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THERMODYNAMIC DATABASE, LOWER LENGTH SCALE, PART II: THERMODYNAMIC ASSESSMENT OF AL-MO-SI-U (M3MS-12LL0602092)

P. E. A. Turchi, A. I. Landa

November 19, 2012

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THERMODYNAMIC DATABASE, LOWER LENGTH SCALE (MS-12LL060209)
Part II: Thermodynamic Assessment of Al-Mo-Si-U (M3MS-12LL0602092)

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Project Objective:

The goal of this project is to predict thermodynamics and structure-properties relationships of metallic nuclear fuels. This project makes use of improved coupling between *ab initio* energetic output, phenomenological thermodynamics based on CALPHAD, and experimental data with two deliverables for FY12: (1) the thermodynamic assessment of the ternary alloy system Mo-Pu-U (D1, M3MS-12LL0602091), due at the end of March 2012, and (2) the thermodynamic assessment of the quaternary alloy system Al-Mo-Si-U (M3MS-12LL0602092) due at the end of September 2012.

Milestone 1: Thermodynamic assessment of Mo-Pu-U (D2, M3MS-12LL0602091)

See previous report submitted in April 2012 (LLNL-TR-553775). The thermodynamic database for the binary Mo-Pu alloy system is reported in Appendix II.

Milestone 2: Thermodynamic assessment of Al-Mo-Si-U (D2, M3MS-12LL0602092)

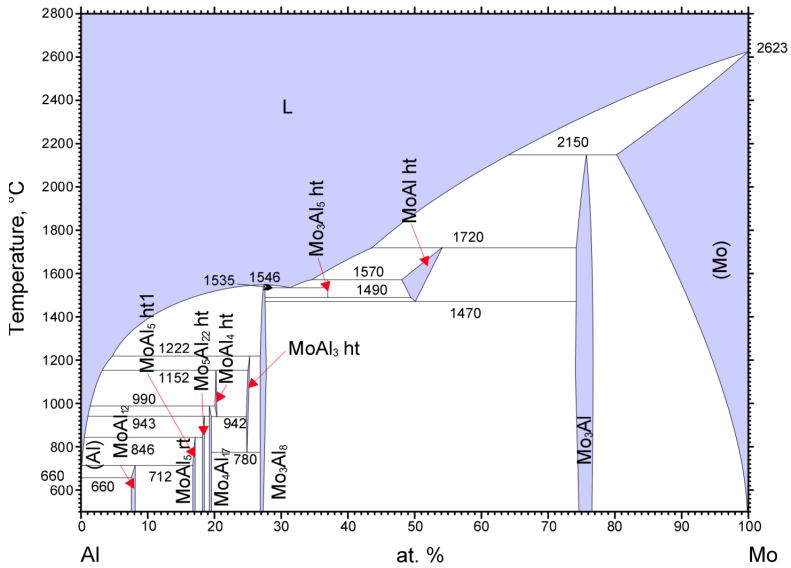
In the framework of the RERTR program there is a need to acquire some fundamental knowledge on U-Mo fuel kernel interacting with the surrounding cladding materials, mostly Al with Si as solute. Based on an improved coupling between *ab initio* energetics output, phenomenological thermodynamics based on the CALPHAD (CALculation of Phase Diagrams) approach, and the use of the Thermo-Calc® software, together with experimental data (whenever available), the final objective of this task is to carry out a thermodynamic assessment of the Al-Mo-Si-U alloy system, as part of the development of a self-consistent and validated thermodynamic database that includes the following actinide elements {U, Np, Pu, Am} forming mixtures among themselves or with the following elements {Al, Be, Cu, Fe, Mo, Nb, Si, Ta, Ti, W, Zr}. This quaternary Al-Mo-Si-U alloy system is comprised of 6 binary alloys: Al-Mo, Al-Si, Al-U, Mo-Si, Mo-U, and Si-U, and 4 ternary alloys: Al-Mo-Si, Al-Mo-U, Al-Si-U, and Mo-Si-U that need to be thermodynamically described by a self-consistent database. For completeness we recall in Appendix I the basics of CALPHAD Modeling and its application to Thermo-Calc® Application Software. The few known phase diagrams are from Refs. [1.2].

I. CALPHAD-based thermodynamic modeling of the 6 binaries of Al-Mo-Si-U

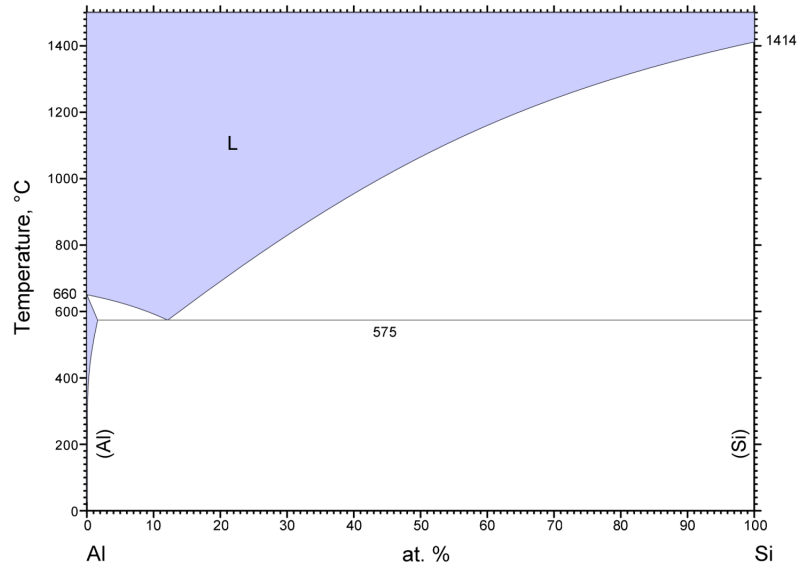
The bibliography related to the 6 binary alloys is summarized in Table I, and the most recent phase diagrams from the ASM Alloy Phase Diagram Center are given in Figure 1.

Binary Alloy	References	Reference for Assessment
Al-Mo	2-6	6
Al-Si	6, 7-8	6
Al-U	8-18	14
Mo-Si	6, 19-20	6
Mo-U	21-40	40
Si-U	41-45	44

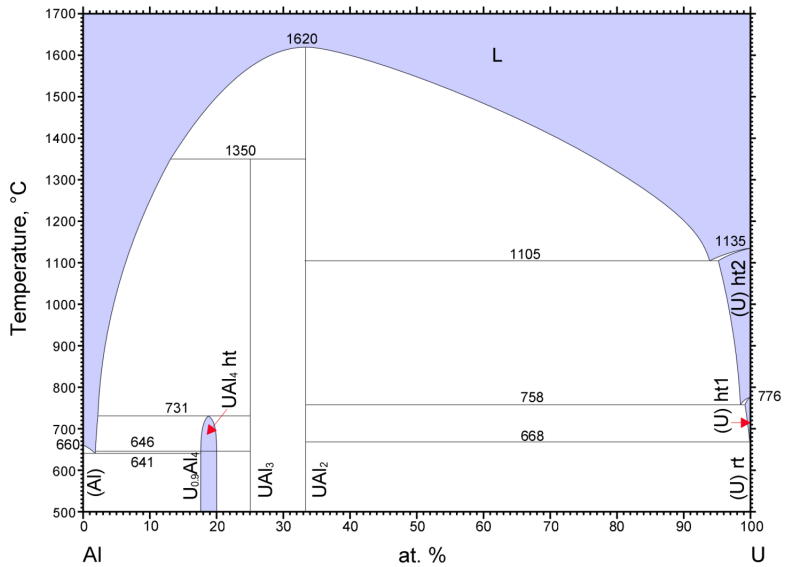
Table I. For each of the six binary alloys that make up the quaternary Al-Mo-Si-U systems, the major references are cited in addition to the one that was used to carry out the thermodynamic assessment.



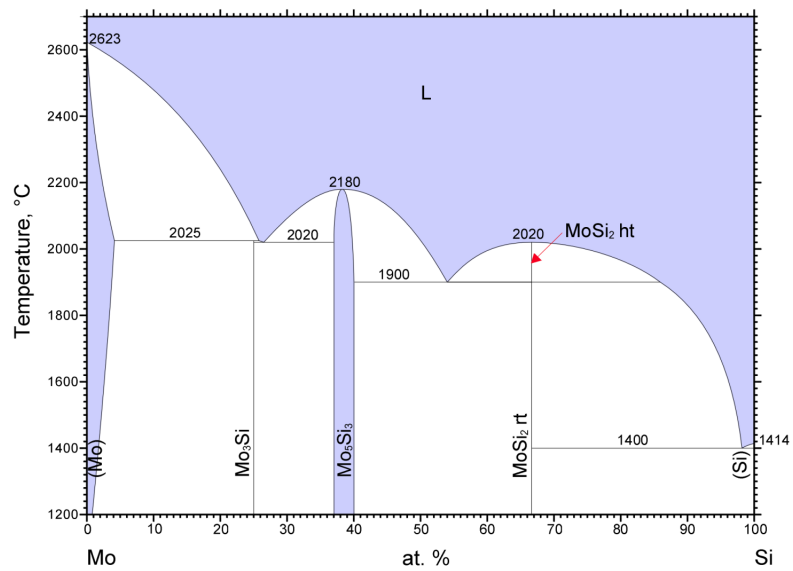
Al-Mo phase diagram from M. Eumann *et al*. (2006) [2].



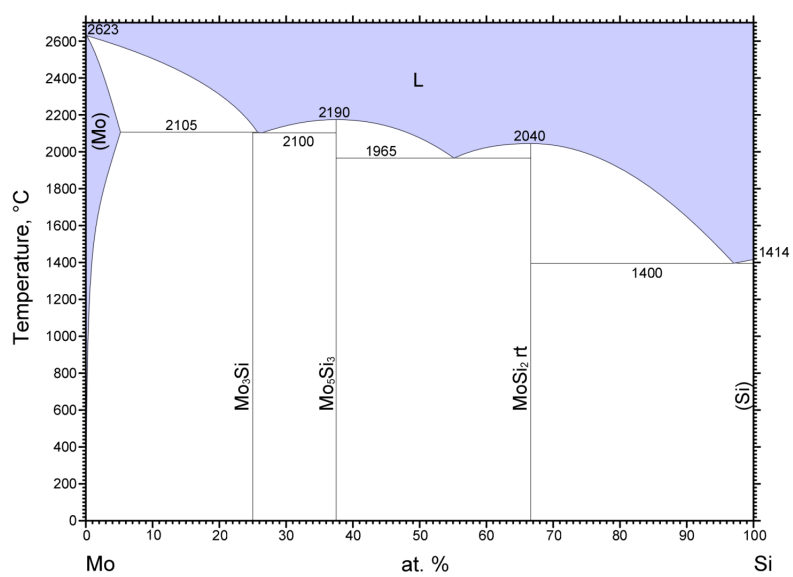
Al-Si phase diagram from A. L. Udovskii *et al*. (1995) [2].



