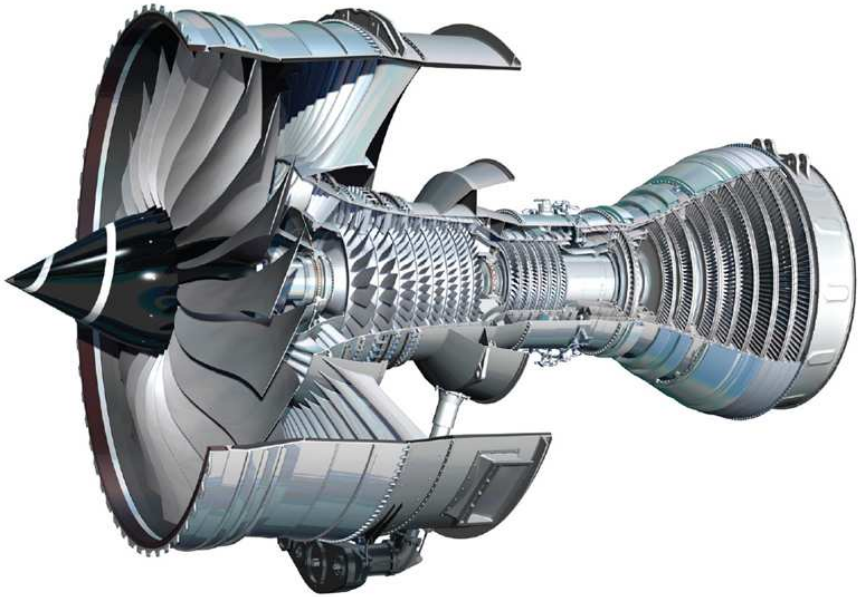
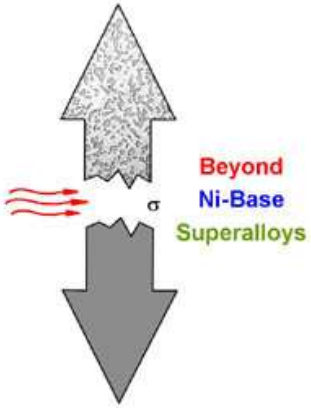
Introduction

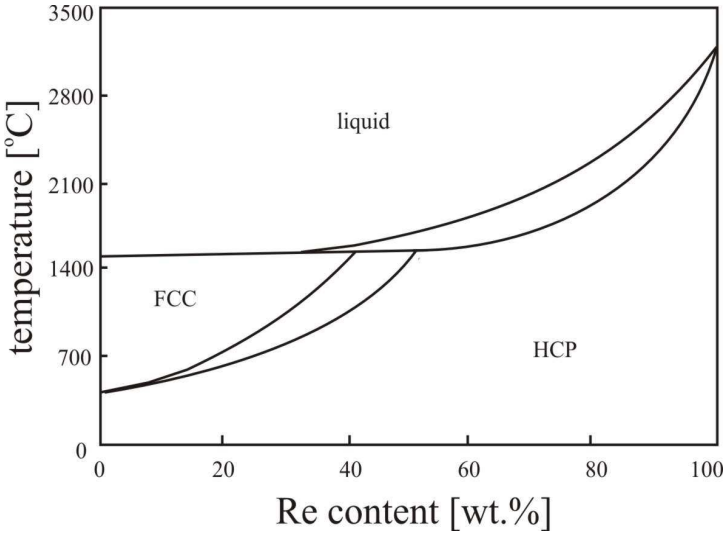


Jet EngineTrent XWB (Rolls-Royce)

Co-Re-based Alloys

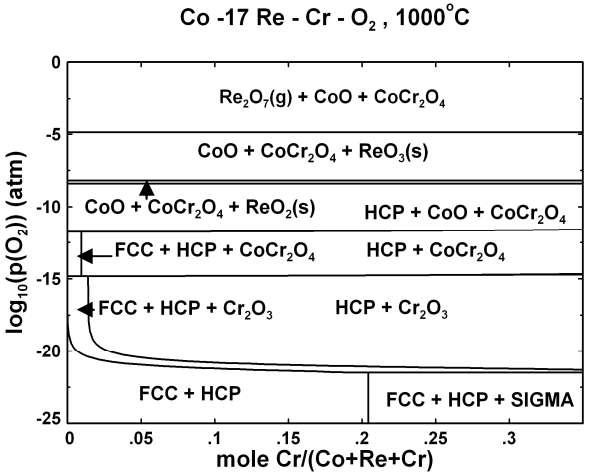


Co-Re

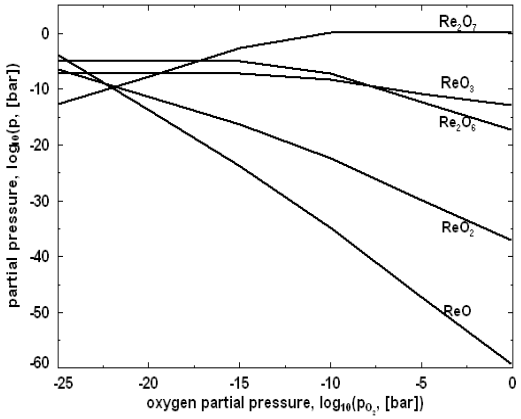


Motivation

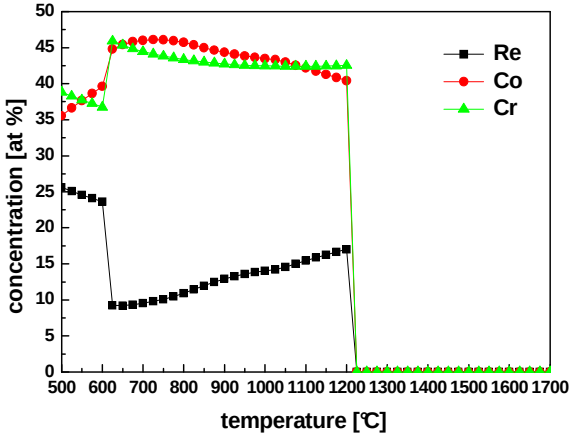
•Previous history: ordering of the data-file Co-Re-Cr-C-O by GTT-Technologies



Corrosion Engineering, Science and Technology **44** (2009) 176



Oxidation of Metals **71** (2009) 157



Materials and Corrosion (2009) DOI: 10.1002/maco.200905412

• Current task – addition of Si to the existing data-file

• Strategy:

- understanding of the thermodynamic basics
- understanding of the main modelling principles
- comprehension of the data-file construction
- literature research

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Theoretical Background

Elements and stoichiometric compounds

$$C_p = -C - 2DT - 2ET^{-2} - 6FT^2$$

$$H(T) = H(T_0) + \int_{T_0}^{T} C_P dT = A - CT - DT^2 + 2ET^{-1} - 2FT^3$$

$$S(T) = S(T_0) + \int_{T_0}^{T} \frac{C_P}{T} dT = -B - C(1 + \ln(T)) - 2DT + ET^{-2} - 3FT^2$$

$$G = H - TS$$ **(Gibbs-Helmholz)**

$$G(T) = A + BT + CT\ln T + DT^2 + FT^3 + ET^{-1}$$

Solutions

1) ideal solutions (gas phases)

$$G^{\Phi} = {}^{ref}G^{\Phi} + {}^{id}G^{\Phi}$$

$${}^{ref}G^{\phi} = \sum_{i=1}^{n} x_i \cdot {}^{0}G_i$$

$${}^{id}G^{\phi} = -TS_c = RT\sum_{i=1}^{n} x_i \ln x_i$$

2) nonideal solutions (condensed phases)

$$G^{\Phi} = {}^{ref}G^{\Phi} + {}^{id}G^{\Phi} + {}^{ex}G^{\Phi}$$

Regular solution (liquid phases)

$${}^{ex}G^{\Phi} = x_A x_B \sum_{\nu=0}^{n} {}^{\nu}L(T) \cdot (x_A - x_B)^{\nu}.$$

(Redlich-Kister polynomial)

Phases with sublattices (bcc,fcc,..)

⇩

Compound energy fomalism

$$G^{\Phi} = {}^{ref}G^{\Phi} + {}^{id}G^{\Phi} + {}^{ex}G^{\Phi}$$

$$(A,B)_p(B,A)_q$$

Compound energy formalism

$$G^{\Phi}(T,x) - H^{SER}(298{,}15K) =$$

$$\left.\begin{aligned}
&{}^{\circ}G^{\Phi}_{A:B}\cdot(1-y_B')y_B'' \\
&+{}^{\circ}G^{\Phi}_{A:A}\cdot(1-y_B')(1-y_B'') \\
&+{}^{\circ}G^{\Phi}_{B:B}\cdot y_B'y_B'' \\
&+{}^{\circ}G^{\Phi}_{B:A}\cdot y_B'(1-y_B'')
\end{aligned}\right\} \; {}^{ref}G^{\Phi}$$

$$\left.\begin{aligned}
&+RT[\,p((1-y_B')\ln(1-y_B')+y_B'\ln y_B') \\
&+\quad q((1-y_B'')\ln(1-y_B'')+y_B''\ln y_B'')]
\end{aligned}\right\} \; {}^{id}G^{\Phi}$$

$$\left.\begin{aligned}
&+{}^{\circ}L^{\Phi}_{A,B:B}\cdot(1-y_B')y_B'y_B'' \\
&+{}^{\circ}L^{\Phi}_{A,B:A}\cdot(1-y_B')y_B'(1-y_B'') \\
&+{}^{\circ}L^{\Phi}_{A:B,A}\cdot(1-y_B')y_B''(1-y_B'') \\
&+{}^{\circ}L^{\Phi}_{B:B,A}\cdot y_B'y_B''(1-y_B'') \\
&+{}^{1}L^{\Phi}_{A,B:B}\cdot(1-y_B')y_B'(1-2y_B')y_B'' \\
&+{}^{1}L^{\Phi}_{A,B:A}\cdot(1-y_B')y_B'(1-2y_B')(1-y_B'') \\
&+{}^{1}L^{\Phi}_{A:B,A}\cdot(1-y_B')y_B''(1-y_B'')(1-2y_B'') \\
&+{}^{1}L^{\Phi}_{B:B,A}\cdot y_B'y_B''(1-y_B'')(1-2y_B'') \\
&+\ldots
\end{aligned}\right\} \; {}^{ex}G^{\Phi}$$

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Construction of the FactSage data-files

9151b16g.dat - Editor

Datei Bearbeiten Format Ansicht ?

```
Ar-Al-Cr-N-Ni-Ti-O              See commentary below !       GTT 2.7.2004
   7  12  37   5   4   4   4   8   12   4   8   4   4   2  39
Ar                          Al                          Cr
N                           Ni                          Ti
O
     39.9480       26.9815       51.9960       14.0067       58.6900       47.8800
     15.9994
   6   1   2   3   4   5   6
   4   1   2   3   4
GAS
IDMX
Cr
 4 6   0.0   0.0   1.0   0.0   0.0   0.0   0.0
 800.00000       391905.70       65.023778      -20.786100      0.00000000
0.00000000      0.00000000
3 0.00000000       0.0 0.00000000       0.0 0.00000000       0.0
 1200.0000       391703.80       69.012778      -21.428800      0.82355800E-03
-.18278500E-06  11071.900
3 0.00000000       0.0 0.00000000       0.0 0.00000000       0.0
 2200.0000       401183.50       10.950778      -13.833600      -.10803500E-02
-.22069200E-06 -1931730.0
3 0.00000000       0.0 0.00000000       0.0 0.00000000       0.0
 3600.0000       393019.00      -2.4932223      -10.996000      -.44812700E-02
0.11658000E-06  3710580.0
3 0.00000000       0.0 0.00000000       0.0 0.00000000       0.0
 4800.0000       304527.70       256.69648      -55.864800      0.53938000E-02
-.28363300E-06  35390400.
3 0.00000000       0.0 0.00000000       0.0 0.00000000       0.0
 6000.0000       853670.90      -1195.0162       115.37800      -.18385300E-01
0.33669000E-06 -.29543200E+09
3 0.00000000       0.0 0.00000000       0.0 0.00000000       0.0
N2
 4 3   0.0   0.0   0.0   2.0   0.0   0.0   0.0
 950.00000      -7501.3500      -18.908500      -25.563800      -.35337200E-02
0.53620000E-08 -64748.000
3 0.00000000       0.0 0.00000000       0.0 0.00000000       0.0
 3350.0000      -14717.700       34.400600      -32.739800      -.13021400E-02
0.60194000E-07  1126140.0
3 0.00000000       0.0 0.00000000       0.0 0.00000000       0.0
 6000.0000      -32785.600       100.52000      -40.939000      0.47950800E-03
-.16666000E-07  9192750.0
3 0.00000000       0.0 0.00000000       0.0 0.00000000       0.0
O2
 4 3   0.0   0.0   0.0   0.0   0.0   0.0   2.0
 1000.0000      -6961.7400      -51.006076      -22.272000      -.10197776E-01
0.13236920E-05 -76730.000
```

Construction of the FactSage data-files

HEADER

DATA BLOCK(S) FOR MIXTURE PHASES

- **Mixture Phase 1**
- **Mixture Phase 2**
- .
- .
- **Mixture Phase n**

DATA BLOCK(S) FOR STOICHIOMETRIC CONDENCED PHASES

- **Stoichiometric Condenced Phase 1**
- **Stoichiometric Condenced Phase 2**
- .
- .
- **Stoichiometric Condenced Phase n**