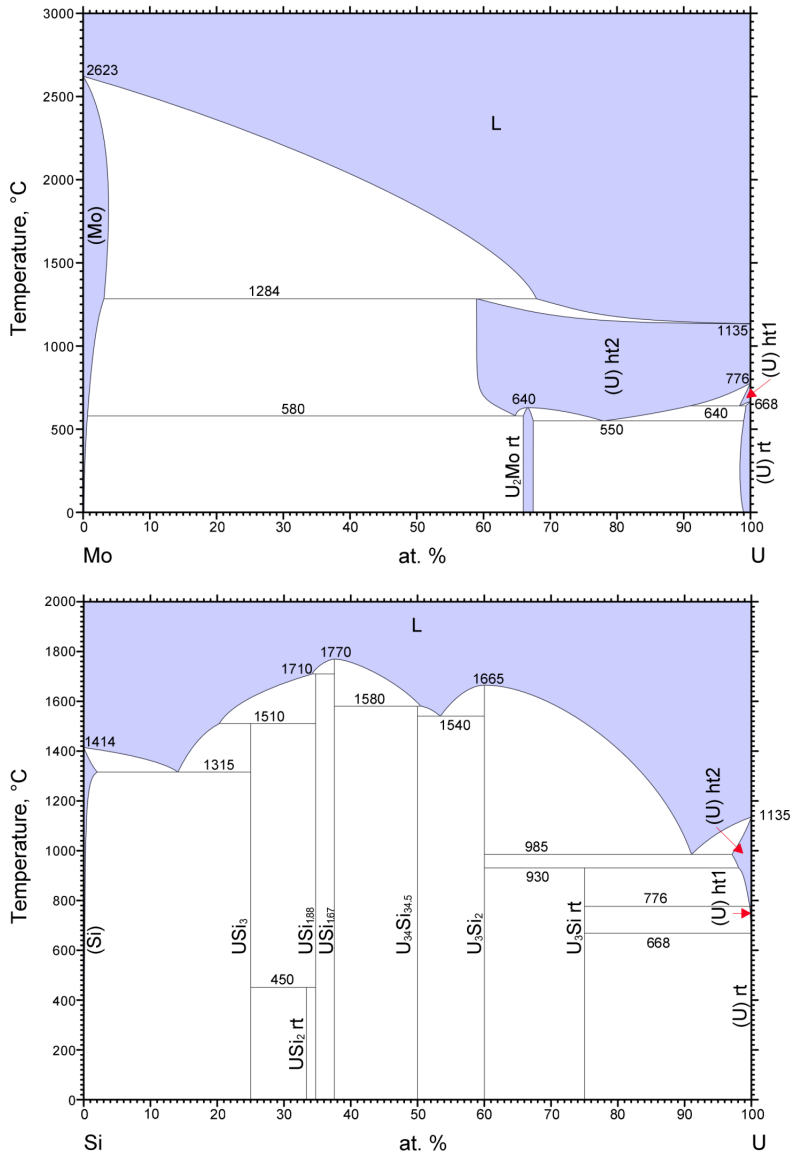
Al-U phase diagram from M. E. Kassner *et al*. (1990) [2].



Mo-Si phase diagram from C. Vahlas *et al*. (1989) [2].



Mo-Si phase diagram from A. B. Gokhale *et al*. (1990) [2].



Mo-U phase diagram from L. Brewer *et al*. (1980), reported by H. Okamoto (1990) [2].

Si-U phase diagram from H. Okamoto (1990) [2].

Figure 1. Phase diagrams of the 6 binaries alloys of the Al-Mo-Si-U quaternary system from the ASM Alloy Phase Diagram Center [2]. Note that for Mo-Si there are two versions of the phase diagrams.

For each of the six binaries, the phases that have been considered are:

Al-Mo: all nine compounds have been considered $Al_{12}Mo$ (cI26, $Im\overline{3}$), Al_5Mo (hP12, $P6_3$), $Al_{22}Mo_5$, $Al_{17}Mo_4$, Al_4Mo (mC30, Cm), Al_3Mo, $Al_{63}Mo_{37}$, AlMo (CI2, bcc), and $AlMo_3$ (A15) that decomposes in a peritectic reaction at the high temperature of 2150 ºC, as well as the two solid solutions, fcc (A1) and bcc (A2), and the liquid phase.

Al-Si: this is a simple eutectic-like alloy, with only the two solid solutions, fcc (A1) and diamond (A4), and the liquid phase.

Al-U: the three compounds Al_4U ($D1_b$), Al_3U ($L1_2$), and Al_2U (C15) that melts congruently at the high temperature of 1620 ºC, the four solid solutions: fcc (A1) and the three phases of U,

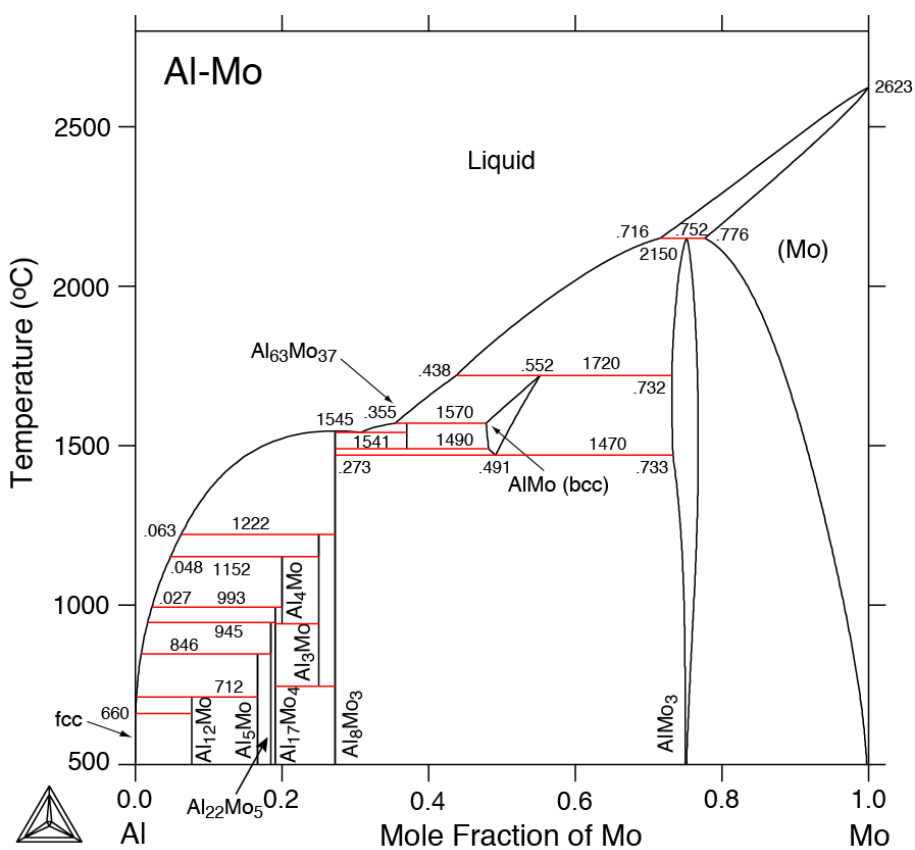
namely orthorhombic (A20), tetragonal (A_b), and bcc (A2), and the liquid state have been considered.

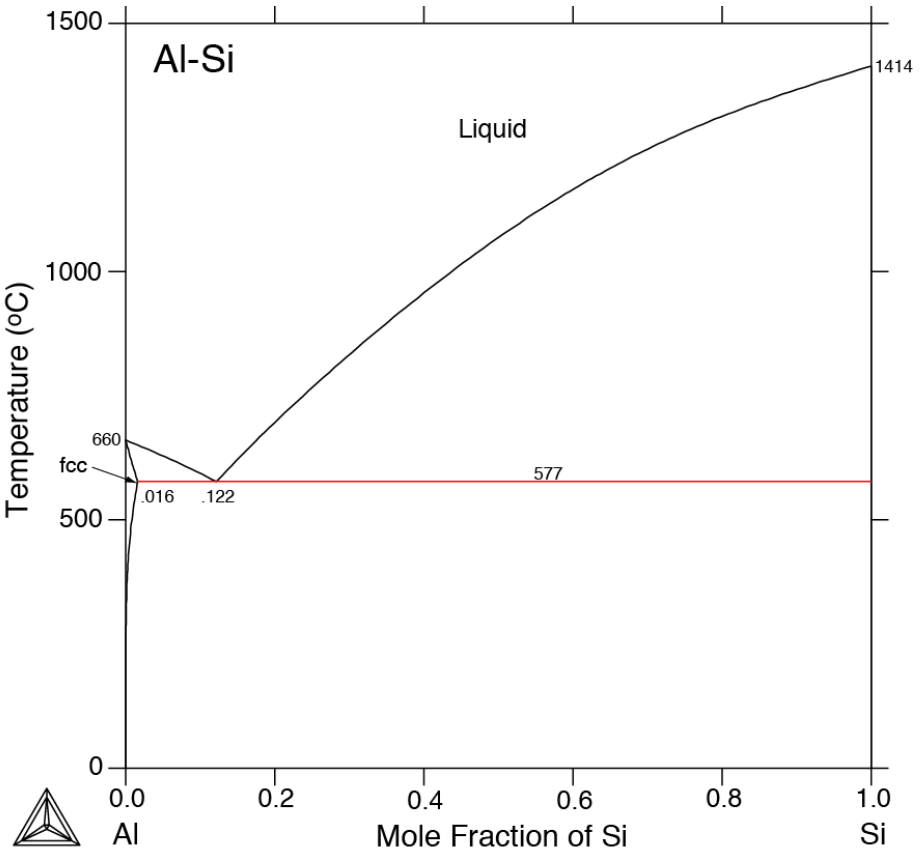
Mo-Si: the three compounds Mo_3Si (A15), Mo_5Si_3 ($D8_m$) that melts at the high temperature of 2180 ºC, and $MoSi_2$ ($C11_b$), the two solid solutions, fcc (A1) and diamond (A4), and the liquid state have been considered.

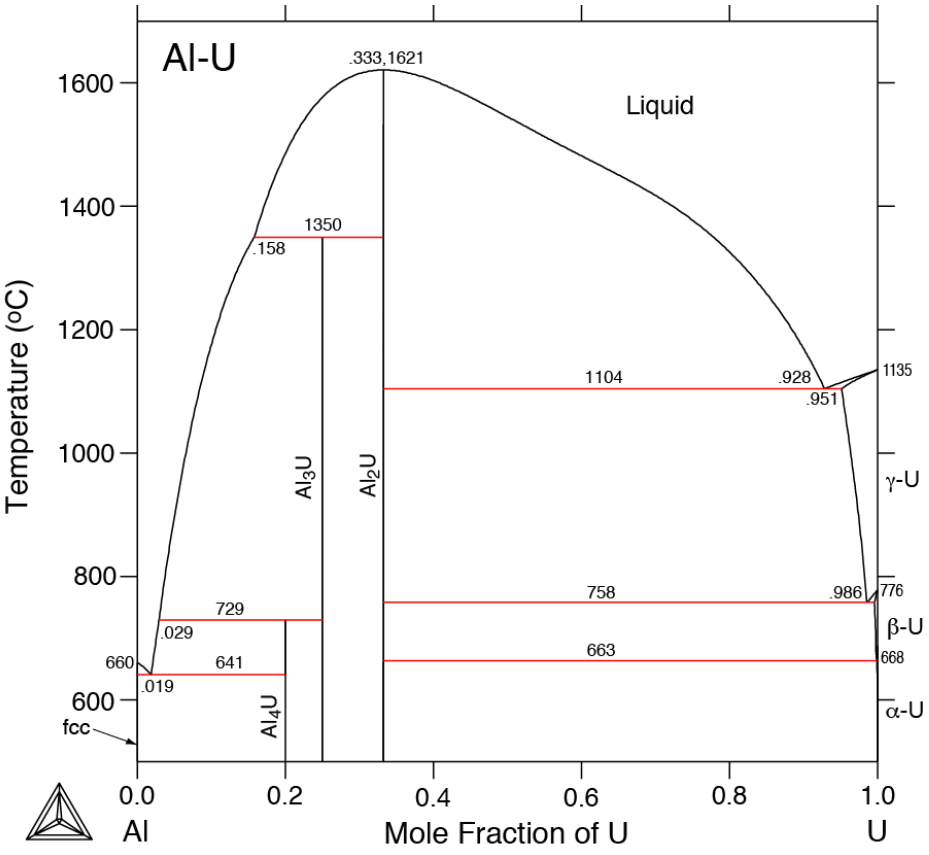
Mo-U: the compound MoU_2 ($C11_b$), the three solid solutions, fcc (A1) and the two extra phases of U, namely orthorhombic (A20) and tetragonal (A_b), and the liquid state has been considered.