COMMENTARY BLOCK

Construction of the FactSage data-files

HEADER

DATA BLOCK(S) FOR MIXTURE PHASES

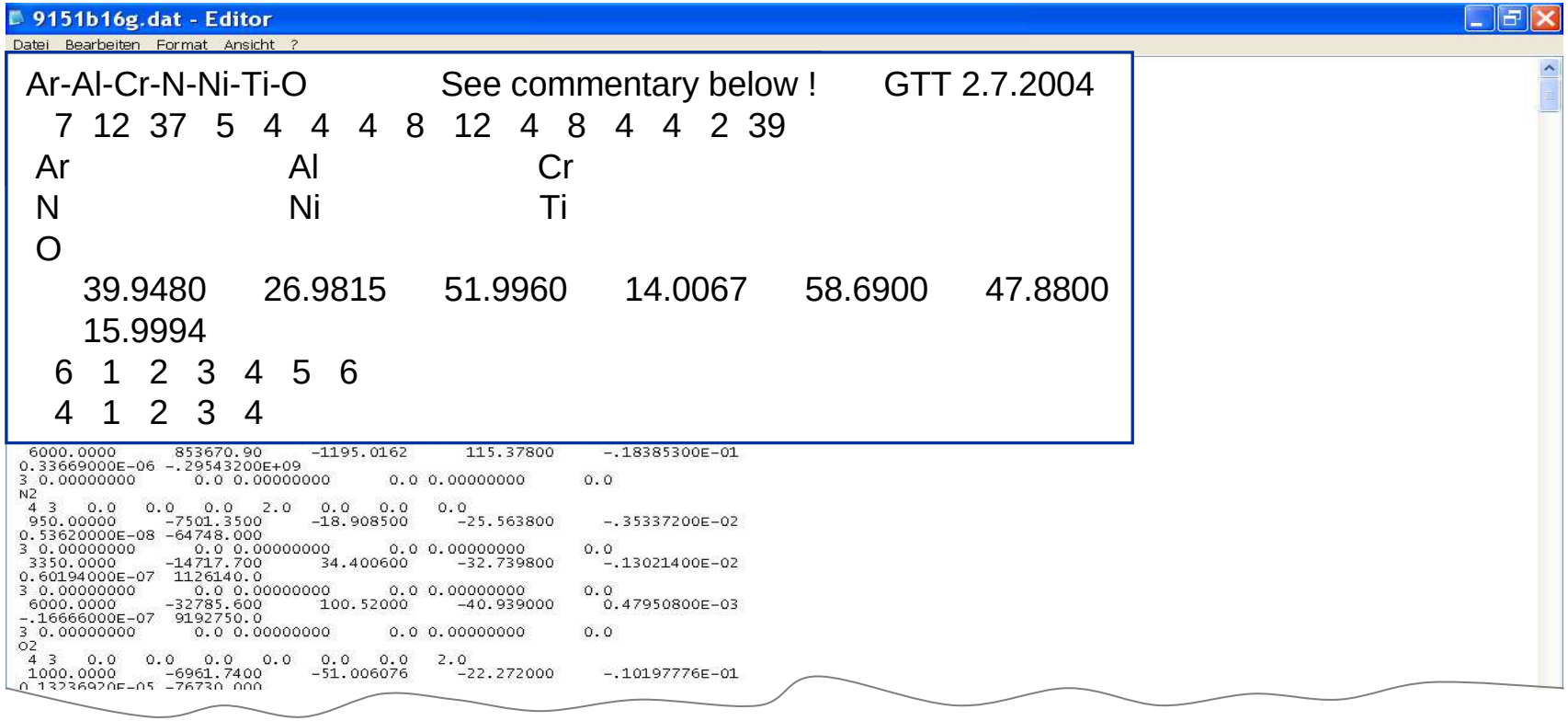
- Mixture Phase 1
- Mixture Phase 2
- .
- .
- Mixture Phase n

DATA BLOCK(S) FOR STOICHIOMETRIC CONDENCED PHASES

- Stoichiometric Condenced Phase 1
- Stoichiometric Condenced Phase 2
- .
- .
- Stoichiometric Condenced Phase n

COMMENTARY BLOCK

Construction of the FactSage data-files



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- Stoichiometric Condenced Phase 2
- .
- .
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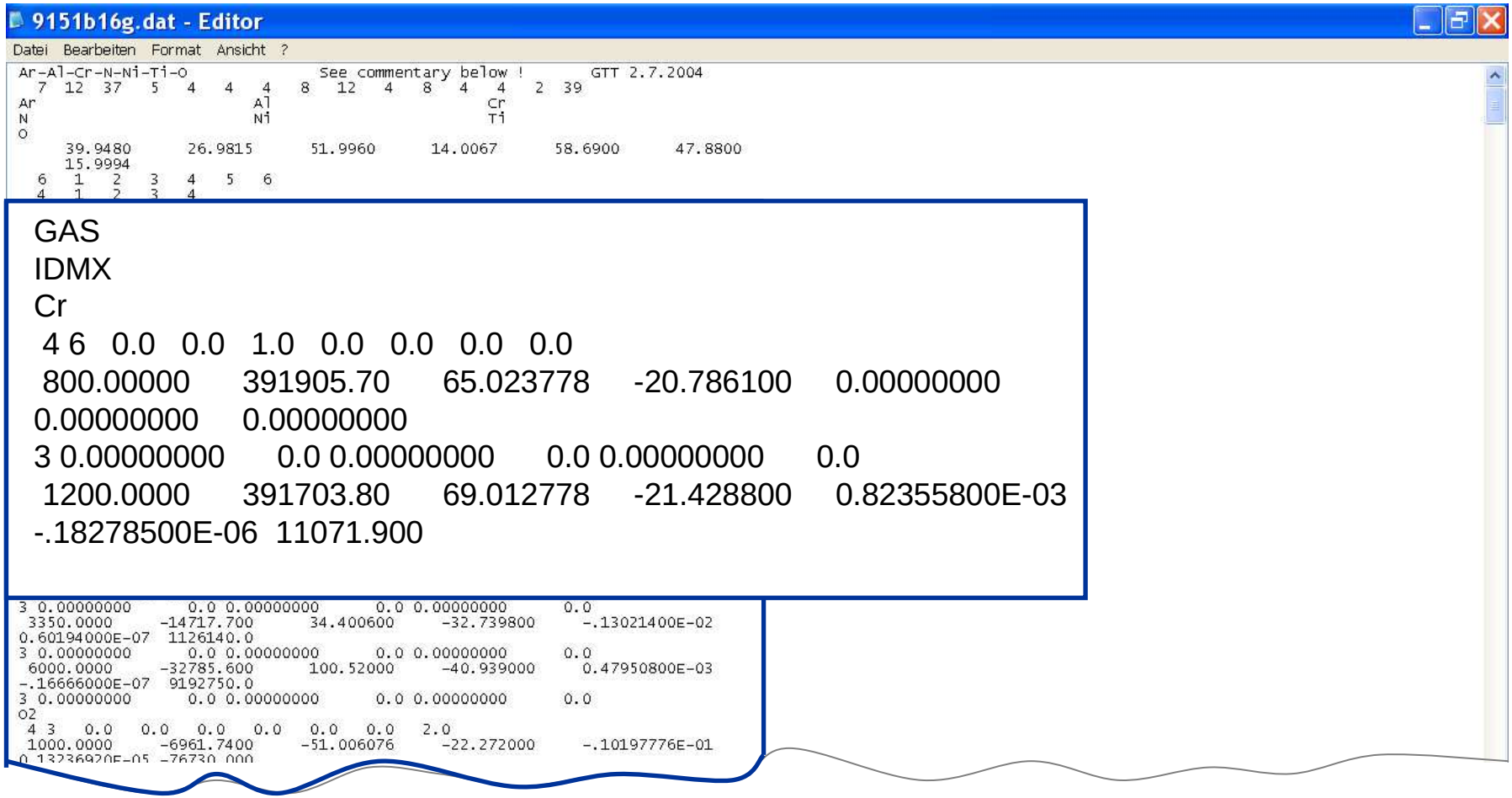
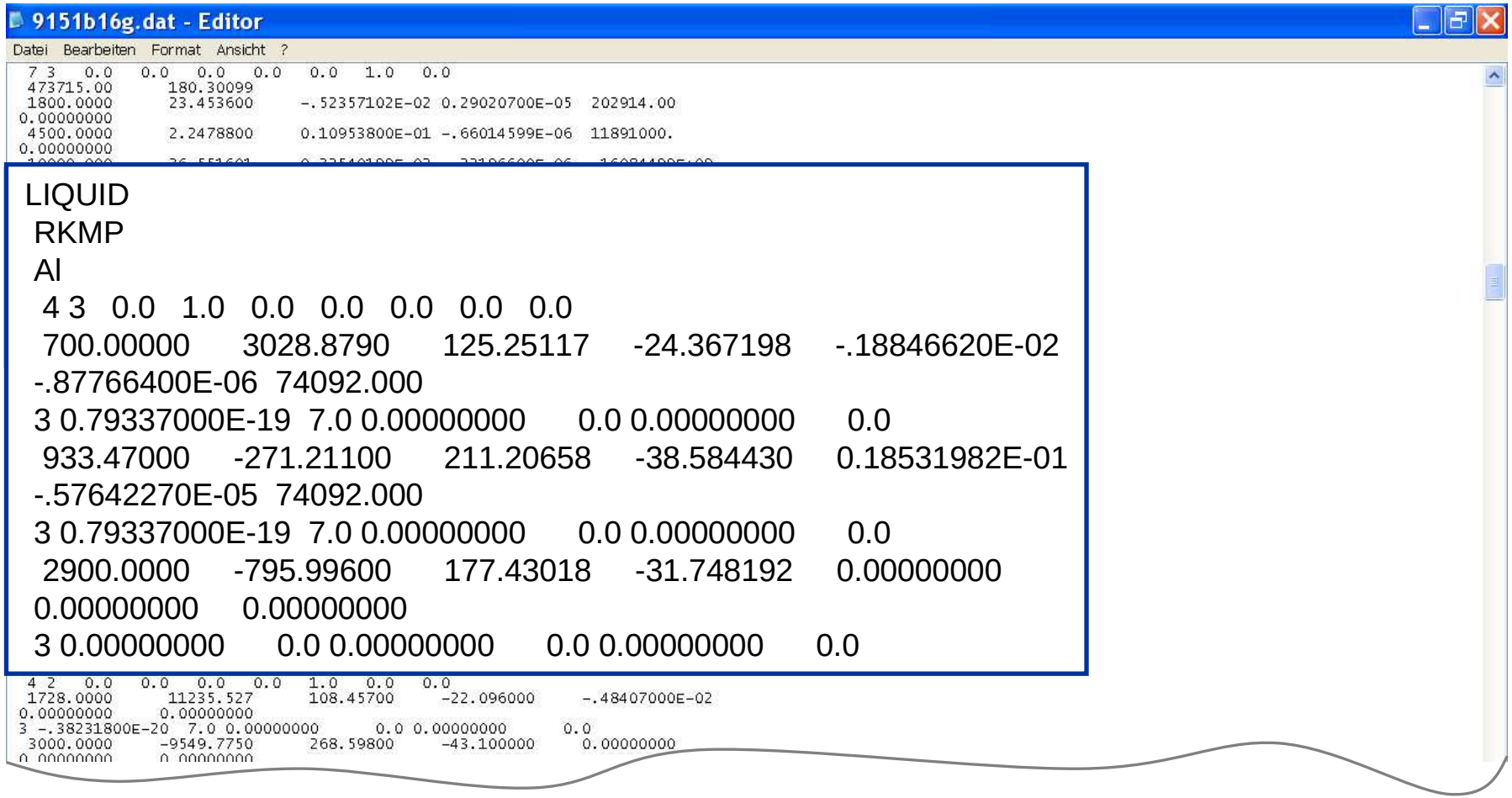
COMMENTARY BLOCK