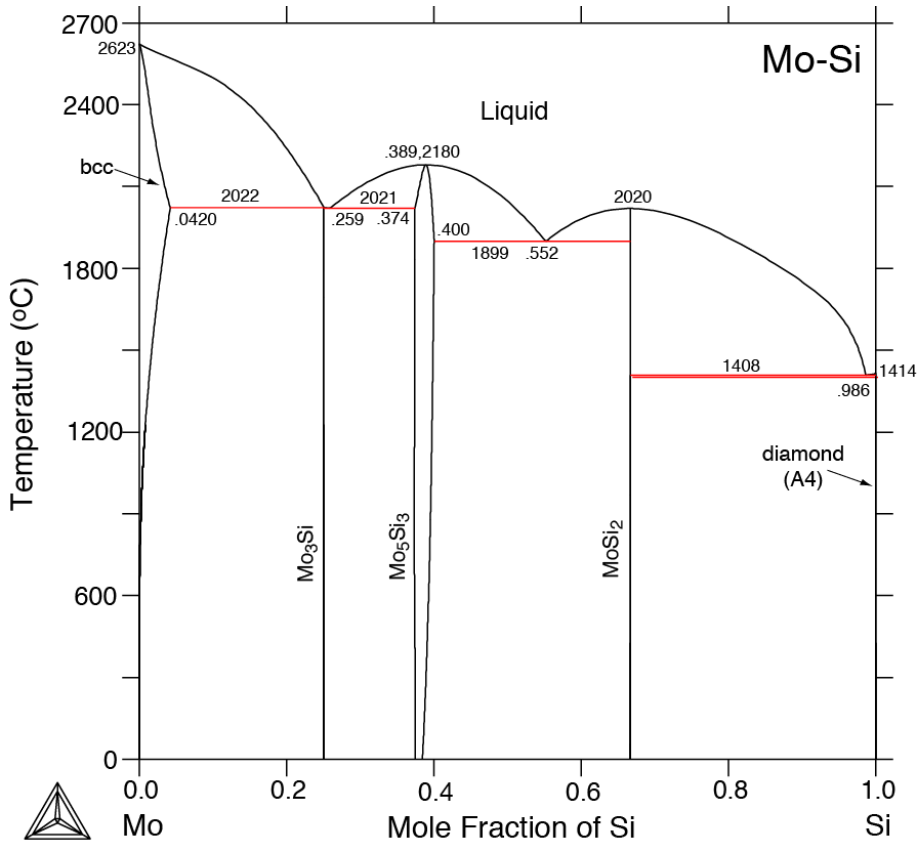
Si-U: all seven compounds have been considered Si_3U ($L1_2$), Si_2U (C32), $Si_{1.88}U$ (C_c), $Si_{\backslash 5}U_3$ (C32), SiU (B27), Si_2U_3 ($D5_a$) and SiU_3 ($L1_2$ or $D0_c$), as well as the two solid solutions, diamond (A4) and the three phases of U, namely orthorhombic (A20), tetragonal (A_b), and bcc (A2), and the liquid phase.

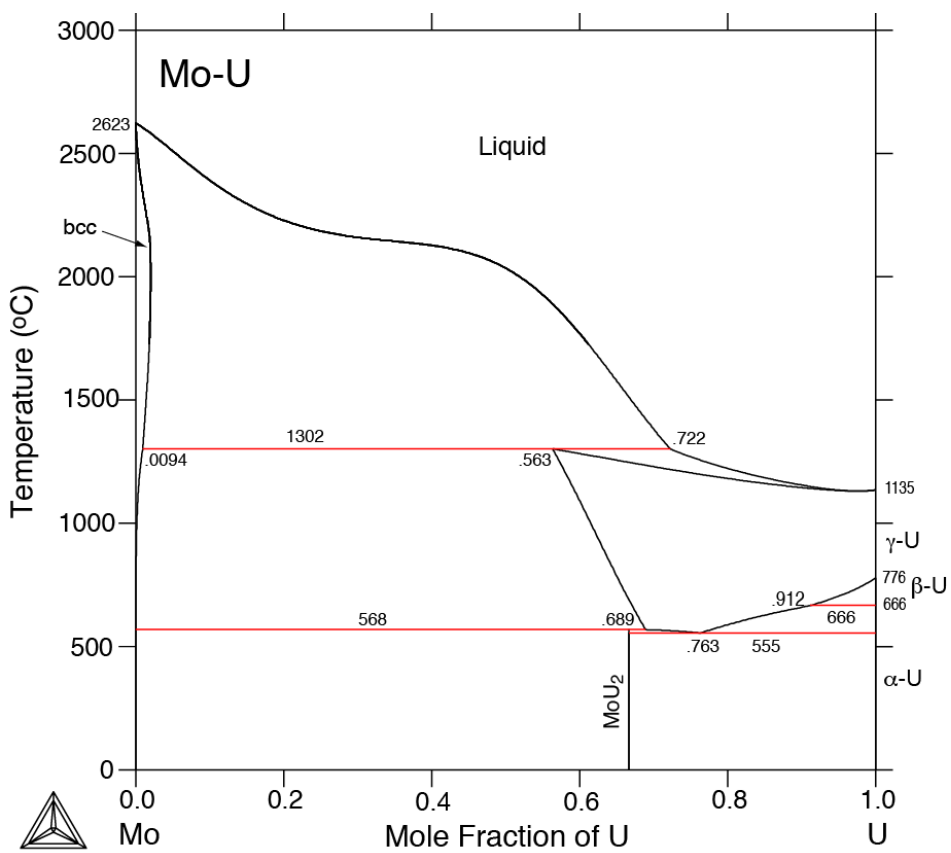
The thermodynamic database has been assembled for all 6 binary alloys, and the phase diagram results are shown in Fig. 2. Note that with U, the solutes Al, Mo, and Si primarily form Al_2U (C15) that melts congruently at the high temperature of 1620 ºC, MoU_2 that decomposes in two bcc phases at about 689 ºC, and SiU_3 that decomposes in an eutectoid reaction in γ-U (bcc) and Si_2U_3 at a temperature of 920 ºC, respectively.




Al-Si
Liquid
1414
660
fcc
.016
.122
577
Temperature (°C)
1500
1000
500
0
0.0
0.2
0.4
0.6
0.8
1.0
Al
Mole Fraction of Si
Si


Al-U
.333,1621
Liquid
1350
.158
1104
.928
.951
1135
γ-U
Al3U
Al2U
758
.986
776
β-U
729
.029
660
641
.019
663
668
α-U
Al4U
fcc
Temperature (°C)
1600
1400
1200
1000
800
600
0.0
0.2
0.4
0.6
0.8
1.0
Al
Mole Fraction of U
U


Mo-Si
Liquid
2700
2400
1800
1200
600
0
Temperature (°C)
2623
bcc
2022
.0420
2021
.259
.374
.389,2180
.400
1899
.552
2020
1408
1414
.986
diamond
(A4)
Mo3Si
Mo5Si3
MoSi2
0.0
0.2
0.4
0.6
0.8
1.0
Mo
Mole Fraction of Si
Si


Mo-U
Liquid
3000
2500
2000
1500
1000
500
0
Temperature (°C)
2623
bcc
1302
.0094
.563
.722
1135
γ-U
776
β-U
.912
666
568
.689
.763
555
α-U
MoU2
0.0
0.2
0.4
0.6
0.8
1.0
Mo
Mole Fraction of U
U

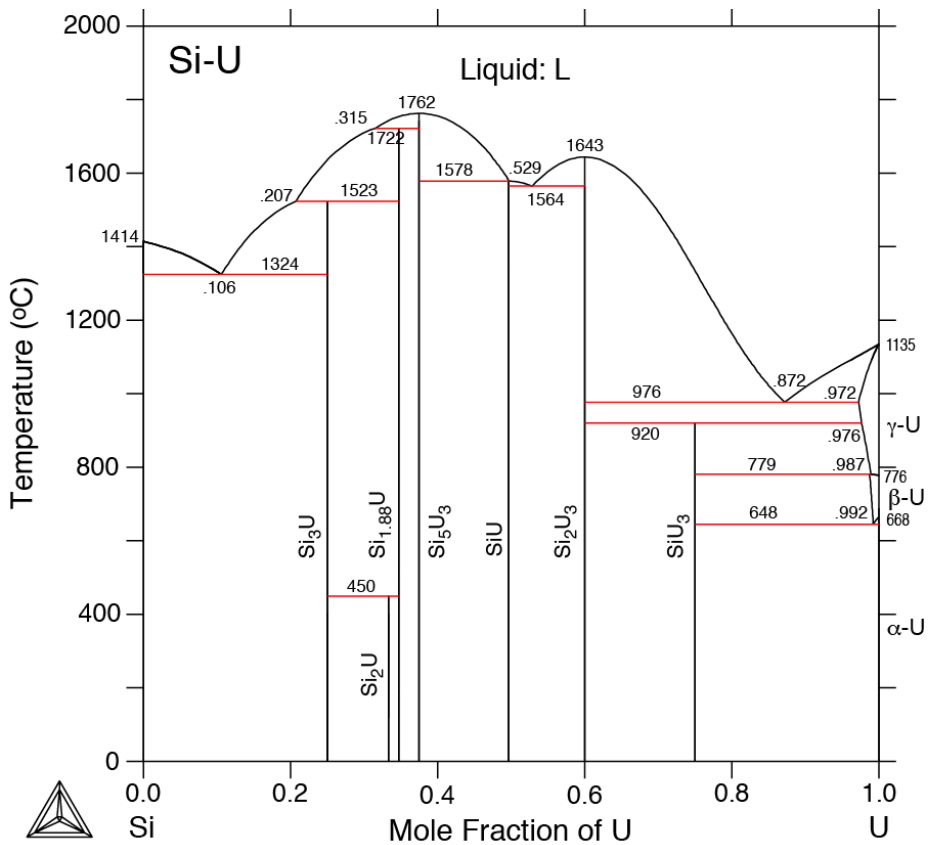


Figure 2. CALPHAD assessment of the six binaries subsystems of the Al-Mo-Si-U alloy.

II. CALPHAD-based thermodynamic modeling of the 4 ternaries of the quaternary Al-Mo-Si-U system

The bibliography related to the 4 ternary alloys and the quaternary system is summarized in Table II.

Ternary Alloy	References	Reference for Assessment
Al-Mo-Si	46-49	48
Al-Mo-U	50-67	63
Al-Si-U	68-71	N/A
Mo-Si-U	72-73	N/A
Al-Mo-Si-U	74-80	N/A

Table II. For each of the four ternary alloys that make up the quaternary Al-Mo-Si-U systems, the major references are cited in addition to the one (if any) that was used to carry out the thermodynamic assessment.

For each of the four ternary systems we considered the compounds that form in the binaries, and only in a few cases we had a few ternary compounds for which enough experimental data were available. This includes:

• for Al-Mo-Si system the C40 and C54 phases, $(Al,Si)_2Mo$ treated with a two-sublattice model, $(Al,Si)_{.667}:Mo_{.333}$, and

• for the Al-Mo-U, the two phases $Al_{43}Mo_4U_6$ and $Al_{20}Mo_2U$, treated with a four-sublattice model, $Al_{.566}:(Al,Mo)_{.208}:(Al,Mo)_{.113}:U_{.113}$, and a three sublattice model, $Al_{.783}:(Al,Mo)_{.174}:U_{.043}$, respectively.

Because of the complexity of the ternary systems, it is anticipated that other compounds that strictly form in the ternary systems may exist. For example, in the case of the Mo-Si-U ternary system, according to Ref. 72, ternary phases are found stable, including the stoichiometric compound $Mo_3Si_4U_2$ and the ternary $U(Mo_{1-x}Si_x)_2$ of $MgZn_2$-type (or C14, Laves) phase extending from x=.25 to x=.38 at 1400 ºC. This implies that the isothermal sections that are presented for each of the ternary system should be considered as representations, if not of the stable equilibrium, at least of the metastable equilibrium state. When more experimental data on new compounds in the ternary systems will be available, it will be relatively easy to introduce their thermodynamic description in the database.

The thermodynamic database has been assembled for all 4 ternary alloys, and the phase diagram results in terms of four isothermal sections at 400, 800, 1200, and 1600 ºC are shown in Figs. 3-6. It should be mentioned that because of the complexity of these phase diagrams in terms of the number of phases that can form at various temperatures, only a few major phase equilibria, in some instances, have been indicated in the isothermal sections for the sake of clarity.

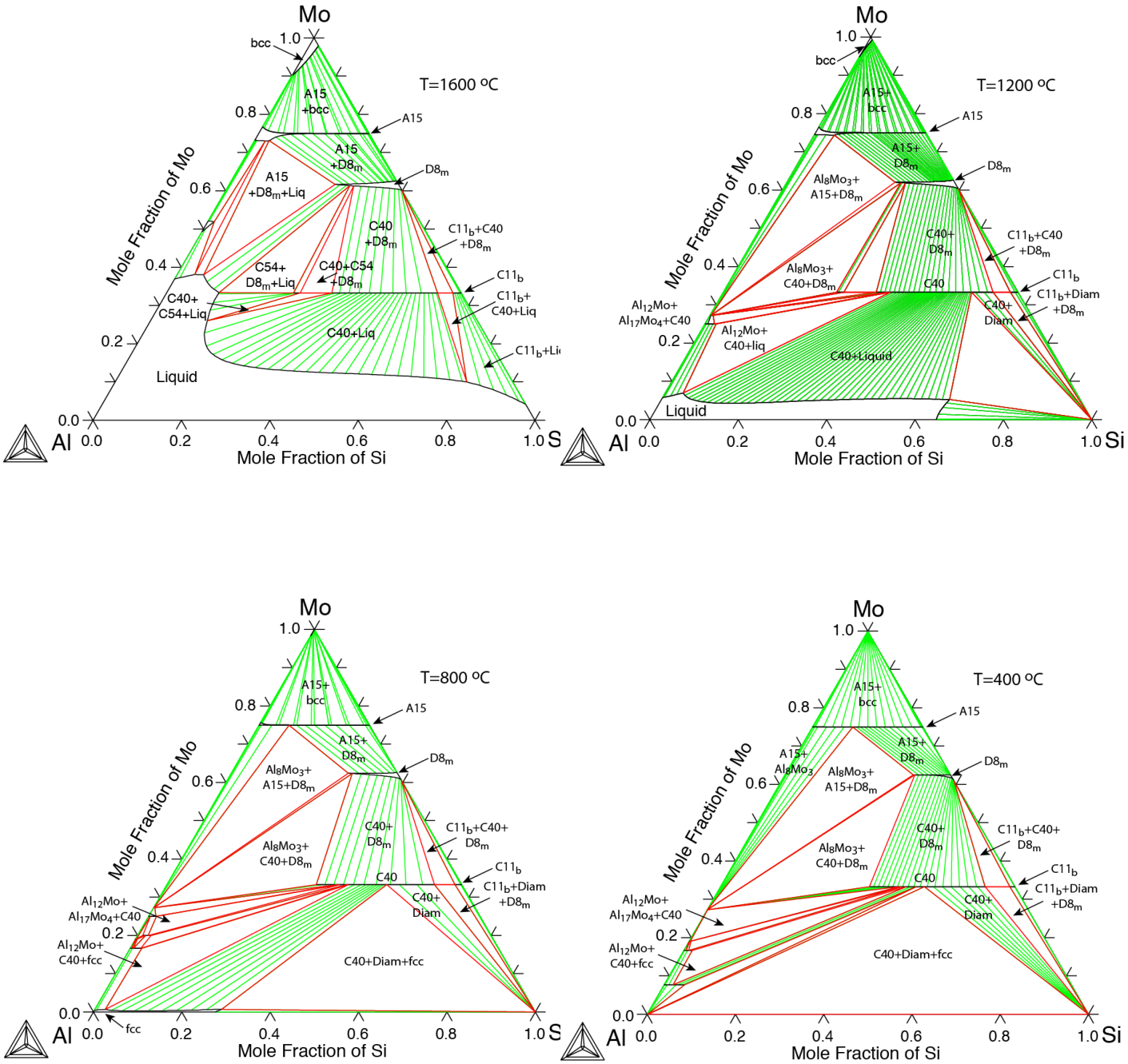


Figure 3. Thermodynamic assessment of the Al-Mo-Si phase diagram with representation of 4 isothermal sections at 1600, 1200, 800, and 400 ºC.

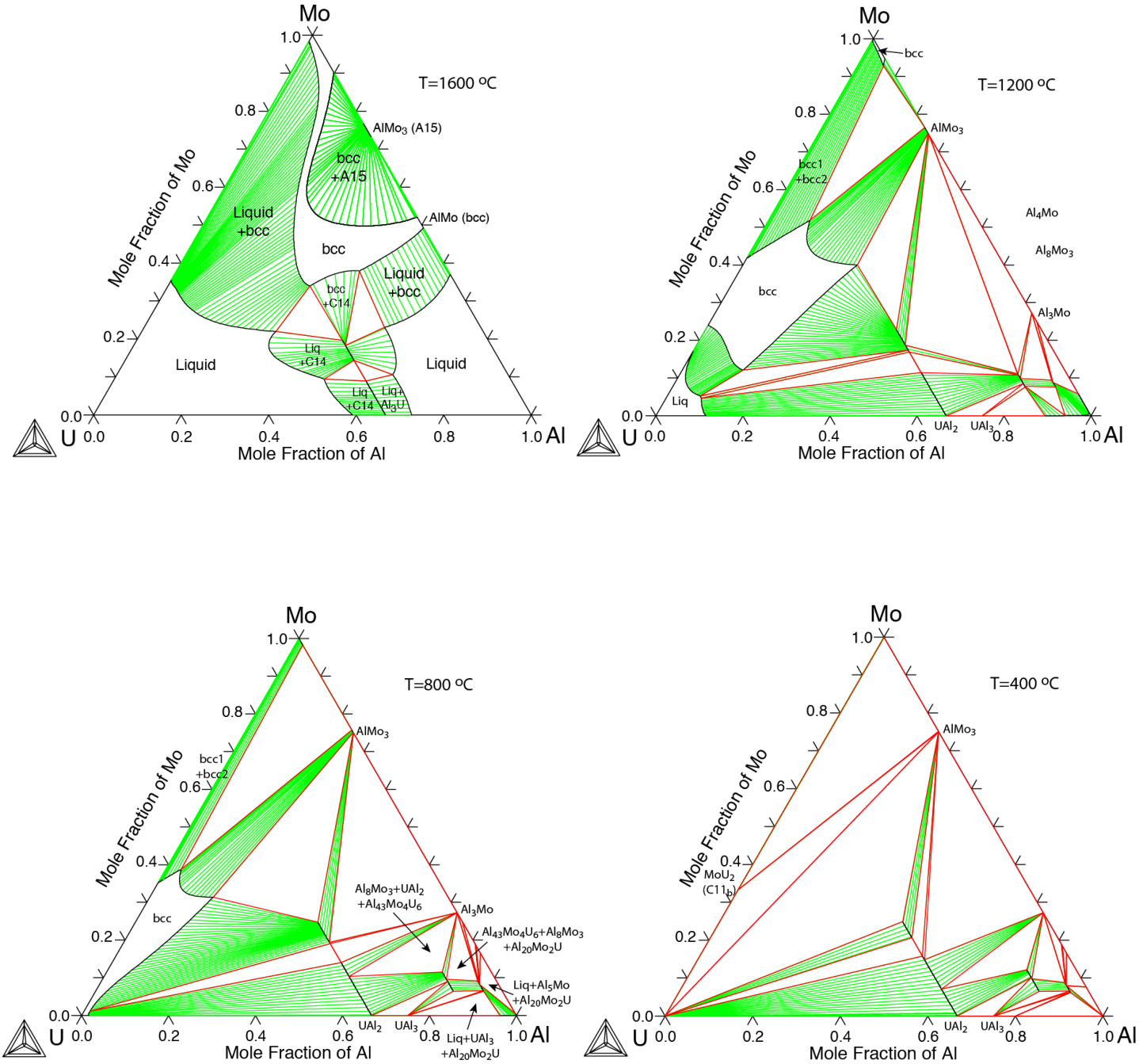


Figure 4. Thermodynamic assessment of the Al-Mo-U phase diagram with representation of 4 isothermal sections at 1600, 1200, 800, and 400 ºC.

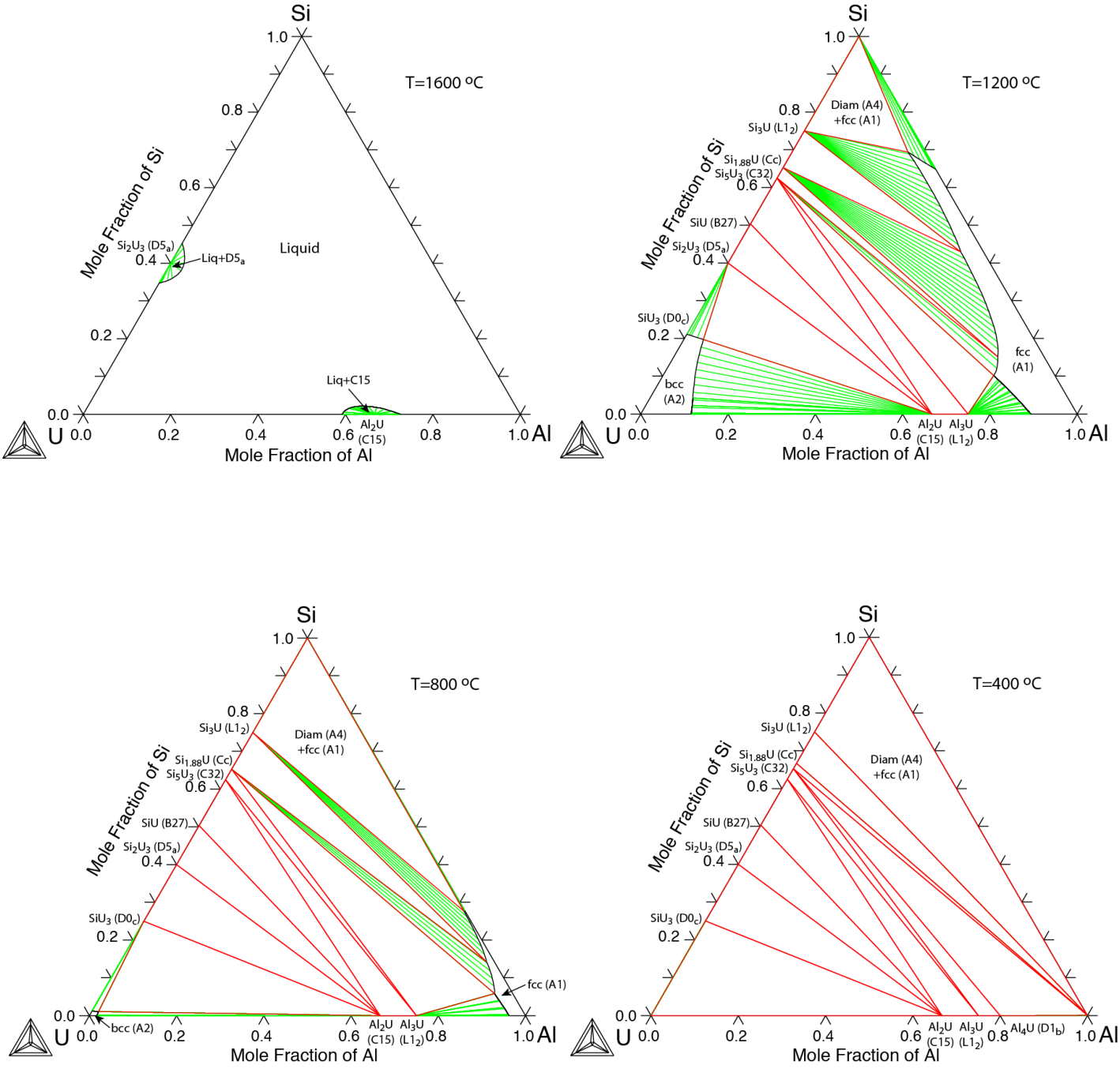


Figure 5. Thermodynamic assessment of the Al-Si-U phase diagram with representation of 4 isothermal sections at 1600, 1200, 800, and 400 ºC.