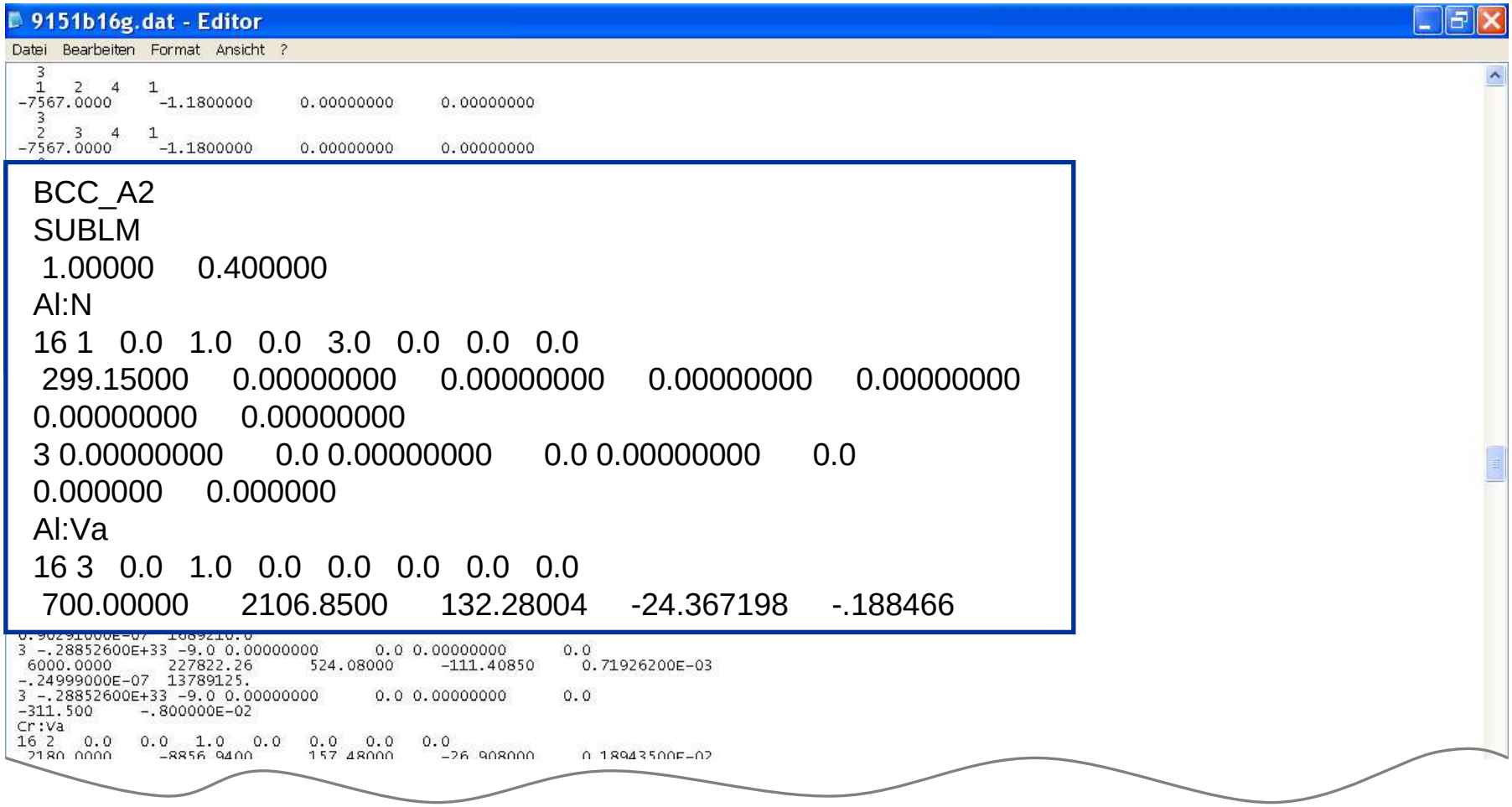
Construction of the FactSage data-files



Construction of the FactSage data-files



Construction of the FactSage data-files



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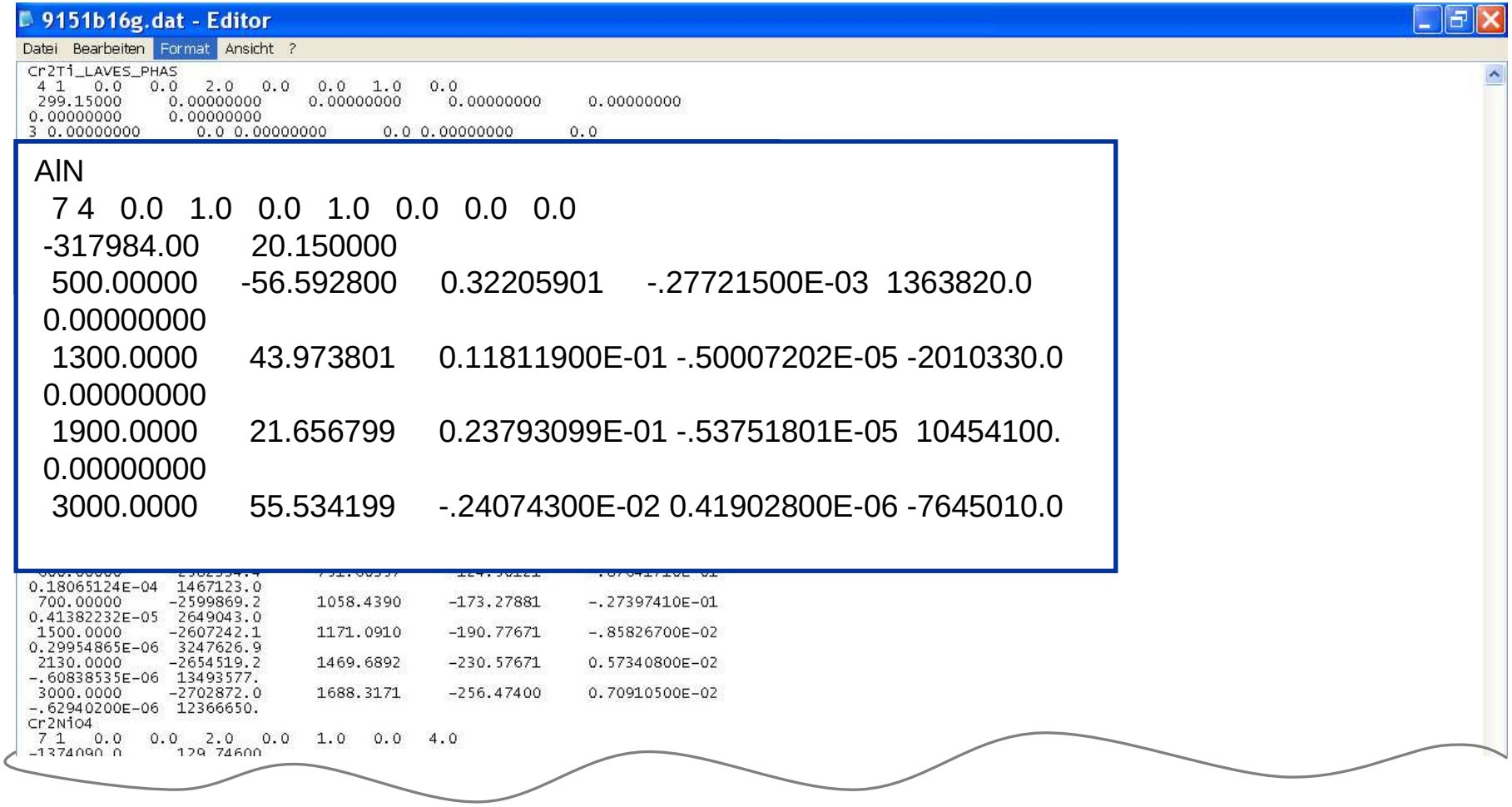
- Stoichiometric Condenced Phase 2
- .
- .
- Stoichiometric Condenced Phase n

COMMENTARY BLOCK

Construction of the FactSage data-files



Construction of the FactSage data-files

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- .
- .
- Mixture Phase n

DATA BLOCK(S) FOR STOICHIOMETRIC CONDENCED PHASES

- Stoichiometric Condenced Phase 1
- Stoichiometric Condenced Phase 2
- .
- .
- Stoichiometric Condenced Phase n

COMMENTARY BLOCK

Construction of the FactSage data-files

9151b16g.dat - Editor

Datei Bearbeiten Format Ansicht ?

```
################################################################################

Date            : 07.04.1997
Originator      : KH
Serial No       : 9151B17G.DAT
Quality Status  : B
ChemSage Vers.  : 3.0

Temperatures    : Below liquidus of the metallic subsystem
Compositions    : Ni-rich
Applications    : Oxidation and nitride formation


Sources of data

Unary           : 94SGT, 95Hac (for Ni3Al and Ni3Ti)

Binary          : 92SGT, 95Dup (for Ti in solid Ni)

                  NOTE: The elementary components contained in
                        the set of Stoichiometric Condensed Phases
                        are given to simplify input of the system
                        composition. They are suppressed from the
                        equilibrium calculations by use of the
                        exclamation mark in the names. Do not change
                        the "!".


System components:

 1: Ar                    2: Al                    3: Cr
 4: N                     5: Ni                    6: Ti
 7: O

Phases:

 1: GAS                   2: LIQUID                3: AL3NI2
 4: TI3AL                 5: TIAL                  6: BCC_A2
 7: FCC_A1                8: ALNI_B2               9: HCP_A3
10: (Cr,Ti)N             11: (Cr,Ni)2N:2          12: M2O3_alpha
13: Cr12.8Ni7.2N4_PI     14: Al.8667Cr.1333_A     15: Al.8Cr.2_AL4CR
16: Al.616Cr.384         17: Al.692Cr.308_h       18: Al.692Cr.308_l
19: Al.333Cr.667         20: Al.769Al.077Cr.154   21: Al.75Ni.25_AL3NI
22: Al.68Ti.32           23: Al.667Ti.333         24: Al.75Ti.25
25: Ti2N_TI2N            26: Cr2Ti_LAVES_PHAS     27: AlN
28: AlNi3                29: Al2NiO4              30: Al2O3
```

Construction of the FactSage data-files

$$G(T) = A + BT + CT\ln T + DT^2 + FT^3 + ET^{-1}$$

```
System Re-Co-Cr-O-C
 5  8 20  4  6  6  6  4  2  6 30
Re                  Co                  Cr
O                   C
  186.207000           58.933200           51.996100
   15.999400           12.011000
  6  1  2  3  4  5  6
  6  1  2  3  4  5  6
gas_ideal
IDMX
O2
  4  5    0.0    0.0    0.0    2.0    0.0
ΔT1→ 900.00000   -6960.6927   -51.183147   -22.258620   -.10238670E-01
     0.13399470E-05 -76749.550
ΔT2→ 3700.0000   -13136.017    24.743297   -33.557260   -.12348985E-02
     0.16694333E-07  539886.00
ΔT3→ 9600.0000    14154.646   -51.485458   -24.479780   -.26347590E-02
     0.60154433E-07 -15120935.
ΔT4→ 18500.000   -314316.63    515.06804   -87.561430    0.25787245E-02
     -.18787650E-07 0.29052515E+09
ΔT5→ 20000.000   -108797.18    288.48302   -63.737000    0.14375000E-02
     -.90000000E-08 0.25153895
     1 0.00000000       0.00
```