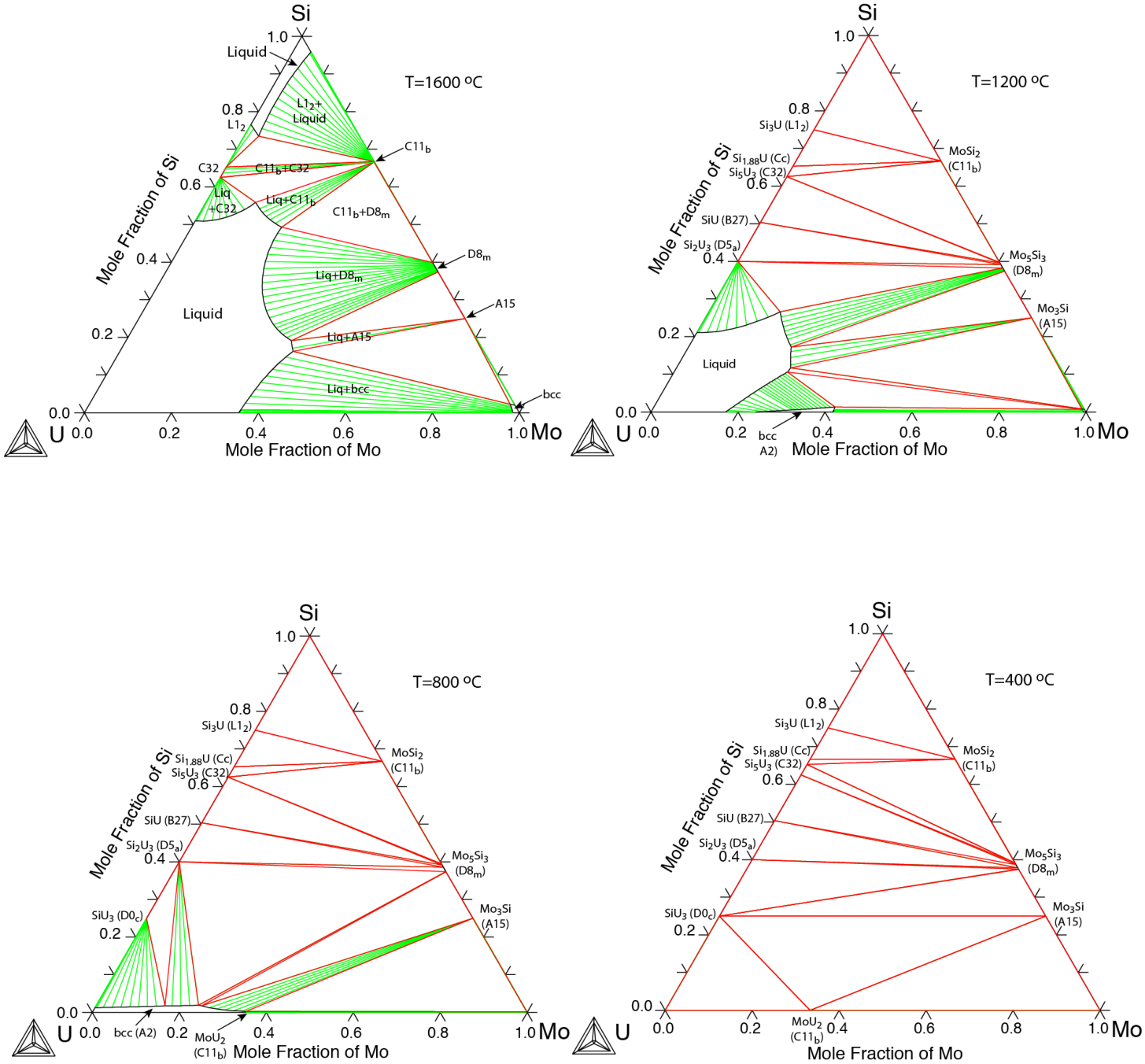


Figure 6. Thermodynamic assessment of the Mo-Si-U phase diagram with representation of 4 isothermal sections at 1600, 1200, 800, and 400 ºC.

With the knowledge gained on phase equilibria in these four ternary systems, one can find out which equilibrium phases are likely to form as function of temperature at a given alloy composition. For example, it has been reported [61] that considering two Al-Mo-U alloys, $Al_{85.7}Mo_{2.86}U_{11.44}$ and $Al_{87.5}Mo_{2.5}U_{10}$ (in at.%), the phases that are observed are fcc (Al-rich) solid solution, Al_4U, Al_3U, $Al_{43}Mo_4U_6$ and $Al_{20}Mo_2U$, except that for the second alloy the Al_3U is not observed. Using our thermodynamic database the property diagram of each of these two alloys was calculated. As a reminder, for a complex multi-component alloy at a specific alloy composition, the property diagram conveniently shows the phase fraction of each phase that forms as a function of temperature. This can be directly compared with experimental results, and as such constitutes a way of validating a thermodynamic database. In Fig. 7, the property diagram of each of the mentioned alloys is shown.

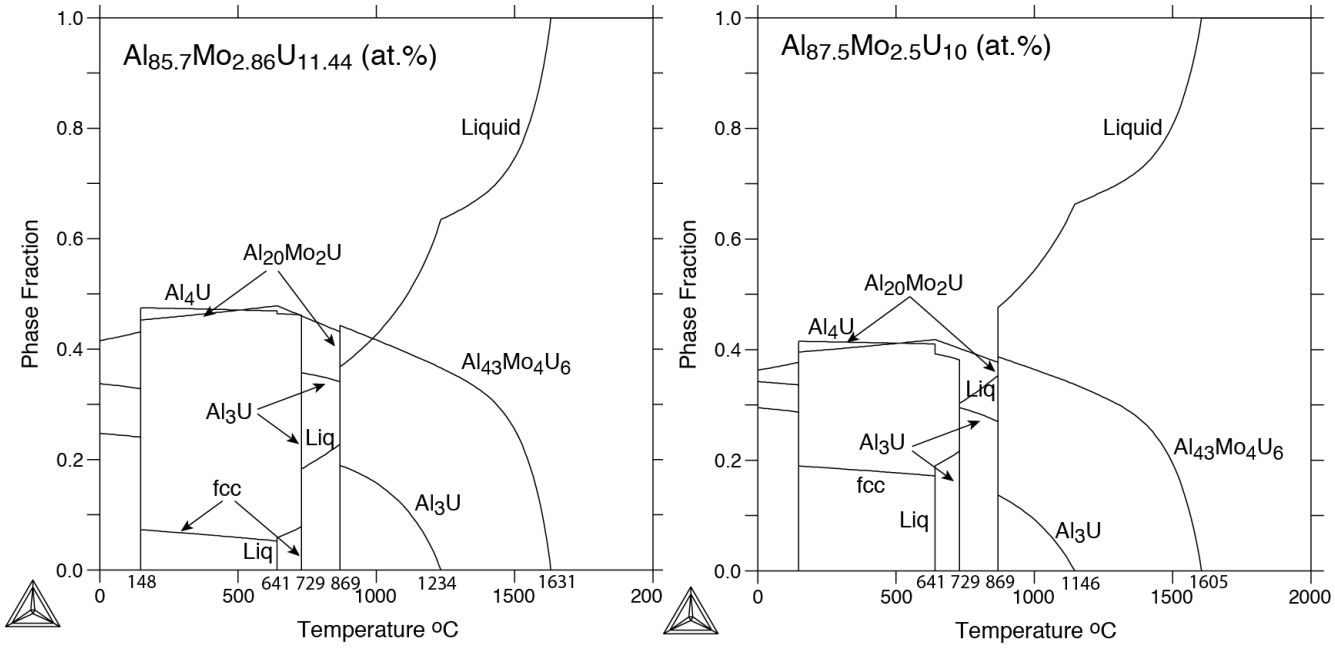


Figure 7. Based on the newly built thermodynamic database, property diagram of $Al_{85.7}Mo_{2.86}U_{11.44}$ (left) and $Al_{87.5}Mo_{2.5}U_{10}$ (right), in at.%.

Although for both alloy compositions the phases that form as functions of temperature are the same, their phase fractions are different. It is worth mentioning that the first phases to form are Al_3U and $Al_{43}Mo_4U_6$, and the phase fraction of Al_3U is lower for the slightly lower U-content alloy (right panel): This may explain why for this alloy this Al_3U phase is more difficult to observe. Also, one should note that crystallization occurs at similar temperatures, of about 1600 ºC whereas the last drop of liquid is observed down to 641 ºC, hence a huge undercooling in these alloys. This has consequences on how alloys at these compositions

should be treated as functions of temperature to ensure that true phase equilibrium is observed. Finally the phases that sequentially form below the liquidus surface are, in order of decreasing temperatures: $Al_{43}Mo_4U_6$ – Al_3U – $Al_{20}Mo_2U$ – {Al_4U, fcc solid solution}.
This proposed thermodynamic database for the quaternary Al-Mo-Si-U ally system can be used to predict the phases that may form under equilibrium condition for any alloy composition and temperature.

Conclusions and Recommendations

The thermodynamic properties of the six binary Al-Mo, Al-Si, Al-U, Mo-Si, Mo-U, and Si-U alloy systems have been reported in a single consistent thermodynamic database that is given in Appendix II, and without additional assumption on ternary interactions to describe the excess Gibbs energy, G_{mix}^{xs} (see Appendix I), of the four ternary Al-Mo-Si, Al-Mo-U, Al-Si-U, and Mo-Si-U and the quaternary Al-Mo-Si-U alloy systems, isothermal sections of the ternary phase diagrams that are relevant for the RERTR program have been proposed to predict phase occurrence as a function of temperature and thermodynamic properties.

In summary, for the second semester the accomplishments are:

1. An extensive literature search on phase stability properties of Al-Mo, Al-Si, Al-U, Mo-Si, Mo-U, Si-U, Al-Mo-Si, Si-Mo-U, Al-Si-U, Mo-Si-U, and Al-Mo-Si-U alloys has been completed.
2. Within the CALPHAD framework, the six binary phase diagrams and isothermal sections of the ternary alloys have been predicted.
3. A database has been built in a consistent way to predict the thermodynamic properties of the quaternary Al-Mo-Si-U alloy system.

Additional funding would have been needed to explicitly show the critical knowledge that one could gain from this newly developed database for the purpose of licensing an adequate fuel form and evaluating fuel performance on a sound scientific basis, themes that are of interest to those involved in various NE programs, and especially the Advanced Fuel Cycle R&D (AFCRD) and the Reduced Enrichment for Research and Test Reactors (RERTR) programs.

The two thermodynamic databases[‡] that have been built this year to study Mo-Pu-U (cf. Appendix II for a description of the thermodynamic database for the Mo-Pu alloy system), and Al-Mo-Si-U alloys are crucial for understanding phase formation in complex actinide mixtures as a function of burn-up, and also provide important input data in terms of thermodynamic driving forces for kinetic modeling of phase transformations, and meso-scale modeling of microstructure evolution, both crucially contributing to building up a physics-based assessment of nuclear fuel performance. All these results could be explored for practical applications to fuel performance modeling if funding had been allocated for FY13 and beyond. It is also important that the role of fission products, including transuranic elements on fuel stability and its evolution as a function of burn-up, even in the case of the more popular {Pu,U,O} MOX fuels remain to be thoroughly studied, and this effort should start with the detailed development of a validated thermodynamic database.

Acknowledgements

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Work at LLNL was funded by the DOE-NE NEAMS program. Part of the *ab initio* work has been funded by the Laboratory Directed Research and Development Program at LLNL under project tracking code 12-SI-008.

[‡] An electronic version of the thermodynamic databases for Mo-Pu and Al-Mo-Si-U, to be directly used with Thermo-Calc® software, are electronically available by contacting the PI of this project at <turchi1@llnl.gov>.

Publications

1. "Thermodynamic study of the Mo-Pu system", P. E. A. Turchi, A. I. Landa, and P. A. Söderlind, to be published in Journal of Nuclear Materials (2012).
2. "Density-functional study of bcc U-Mo, Np-Mo, Pu-Mo, and Am-Mo alloys", A. Landa, P.E.A. Turchi, and P. Söderlind, accepted for publication in Journal of Nuclear Materials (2012).
3. "Thermodynamic re-assessment of the Mo-U system with input from *ab initio*", P. E. A. Turchi, A. I. Landa, and P. A. Söderlind, to be submitted to Journal of Nuclear Materials (2012).

Invited Presentations

1. October 2011: One invited presentation at the Symposium on "Phase Stability, Kinetics, and their Applications (PSDK-VI)" at MS&T'11 in Columbus (OH), October 16-20, 2011, organized by J. C. Lacombe, Y. H. Sohn, U. Kattner, R. Arroyave, A. Misra, and J. Morral:
P. E. A. Turchi, A. I. Landa, and P. Söderlind, "Thermodynamic database validation and the role of *ab initio*".

2. November 2011: One invited lecture at the Materials Science Program seminar series at the University of Wisconsin-Madison (WI), November 10, 2011, hosted by Prof. J. H. Perepezko:
P. E. A. Turchi, "Thermodynamics of alloys: The road from *ab initio* to phenomenology".

3. November 2011: One invited lecture at Idaho National Laboratory, Idaho Falls (ID), November 16, 2011, hosted by Dr. Rory Kennedy, head of the Metal Fuel Development Technical Area:
P. E. A. Turchi, "The Science of advanced nuclear fuels: Opportunities for collaboration".

4. March 2012: Two oral presentations at the Symposium on "Materials for the Current and Advanced Nuclear Reactors", at TMS 2012 Annual Meeting and Exhibition, in Orlando (FL), March 11-15, 2012, organized by R. Prabhakaran, D. Keiser, and R. Rebak:
• P. E. A. Turchi, A. I. Landa, and P. Söderlind: "Thermodynamic properties of complex actinide alloys". (LLNL-PRES-535971)
• V. Lordi, M. Wall, L. Hsiung, R. Foreman, and P. E. A. Turchi, "Inter-diffusion kinetics in U-Zr". (LLNL-ABS-491639)
• Session Chair for the Thursday session on "Materials for the Current and Advanced Nuclear Reactors: Modeling II", March 15, 2012.

5. March 2012: One oral presentation at the Symposium on "Computational Thermodynamics and Kinetics: Cluster Expansion, Kinetic Monte Carlo, and First-principles", at TMS 2012 Annual Meeting and Exhibition, in Orlando (FL), March 11-15, 2012, organized by Z.-K. Liu, M. Asta, J. Warren, Y. Wang, R. Arroyave, and Yu Wang:
A. I. Landa, P. Söderlind, P. E. A. Turchi, A. Ruban, and L. Vitos: "*Ab initio* study of advanced metallic nuclear fuels for fast breeder reactors". (Abs: LLNL-ABS-490670, Pres: LLNL-PRES-535793)

7. April 2012: One invited oral presentation at Symposium Y on "Actinides – Basic Science, Applications, and Technology", at the Spring MRS Meeting in San Francisco, April 9-13, 2012, organized by Sung Woo Yu, Tomasz Durakiewicz, Corwin Booth, Peter C. Burns, and Roberto Caciuffo:
A. Landa, P. Söderlind, B. Grabowski, P.E. A. Turchi, A. V. Ruban, and L. Vitos, "*Ab initio* study of advanced metallic nuclear fuels for fast breeder reactors". (LLNL-ABS-508933)

8. May 2012: One invited presentation at the "2012 NIST Diffusion Workshop" in Gaithersburg (MD), May 3-5, 2012, organized by C. Campbell:
P. E. A. Turchi, "Pseudo-potential method and its limitations". (LLNL-PRES-553992).

9. June 2012: One invited presentation at the International CALPHAD XLI Conference organized by Mark Asta and Patrice E.A. Turchi, in Berkeley (CA), June 3-8, 2012:
A.I. Landa, P. Söderlind, B. Grabowski, P.E.A. Turchi, A.V. Ruban, and L. Vitos, "*Ab Initio* Study of Advanced Metallic Nuclear Fuels for Fast Breeder Reactors" (LLNL-ABS-541312).

10. July 2012: One Invited presentation at the International Workshop on "Electron Correlations and Materials Properties of Compounds and Alloys", organized by Igor Abrikosov, Nikitas Gidopoulos, Tony Gonis, G. M. Stocks, and P. E. A. Turchi, in Porto Heli (Greece), July 9-13, 2012:
P. E. A. Turchi, A. I. Landa, V. Lordi, Per Söderlind, "Electronic Structure and Thermodynamics of Actinide-based Alloys".

11. October 2012: One poster presentation at the session on "Energy Issues", at MS&T 2012 Conference and Exhibition, in Pittsburgh (PA), October 07-11, 2012:
T. Duong, S. Bajaj, A. Landa, P. E. A. Turchi, and R. Arroyave "Density functional study of Uranium-Niobium system".

12. October 2012: One oral presentation at the Symposium on "Materials Development for Nuclear Applications and Extreme Environments", at MS&T 2012 Conference and Exhibition, in Pittsburgh (PA), October 07-11, 2012, organized by R. Rebak, K. Fox, R. Prabhakaran, A. A. Csontos, K. Sridharan, B. Lee, E. Hoffman, and E. G. Reddy:
J. T. McKeown, S. Ahn, S. Irukuvarghula, M. Wall, L. L. Hsiung, S. McDeavitt, P. E. A. Turchi, "Characterization of U-Zr alloys for ultra-high burn-up nuclear fuels".

13. October 2012: One invited presentation at the Symposium on "Materials Development for Nuclear Applications and Extreme Environments", at MS&T 2012 Conference and Exhibition, in Pittsburgh (PA), October 07-11, 2012, organized by R. Rebak, K. Fox, R. Prabhakaran, A. A. Csontos, K. Sridharan, B. Lee, E. Hoffman, and E. G. Reddy:
P. E. A. Turchi, A. I. Landa, and P. A. Söderlind, "Thermodynamics of Actinide Alloys: Application to RERTR Nuclear Fuels".

14. October 2012: One invited presentation at the 6th International Conference on Multiscale Marterials Modeling (MMM 2012), in Singapore, October 15-19, 2012:
P. E. A. Turchi, A. I. Landa, P. A. Söderlind, J.-L. Fattebert, V. Lordi, and M. Tang, "Thermodynamics, Kinetics, and Microstructures of Actinide-based Materials".

15. October 2012: One keynote presentation at the Nuclear Materials Conference, NuMat 2012, "Materials Development for Nuclear Applications and Extreme Environments", in Osaka (Japan), October 21-25, 2012:
P. E. A. Turchi, A. I. Landa, J.-L. Fattebert, V. Lordi, M. Tang, and P. A. Söderlind, "*Ab Initio* Properties and Thermodynamics of Metallic Nuclear Fuels – A Current Status".

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APPENDIX I. Thermo-Calc Application Software and CALPHAD Modeling

Thermo-Calc® version S [A1.1] is a commercially available software code that fulfills the need for critical modeling and analysis of data to:

• Produce, refine, and analyze multi-component phase diagrams of alloys at relevant temperatures for predicting phase stability properties.

• Determine the solidification path and long-term aging of alloys.

• Generate isothermal sections of multi-component alloy phase diagrams at relevant temperatures, isopleths, and property diagrams (phase fractions as functions of temperature), and composition versus temperature for all stable and metastable phases forming.

• Simulate phase transformations according to the Scheil-Gulliver model (for which local equilibria, infinite diffusion in the liquid phase, and no back diffusion in the solid phase are assumed).

Thermo-Calc® is specially designed for systems with strongly non-ideal phases. It has gained a worldwide reputation as the best software application for calculation of multi-component phase diagrams. It is the only commercially available software that can calculate arbitrary phase diagram sections with up to five independent variables in multi-component systems. There are also modules to calculate many other types of properties, such as, Scheil-Gulliver solidification simulations, Pourbaix diagrams, partial pressures in gases, and more [A1.1].

In the CALPHAD approach [A1.2-A1.7], the Gibbs energy of individual phases is modeled, and the model parameters are collected in a thermodynamic database. It is the modeling of the Gibbs energy of individual phases and the coupling of phase diagram and thermo-chemistry that make the CALPHAD a powerful technique in computational thermodynamics of multi-component materials. Models for the Gibbs energy are based on the crystal structures of the phases. For pure elements and stoichiometric compounds, the most commonly used model is the one suggested by the Scientific Group Thermodata Europe (SGTE) [A8] and has the following form (for simplicity, the pressure dependence and the magnetic contribution are not shown here),

$$G_m - H_m^{SER} = a + bT + cT\ln(T) + \sum d_i T^i \qquad \text{(A.1)}$$

The left-hand side of Eq. A.1 is defined as the Gibbs energy relative to a standard element reference state (SER), where H_m^{SER} is the enthalpy of the element in its stable state at 298.15 K and 1 bar of pressure. Coefficients, a, b, c, and d_i are the model parameters. The SGTE data for all the pure elements of the periodic table have been compiled by Dinsdale [A1.8].