Sources of thermochemical data-files

1). SGTE, SGUN Pure Substances and Solution databases

Compound.txt - Editor

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Si Units: P(bar) Energy(J)
Name: Si

$$G(T) = A + BT + CT\ln T + DT^2 + FT^3 + ET^{-1}$$

G(T) J/mol - 1 bar

		G(T)		G(T)	G(T)	T(K)
S1	1	- 8162.60806		+ 137.236860 T	- 1.912904000E-03 T^ 2	298 - 1687
S1	1	+ 176667.000	T^-1	- 3.552000000E-09 T^ 3	- 22.8317530 T ln(T)	298 - 1687
S1	2	- 9457.63976		+ 167.281369 T	- 4.203690000E+30 T^-9	1687 - 3600
S1	2	- 27.1960000	T ln(T)			1687 - 3600
S2	3	38837.3909		+ 114.736860 T	- 1.912904000E-03 T^ 2	298 - 1687
S2	3	+ 176667.000	T^-1	- 3.552000000E-09 T^ 3	- 22.8317530 T ln(T)	298 - 1687
S2	4	37542.3592		+ 144.781369 T	- 4.203690000E+30 T^-9	1687 - 3600
S2	4	- 27.1960000	T ln(T)			1687 - 3600
S3	5	42045.3909		+ 116.859860 T	- 1.912904000E-03 T^ 2	298 - 1687
S3	5	+ 176667.000	T^-1	- 3.552000000E-09 T^ 3	- 22.8317530 T ln(T)	298 - 1687
S3	6	40750.3592		+ 146.904369 T	- 4.203690000E+30 T^-9	1687 - 3600
S3	6	- 27.1960000	T ln(T)			1687 - 3600
S4	7	39116.3909		+ 116.859860 T	- 1.912904000E-03 T^ 2	298 - 1687
S4	7	+ 176667.000	T^-1	- 3.552000000E-09 T^ 3	- 22.8317530 T ln(T)	298 - 1687
S4	8	37821.3592		+ 146.904369 T	- 4.203690000E+30 T^-9	1687 - 3600
S4	8	- 27.1960000	T ln(T)			1687 - 3600
S5	9	42837.3909		+ 115.436860 T	- 1.912904000E-03 T^ 2	298 - 1687
S5	9	+ 176667.000	T^-1	- 3.552000000E-09 T^ 3	- 22.8317530 T ln(T)	298 - 1687
S5	10	41542.3592		+ 145.481369 T	- 4.203690000E+30 T^-9	1687 - 3600
S5	10	- 27.1960000	T ln(T)			1687 - 3600
S6	11	41037.3909		+ 116.436860 T	- 1.912904000E-03 T^ 2	298 - 1687
S6	11	+ 176667.000	T^-1	- 3.552000000E-09 T^ 3	- 22.8317530 T ln(T)	298 - 1687
S6	12	39742.3592		+ 146.481369 T	- 4.203690000E+30 T^-9	1687 - 3600
S6	12	- 27.1960000	T ln(T)			1687 - 3600
S7	13	41038.3909		+ 116.436860 T	- 1.912904000E-03 T^ 2	298 - 1687
S7	13	+ 176667.000	T^-1	- 3.552000000E-09 T^ 3	- 22.8317530 T ln(T)	298 - 1687
S7	14	39743.3592		+ 146.481369 T	- 4.203690000E+30 T^-9	1687 - 3600
S7	14	- 27.1960000	T ln(T)			1687 - 3600
L	15	42533.7506		+ 107.137420 T	- 1.912904000E-03 T^ 2	298 - 1687
L	15	+ 176667.000	T^-1	- 3.552000000E-09 T^ 3	+ 2.093070000E-21 T^ 7	298 - 1687
L	15	- 22.8317530	T ln(T)			298 - 1687
L	16	40370.5233		+ 137.722299 T	- 27.1960000 T ln(T)	1687 - 3600

A B D E C F

Sources of thermochemical data-files

1). SGTE, SGUN Pure Substances and Solution databases (thermochemical data for pure substances in the system Co-Re-Cr-O-C-Si)

2). Ready-made data-files (thermochemical data for compounds, solutions, and interaction coefficients between constituents in the system Co-Cr-O-C-Si, without Re!)

- FRAN (Co, Cr, Si, C O)
- MoSi (Si, Cr, O)

4). Phase diagrams

3). Literature (Re,Si)

Sources of thermochemical data-files

ELSEVIER

Intermetallics 9 (2001) 1063–1068

Intermetallics

www.elsevier.com/locate/intermet

Thermodynamic analysis of the Re–Si system

G. Shao*

School of Mechanical and Materials Engineering, University of Surrey, Guildford, Surrey GU2 7XH, UK

Received 31 July 2001; accepted 13 September 2001

Abstract

The Re–Si system is assessed thermodynamically, using the CALPHAD method. The calculated phase diagram and thermodynamic properties are in good agreement with available experimental data. Calculated enthalpies and entropies of fusion are compared with available data for other transition metal silicides, against melting points, showing good agreement with the general trends. This is a useful approach for thermodynamic assessment of alloy systems, where experimentally measured thermodynamic data are limited. The stability of the amorphous phase in this system has also been discussed.

Keywords: A. Silicides, various; B. Phase diagram; B. Thermodynamic and thermochemical properties

1. Introduction

this phase is Re_2Si [4]. The latest version of the Re–Si phase diagram [5,6] is redrawn and shown in Fig. 1. The

Sources of thermochemical data-files

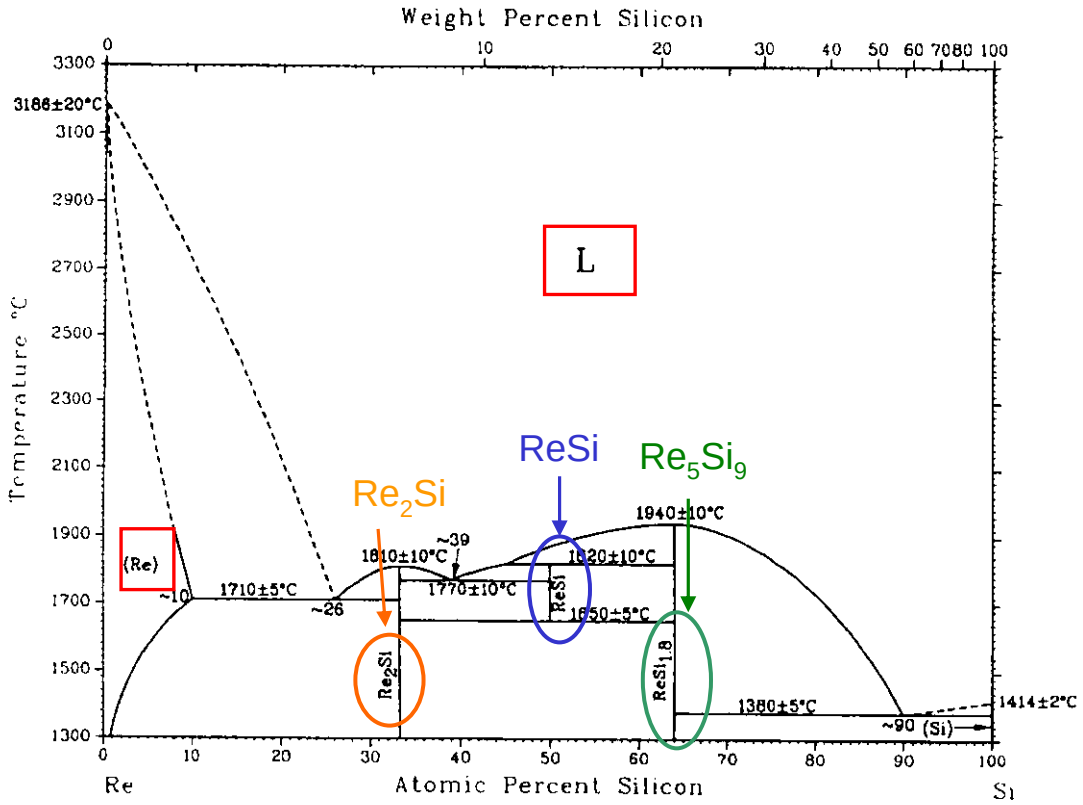

Fig. 1. Experimentally determined Re–Si phase diagram redrawn from Refs. [5,6].