For multi-component solution phases, the Gibbs energy has the following general expression [A1.2,A1.3,A1.6,A1.7],

$$G = G^o + G_{mix}^{ideal} + G_{mix}^{xs} \tag{A.2}$$

where G^o is the contribution from the mechanical mixing of the pure components, G_{mix}^{ideal} is the ideal mixing contribution, and G_{mix}^{xs} is the excess Gibbs energy of mixing due to non-ideal interactions. Sublattice models have been widely used to describe solution phases [A1.3, A1.6, A1.7]. For example, for a simple phase with two sublattices in an A-B binary system where the two components enter both sublattices, the sublattice model is written as $(A,B)_p(A,B)_q$, where subscripts p and q denote the number of sites of each sublattice. More specifically, the three terms in Eq. A.2 are written as,

$$G^o = y_A^I y_A^{II} G_{A:A}^o + y_A^I y_B^{II} G_{A:B}^o + y_B^I y_A^{II} G_{B:A}^o + y_B^I y_B^{II} G_{B:B}^o \tag{A.3}$$

$$G_{mix}^{ideal} = pRT\left(y_A^I \ln y_A^I + y_B^I \ln y_B^I\right) + qRT\left(y_A^{II} \ln y_A^{II} + y_B^{II} \ln y_B^{II}\right) \tag{A.4}$$

$$\begin{aligned} G_{mix}^{xs} = {} & y_A^I y_B^I \left(y_A^{II} \sum_{k=0} L_{A,B:A}^k (y_A^I - y_B^I)^k + y_B^{II} \sum_{k=0} L_{A,B:B}^k (y_A^I - y_B^I)^k \right) \\ & + y_A^{II} y_B^{II} \left(y_A^I \sum_{k=0} L_{A:A,B}^k (y_A^{II} - y_B^{II})^k + y_B^I \sum_{k=0} L_{B:A,B}^k (y_A^{II} - y_B^{II})^k \right) \end{aligned} \tag{A.5}$$

where y^I and y^{II} are the site fractions of A or B in the first and second sublattices, respectively. $G_{I:J}^o$ is the Gibbs energy of the compound I_pJ_q, expressed by Eq. 1. $L_{A,B:*}^k$ ($L_{*:A,B}^k$) is the kth order interaction parameter between component A and B in the first (second) sublattice. In this notation, a colon separates components occupying different sublattices, and a comma separates interacting components in the same sublattice. These equations can be generalized for phases with multi-components and multi-sublattices, and they reduce to a random substitutional model when there is only one sublattice.

For a multi-component solution in a particular phase Φ described with a single sublattice model, the three contributions to the total Gibbs energy reduce to [A1.3, A1.6, A1.7]:

$$\begin{aligned} {}^{\Phi}G^o &= \sum_I c_I \, {}^{\Phi}G_I^o \\ {}^{\Phi}G_{mix}^{ideal} &= RT \sum_I c_I \ln c_I \\ {}^{\Phi}G_{mix}^{xs} &= \sum_I \sum_{J>I} c_I c_J \sum_k {}^{\Phi}L_{I,J}^k \left(c_I - c_J\right)^k \end{aligned} \tag{A.6}$$

where the molar Gibbs energy of mixing is expressed by a Redlich-Kister expansion [A1.9]. In these expressions c_I is the composition of the alloy in species I, and the $L^k_{I,J}$ is the kth-order binary interaction parameter between species I and J usually expressed as a first-order polynomial in temperature T: $L^k_{I,J} = a^k_{I,J} + b^k_{I,J}T$. Note that in both sets of expressions the excess Gibbs energy due to non-ideal contributions is expressed within the Muggianu approximation [A1.10].

Data generated with the Thermo-Calc® software also provide the basis for more accurate predictions of diffusion kinetics and ultimately TTT (temperature-time-transformations) diagrams with the DICTRA® software [A1.1, A1.11] by assuming diffusion both in the liquid and the solid phase. Note that the results of both equilibrium solidification and Scheil-Gulliver simulations generated by Thermo-Calc® correspond to upper and lower bounds for the DICTRA® results.

Input data files used by Thermo-Calc® are: KP (Kaufman binary alloys database), SSOL4 (Scientific Group Thermodata Europe, or SGTE, solution database), from published journals, and/or from qualified sources. Here to describe the selected alloys systems, a thermodynamic database has been developed.

References

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[A1.11] A. Engström, L. Höglund, and J. Ågren, "Computer simulations of diffusion in multiphase systems", Metall. Mater. Trans. **25A**, 1127-1134 (1994); A. Borgenstam, A. Engström, L. Höglund, and J. Ågren, "DICTRA, a tool for simulation of diffusional transformations in alloys", J. of Phase Equil. **21** (3), 269-280 (2000).

APPENDIX II. Thermodynamic databases for the Al-Mo-Si-U and the Mo-Pu alloy systems

The two database, .TDB, files that have been assembled can be used as input to the Thermo-Calc® software [A2.1] to predict the thermodynamic properties of all subsystems included in the quaternary Al-Mo-Si-U alloy system (an electronic version of this two TDB files is available upon request by contacting the PI).