Sources of thermochemical data-files

shown in Fig 7 in dotted lines, indicating the difficulty in reaching stable metastable equilibrium, as extensive diffusion has to be involved. This explains why other stable phases such e-Si and Re_2Si could not coexist with the amorphous phase in the indicated composition range. Local equilibrium at the Am./$ReSi_{1.8}$ interface is unlikely to be achieved, as the metastable equilibrium Re content in the amorphous Si(Re) is very low as well.

4. Conclusions

The Re–Si system is assessed thermodynamically. The calculated phase diagram and thermodynamic properties are in good agreement with available experimental data. Calculated enthalpies as well as entropies, of fusion, are compared with reported values of various transition metal silicides, showing good agreement with the general trends. The approach of this work is useful for thermodynamic assessment of alloy systems, with limited experimentally measured data. The stability of the amorphous phase in this system has also been discussed.

Appendix

Summary of the optimised thermodynamic parameters for the Re–Si systems. Values are given in SI units and correspond to one mole of atoms.

Phase liquid
description: (Re, Si)

$$L^{liq}_{Re,Si} = -96700 - 45000(x_{Re} - x_{Si}) - 60000(x_{Re} - x_{Si})^2$$

Data for amorphization stabilization in this work are:

$T^{Re}_g = 865$ K $\quad \alpha^{Re} = 2.839$
$T^{Si}_g = 1266$ K $\quad \alpha^{Si} = 3.59$
$A^{Re,Si}_0 = -2.5 \quad A^{Re,Si}_1 = -2.2$

Phase hcp
description: (Re, Si)

$$L^{hcp}_{Re,Si} = -48000 - 3000(x_{Re} - x_{Si})$$

Phase Re_2Si
description: $(Re)_{0.667}(Si)_{0.333}$

$$G_{Re_2Si} - 0.667\ G^0_{Re} - 0.333\ G^0_{Si} = -22700 - 1.86\ T$$

Phase ReSi
description: $(Re)_{0.5}(Si)_{0.5}$

$$G_{ReSi} - 0.5\ G^0_{Re} - 0.5\ G^0_{Si} = -21480 - 5\ T$$

Phase $ReSi_{1.8}$ description: $(Re)_{0.357}(Si)_{0.643}$

$$G_{ReSi_{1.8}} - 0.357\ G^0_{Re} - 0.643\ G^0_{Si} = -31200 - 2.1\ T$$

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Appendix

Summary of the optimised thermodynamic parameters for the Re–Si systems. Values are given in SI units and correspond to one mole of atoms.

Phase liquid
description: (Re, Si)

$$L^{liq}_{Re,Si} = -96700 - 45000(x_{Re} - x_{Si}) - 60000(x_{Re} - x_{Si})^2$$

Data for amorphization stabilization in this work are:

$T^{Re}_g = 865$ K $\quad \alpha^{Re} = 2.839$
$T^{Si}_g = 1266$ K $\quad \alpha^{Si} = 3.59$
$A^{Re,Si}_0 = -2.5 \quad A^{Re,Si}_1 = -2.2$

Phase hcp
description: (Re, Si)

$$L^{hcp}_{Re,Si} = -48000 - 3000(x_{Re} - x_{Si})$$

Phase Re_2Si
description: $(Re)_{0.667}(Si)_{0.333}$

$$G_{Re_2Si} - 0.667\ G^0_{Re} - 0.333\ G^0_{Si} = -22700 - 1.86\ T$$

Phase ReSi
description: $(Re)_{0.5}(Si)_{0.5}$

$$G_{ReSi} - 0.5\ G^0_{Re} - 0.5\ G^0_{Si} = -21480 - 5\ T$$

Phase $ReSi_{1.8}$ description: $(Re)_{0.357}(Si)_{0.643}$

$$G_{ReSi_{1.8}} - 0.357\ G^0_{Re} - 0.643\ G^0_{Si} = -31200 - 2.1\ T$$

Sources of thermochemical data-files

Liquid

Phase liquid
description: (Re, Si)

$$L^{liq}_{Re,Si} = -96700 - 45000(x_{Re} - x_{Si}) - 60000(x_{Re} - x_{Si})^2$$

$$^{ex}G^{\Phi} = x_A x_B \sum_{\nu=0}^{n} {}^{\nu}L(T)\cdot\left(x_A - x_B\right)^{\nu}.$$

```
2
 4  5  3
-96700.000     0.00000000     0.00000000     0.00000000
0.00000000 0.00000000
-45000.000     0.00000000     0.00000000     0.00000000
0.00000000 0.00000000
-60000.000     0.00000000     0.00000000     0.00000000
0.00000000 0.00000000
 0
```

Re_2Si

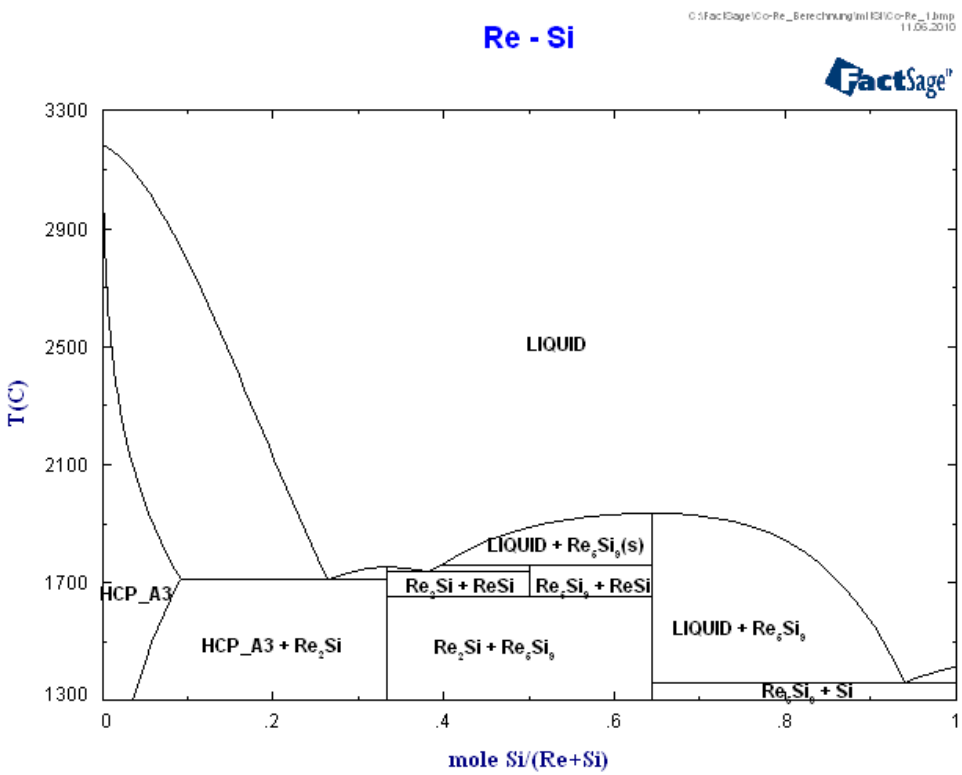
Phase Re_2Si
description: $(Re)_{0.667}(Si)_{0.333}$

$$G_{Re_2Si} - 0.667\ G^0_{Re} - 0.333\ G^0_{Si} = -22700 - 1.86\ T$$

$$\boldsymbol{G = H - TS}$$

$$A_{Re_2Si} = 2A^{Re}_{\Delta T_1} + 1A^{Si}_{\Delta T_1} + H^{Re_2Si} =$$
$$2(-7695,27) + 1(8162) + 3(-22700) = -91653$$

```
Re2Si_re2si(s)
 4  7   2.0    0.0    0.0    1.0    0.0    0.0
1200.0000    -91653.167     388.50004    -71.527753    -.69830040E-02
0.38208400E-06  242497.00
1687.0000    -107814.60     520.99171    -90.003753    0.25783960E-02
-.56722200E-06  2929207.0
2400.0000    -109109.63     551.03622    -94.368000    0.44913000E-02
-.56367000E-06  2752540.0
```



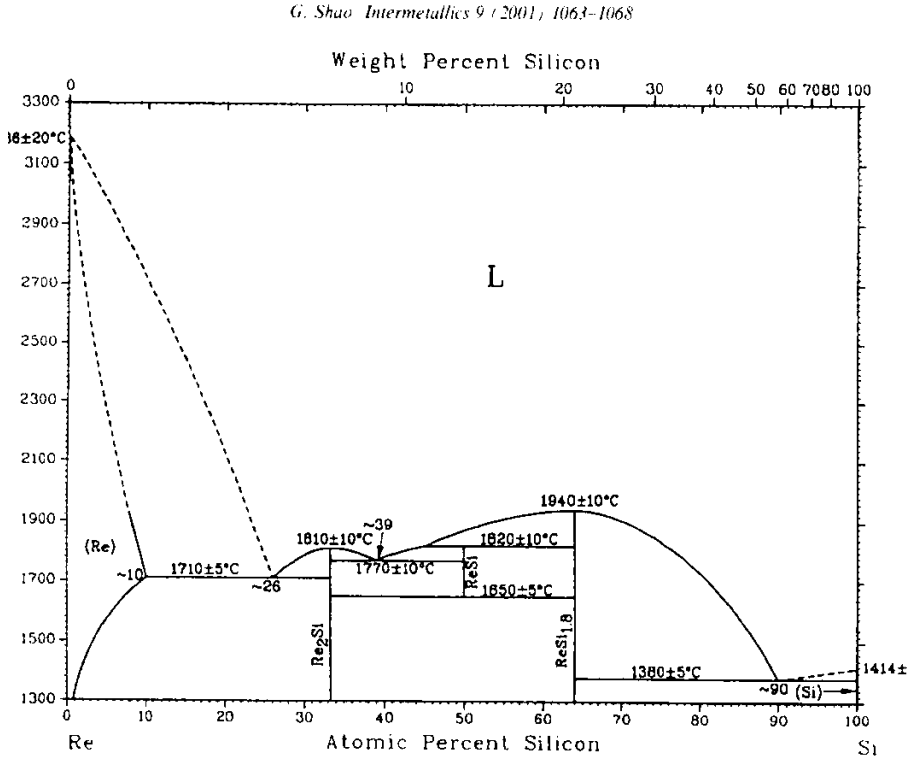


Fig. 1. Experimentally determined Re–Si phase diagram redrawn from Refs. [5,6].

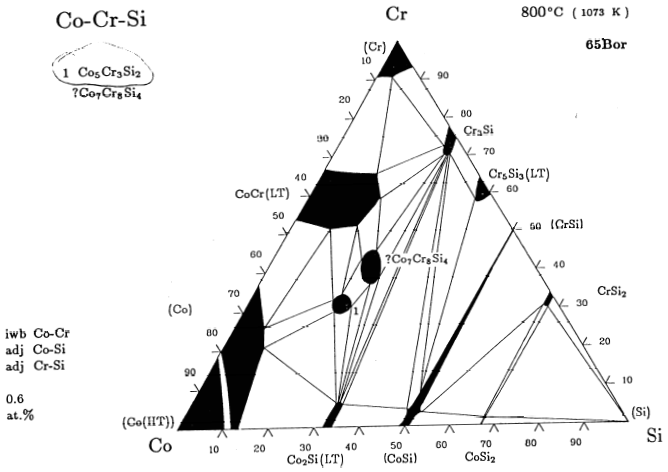
Content

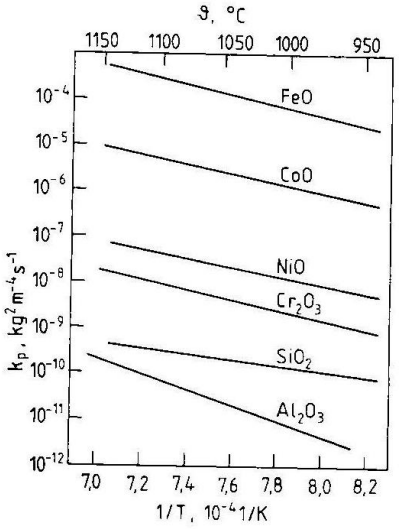
- ✓ Introduction/Motivation
- ✓ Theoretical Background
- ✓ Development of the database
- ✓ Perspectives/Conclusions

Perspectives: An Extension of the Data-file

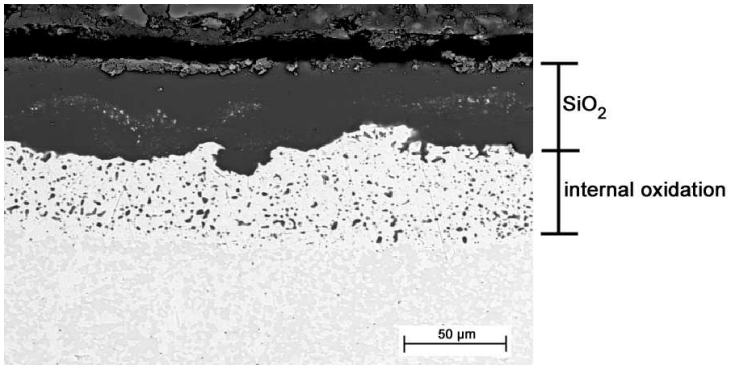
Goals/Perspectives

- Modelling of further phases (primarily in the Co-Cr-Si system)
- Addition of Al to the Co-Re-Cr-C-O-Si data-file
- Addition of B and N to the Co-Re-Cr-C-O-Si data-file
- Literature research
- Critical analysis of calculations





R. Bürgel: Hochtemperaturwerkstofftechnik, Vieweg, Braunschweig, 1998



Mo-9Si-8B, air, 1300℃, 72h

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Conclusions

- There is an urgent need for the development of alloys for temperatures beyond the application range of Ni-based superalloys. Experimental Co-Re-based alloys are potential high-temperature alloys of the new generation.

- Theoretical background of equilibria for stoichiometric reactions and complex systems was presented.

- Models for pure substances and solution phases as well as a basic construction of the FactSage data-files and main sources of the thermochemical data were discussed.

- Perspectives and goals in the further extension of the existing data-files were determined. Al and B should be added to the data-file.

Thank you for your attention!