Reference

[A2.1] The Thermo-Calc and DICTRA applications software are products of Thermo-Calc AB; B. Sundman, B. Jansson, and J.-O. Andersson, "The Thermo-Calc Databank System", CALPHAD **9** (4), 153 (1985); J.-O. Andersson, T. Helander, L. Höglund, Pingfang Shi, and B. Sundman, "THERMO-CALC & DICTRA, computational tools for materials science", CALPHAD **26** (2), 273-312 (2002); cf. also http://www.thermocalc.se.

```
$*********************************************************************
$
$            Database file *** AlMoSiU.TDB *** Assembled by P.E.A. Turchi
$
$                                *** {Al,Mo,Si,U} ***
$
$ With data for the pure elements from the PURE4 database.
```

```
$
$ Al-Mo  Al-Si  Al-U
$        Mo-Si  Mo-U
$               Si-U
$
$ Al-Mo-Si  Al-Mo-U  Al-Si-U
$                    Mo-Si-U
$
$ Al-Mo-Si-U
$
$*********************************************************************

 ELEMENT /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00!
 ELEMENT VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00!
 ELEMENT AL   FCC_A1                    2.6982E+01  4.5773E+03  2.8322E+01!
 ELEMENT MO   BCC_A2                    9.5940E+01  4.5890E+03  2.8560E+01!
 ELEMENT SI   DIAMOND_A4                2.8085E+01  3.2175E+03  1.8820E+01!
 ELEMENT U    ORTHORHOMBIC(A20)         2.3803E+02  0.0000E+00  0.0000E+00!


 FUNCTION GHSERAL    298.15  -7976.15+137.093038*T-24.3671976*T*LN(T)
   -.001884662*T**2-8.77664E-07*T**3+74092*T**(-1);  700  Y
    -11276.24+223.048446*T-38.5844296*T*LN(T)+.018531982*T**2
   -5.764227E-06*T**3+74092*T**(-1);  933.47  Y
    -11278.378+188.684153*T-31.748192*T*LN(T)-1.230524E+28*T**(-9); 2900 N !
 FUNCTION GHSERMO    298.15  -7746.302+131.9197*T-23.56414*T*LN(T)
   -.003443396*T**2+5.66283E-07*T**3+65812*T**(-1)-1.30927E-10*T**4; 2896 Y
    -30556.41+283.559746*T-42.63829*T*LN(T)-4.849315E+33*T**(-9); 5000 N !
 FUNCTION GHSERSI    298.15  -8162.609+137.236859*T-22.8317533*T*LN(T)
   -.001912904*T**2-3.552E-09*T**3+176667*T**(-1); 1687 Y
    -9457.642+167.281367*T-27.196*T*LN(T)-4.20369E+30*T**(-9); 3600 N !
 FUNCTION GHSERUU    298.15  -8407.734+130.955151*T-26.9182*T*LN(T)
    +.00125156*T**2-4.42605E-06*T**3+38568*T**(-1); 955 Y
     -22521.8+292.121093*T-48.66*T*LN(T); 3000 N !
 FUNCTION GLIQAL  298.15  +3028.879+125.251171*T-24.3671976*T*LN(T)
   -.001884662*T**2-8.77664E-07*T**3+74092*T**(-1)+7.9337E-20*T**7; 700 Y
    -271.21+211.206579*T-38.5844296*T*LN(T)+.018531982*T**2-5.764227E-06*T**3
  +74092*T**(-1)+7.9337E-20*T**7;  933.47 Y
   -795.996+177.430178*T-31.748192*T*LN(T); 2900 N REF1 !
 FUNCTION GLIQMO  2.98150E+02  +34085.045+117.224788*T-23.56414*T*LN(T)
   -.003443396*T**2+5.66283E-07*T**3+65812*T**(-1)-1.30927E-10*T**4
   +4.24519E-22*T**7;  2896 Y
    +3538.963+271.6697*T-42.63829*T*LN(T);  5000 N REF1 !
 FUNCTION GLIQSI  2.98150E+02  +42533.751+107.13742*T-22.8317533*T*LN(T)
   -.001912904*T**2-3.552E-09*T**3+176667*T**(-1)+2.09307E-21*T**7; 1687 Y
    +40370.523+137.722298*T-27.196*T*LN(T); 3600 N REF1 !
 FUNCTION GLIQUU  2.98150E+02  +3947.766+120.631251*T-26.9182*T*LN(T)
   +.00125156*T**2-4.42605E-06*T**3+38568*T**(-1); 955 Y
   -10166.3+281.797193*T-48.66*T*LN(T); 3000 N REF1 !
 FUNCTION GBCCAL  298.15  +2106.85+132.280038*T-24.3671976*T*LN(T)
   -.001884662*T**2-8.77664E-07*T**3+74092*T**(-1); 700 Y
    -1193.24+218.235446*T-38.5844296*T*LN(T)+.018531982*T**2
   -5.764227E-06*T**3+74092*T**(-1);  933.47  Y
   -1195.378+183.871153*T-31.748192*T*LN(T)-1.230524E+28*T**(-9); 2900 N REF1 !
 FUNCTION GBCCSI  298.15  +38837.391+114.736859*T-22.8317533*T*LN(T)
   -.001912904*T**2-3.552E-09*T**3+176667*T**(-1); 1687 Y
    +37542.358+144.781367*T-27.196*T*LN(T)-4.20369E+30*T**(-9); 3600 N REF1 !
 FUNCTION GBCCUU  298.15  -752.767+131.5381*T-27.5152*T*LN(T)
   -.00835595*T**2+9.67907E-07*T**3+204611*T**(-1); 1049 Y
    -4698.365+202.685635*T-38.2836*T*LN(T); 3000 N REF1 !
 FUNCTION GDIAAL 298.15  -7976.15+167.093038*T-24.3671976*T*LN(T)
   -.001884662*T**2-8.77664E-07*T**3+74092*T**(-1); 700 Y
   -11276.24+253.048446*T-38.5844296*T*LN(T)+.018531982*T**2
  -5.764227E-06*T**3+74092*T**(-1); 933.47 Y
   -11278.378+218.684153*T-31.748192*T*LN(T)-1.230524E+28*T**(-9); 2900 N REF1 !
 FUNCTION GFCCMO  298.15  +7453.698+132.5497*T-23.56414*T*LN(T)
   -.003443396*T**2+5.66283E-07*T**3+65812*T**(-1)-1.30927E-10*T**4; 2896 Y
    -15356.41+284.189746*T-42.63829*T*LN(T)-4.849315E+33*T**(-9); 5000 N REF1 !
 FUNCTION GFCCSI  298.15  +42837.391+115.436859*T-22.8317533*T*LN(T)
   -.001912904*T**2-3.552E-09*T**3+176667*T**(-1); 1687 Y
```

```
   +41542.358+145.481367*T-27.196*T*LN(T)-4.20369E+30*T**(-9); 3600 N REF1 !
FUNCTION GFCCUU  298.15  -3407.734+130.955151*T-26.9182*T*LN(T)
  +.00125156*T**2-4.42605E-06*T**3+38568*T**(-1); 955 Y
  -17521.8+292.121093*T-48.66*T*LN(T); 3000 N REF1 !
FUNCTION GHCPAL  2.98150E+02  -2495.15+135.293038*T-24.3671976*T*LN(T)
  -.001884662*T**2-8.77664E-07*T**3+74092*T**(-1); 700 Y
   -5795.24+221.248446*T-38.5844296*T*LN(T)+.018531982*T**2
  -5.764227E-06*T**3+74092*T**(-1); 933.47 Y
   -5797.378+186.884153*T-31.748192*T*LN(T)-1.230524E+28*T**(-9); 2900 N REF1 !
FUNCTION GHCPMO  2.98150E+02  +3803.698+131.9197*T-23.56414*T*LN(T)
  -.003443396*T**2+5.66283E-07*T**3+65812*T**(-1)-1.30927E-10*T**4; 2896 Y
   -19006.41+283.559746*T-42.63829*T*LN(T)-4.849315E+33*T**(-9); 5000 N REF1 !
FUNCTION GHCPSI  2.98150E+02  +41037.391+116.436859*T-22.8317533*T*LN(T)
  -.001912904*T**2-3.552E-09*T**3+176667*T**(-1); 1687 Y
   +39742.358+146.481367*T-27.196*T*LN(T)-4.20369E+30*T**(-9); 3600 N REF1 !
FUNCTION GHCPUU  298.15  +4247.233+131.5301*T-27.5152*T*LN(T)
  -.00835595*T**2+9.67907E-07*T**3+204611*T**(-1); 1049 Y
   +301.635+202.677635*T-38.2836*T*LN(T); 2500 N REF1 !
FUNCTION GTETUU  298.15  -5156.136+106.968316*T-22.841*T*LN(T)
  -.01084475*T**2+2.7889E-08*T**3+81944*T**(-1); 941.5 Y
   -14327.309+244.16002*T-42.9278*T*LN(T); 3000 N REF1 !
FUNCTION GMOSI2 298.15   -114762.8-12.8821*T+GHSERMO+2*GHSERSI; 4000 N !
FUNCTION GA15AM 298.15     -95830.9+2.0081*T+GHSERAL+3*GHSERMO; 6000 N !
FUNCTION GA8M3  298.15 -432556.9+99.1737*T+8*GHSERAL+3*GHSERMO; 4000 N !
FUNCTION UN_ASS 298.15 0; 300 N !

TYPE_DEFINITION % SEQ *!
DEFINE_SYSTEM_DEFAULT ELEMENT 2 !
DEFAULT_COMMAND DEF_SYS_ELEMENT VA !


PHASE LIQUID:L %  1  1.0  !
   CONSTITUENT LIQUID:L :AL,MO,SI,U :  !

  PARAM G(LIQUID,AL;0) 298.15  +GLIQAL#; 2900 N REF1 !
  PARAM G(LIQUID,MO;0) 298.15  +GLIQMO#; 6000 N REF1 !
  PARAM G(LIQUID,SI;0) 298.15  +GLIQSI#; 3600 N REF1 !
  PARAM G(LIQUID,U;0)  298.15  +GLIQUU#; 3000 N REF1 !
  PAR L(LIQUID,AL,MO;0) 298.15  -96235.7+20.9416*T; 6000 N !
  PAR L(LIQUID,AL,MO;1) 298.15   -4384.1+12.3636*T; 6000 N !
  PAR L(LIQUID,AL,MO;2) 298.15            -25091.6; 6000 N !
  PAR L(LIQUID,AL,SI;0) 298.15   -11340.1-1.2339*T; 6000 N !
  PAR L(LIQUID,AL,SI;1) 298.15    -3530.9+1.3599*T; 6000 N !
  PAR L(LIQUID,AL,SI;2) 298.15             +2265.4; 6000 N !
  PAR L(LIQUID,AL,U;0)  298.15     -42716+12.376*T; 4000 N !
  PAR L(LIQUID,AL,U;1)  298.15     -66098+20.347*T; 4000 N !
  PAR L(LIQUID,AL,U;2)  298.15       -5000-8.656*T; 4000 N !
  PAR L(LIQUID,MO,SI;0) 298.15  -158013.3+12.0000*T; 6000 N !
  PAR L(LIQUID,MO,SI;1) 298.15   +20000.0-15.0150*T; 6000 N !
  PAR L(LIQUID,MO,SI;2) 298.15    +39026.3+5.1567*T; 6000 N !
  PAR L(LIQUID,MO,SI;3) 298.15     -2461.9+5.5087*T; 6000 N !
  PAR L(LIQUID,MO,U;0)  298.15        +66600-48.5*T; 4000 N !
  PAR L(LIQUID,MO,U;1)  298.15        -17400+35.6*T; 4000 N !
  PAR L(LIQUID,MO,U;2)  298.15          +81300-55*T; 4000 N !
  PAR L(LIQUID,SI,U;0)  298.15      -185537+26.42*T; 6000 N !
  PAR L(LIQUID,SI,U;1)  298.15       -98478+53.79*T; 6000 N !
  PAR L(LIQUID,SI,U;2)  298.15       +47133-16.79*T; 6000 N !
  PAR L(LIQUID,AL,MO,SI;0) 298.15         -133821.6; 4000 N !
  PAR L(LIQUID,AL,MO,SI;1) 298.15         +236641.0; 4000 N !
  PAR L(LIQUID,AL,MO,SI;2) 298.15         -268078.8; 4000 N !


PHASE A15  %  2 1   3 !
   CONSTITUENT A15  :AL,MO,SI : AL,MO :  !

  PARAM G(A15,AL:AL;0) 298.15  +4*GHSERAL#+20000; 6000 N !
  PARAM G(A15,MO:AL;0) 298.15  +3*GHSERAL#+GHSERMO#+135830.9
 -2.0081*T; 6000 N !
  PARAM G(A15,AL:MO;0) 298.15  +GHSERAL#+3*GHSERMO#-95830.9
 +2.0081*T; 6000 N !
  PARAM G(A15,MO:MO;0) 298.15  +4*GHSERMO#+20000; 6000 N !
```

```
 PARAM G(A15,SI:AL;0) 298.15  20000+3*GHSERAL#+GHSERSI#;
4000 N !
 PARAM G(A15,SI:MO;0) 298.15 -117023.4-5.2030*T+3*GHSERMO#
+GHSERSI#; 4000 N !
 PAR L(A15,AL,MO:AL;0)  298.15      +11628.1; 6000 N !
 PAR L(A15,AL:AL,MO;0)  298.15        +52100; 6000 N !
 PAR L(A15,MO:AL,MO;0)  298.15        +52100; 6000 N !
 PAR L(A15,AL,MO:MO;0)  298.15      +11628.1; 6000 N !
 PAR L(A15,AL,SI:MO;0)  298.15   -60000+27*T; 6000 N !
 PAR L(A15,MO,SI:MO;0)  298.15       +200000; 4000 N !


PHASE AL12MO  %  2 12   1 !
   CONSTITUENT AL12MO  :AL,SI : MO :  !

 PARAM G(AL12MO,AL:MO;0)  298.15  +12*GHSERAL#+GHSERMO#-146766.8
+23.1256*T; 6000 N !
 PARAM G(AL12MO,SI:MO;0)  298.15  +10*GHSERSI#+GMOSI2#+65000;
4000 N !
 PAR L(AL12MO,AL,SI:MO;0) 298.15    +313473.3; 4000 N !
 PAR L(AL12MO,AL,SI:MO;1) 298.15    -325095.9; 4000 N !


PHASE AL13FE4  %  3 .6275   .235   .1375 !
   CONSTITUENT AL13FE4  :AL : MO : AL,VA :  !

 PARAM G(AL13FE4,AL:MO:AL;0)  298.15 +.765*GHSERAL#+.235*GHSERMO#
-33963.2+7.2405*T+5000; 6000 N !
 PARAM G(AL13FE4,AL:MO:VA;0)  298.15 +.6275*GHSERAL#+.235*GHSERMO#
+5000; 6000 N !


PHASE AL17MO4  %  2 17   4 !
   CONSTITUENT AL17MO4  :AL,SI : MO :  !

 PARAM G(AL17MO4,AL:MO;0)  298.15  +17*GHSERAL#+4*GHSERMO#
-578455.4+107.4145*T;  6000 N !
 PARAM G(AL17MO4,SI:MO;0)  298.15  +4*GMOSI2#+9*GHSERSI#
+105000;  4000 N !
 PAR L(AL17MO4,AL,SI:MO;0)     298.15  +100000; 4000 N !


PHASE AL22MO5  %  2 22   5 !
   CONSTITUENT AL22MO5  :AL,SI : MO :  !

 PARAM G(AL22MO5,AL:MO;0)  298.15  +22*GHSERAL#+5*GHSERMO#
-723273.3+132.3154*T; 6000 N !
 PARAM G(AL22MO5,SI:MO;0)  298.15  +5*GMOSI2#+12*GHSERSI#
+135000; 4000 N !
 PAR L(AL22MO5,AL,SI:MO;0)     298.15  +517922.1; 4000 N !



PHASE AL3MO  %  2 3   1 !
   CONSTITUENT AL3MO  :AL,SI : MO :  !

 PARAM G(AL3MO,AL:MO;0)  298.15  +3*GHSERAL#+GHSERMO#-143196.7
+30.6912*T; 6000 N !
 PARAM G(AL3MO,SI:MO;0)  298.15  +GMOSI2#+GHSERSI#+20000;
4000 N !
 PAR L(AL3MO,AL,SI:MO:0)     298.15  +40000; 4000 N !


PHASE AL4MO  %  2 4   1 !
   CONSTITUENT AL4MO  :AL,SI : MO :  !

 PARAM G(AL4MO,AL:MO;0)  298.15  +4*GHSERAL#+GHSERMO#-138851.8
+23.112*T; 6000 N !
 PARAM G(AL4MO,SI:MO;0)  298.15  +GMOSI2#+2*GHSERSI#+25000;
4000 N !
 PAR L(AL4MO,AL,SI:MO;0) 298.15  +301099.8+51.4065*T; 4000 N !
```

```
  PAR L(AL4MO,AL,SI:MO;1) 298.15           -426674.9; 4000 N !


PHASE AL63MO37  %  2 63   37 !
   CONSTITUENT AL63MO37  :AL,SI : MO :  !

  PARAM G(AL63MO37,AL:MO;0)  298.15  +63*GHSERAL#+37*GHSERMO#
 -1638310.2-403.7604*T; 6000 N !
  PARAM G(AL63MO37,SI:MO;0)  298.15  +63*GHSERSI#+37*GHSERMO#
 +500000; 4000 N !


PHASE AL8MO3  %  2 8   3 !
   CONSTITUENT AL8MO3  :AL,SI : MO :  !

  PARAM G(AL8MO3,AL:MO;0)  298.15  +8*GHSERAL#+3*GHSERMO#-432556.9
 +99.1737*T; 4000 N !
  PARAM G(AL8MO3,SI:MO;0)  298.15  +3*GMOSI2#+2*GHSERSI#+55000;
 4000 N !
  PAR L(AL8MO3,AL,SI:MO;0)     298.15 +41377.6; 4000 N !
  PAR L(AL8MO3,AL,SI:MO;1)     298.15 +93321.6; 4000 N !


PHASE AL5MO  %  2 5   1 !
   CONSTITUENT AL5MO  :AL,SI : MO :  !

  PARAM G(AL5MO,AL:MO;0)  298.15  +5*GHSERAL#+GHSERMO#-144819.3
 +25.4357*T; 6000 N !
  PARAM G(AL5MO,SI:MO;0)  298.15  +GMOSI2#+3*GHSERSI#+30000;
 6000 N !
  PAR L(AL5MO,AL,SI:MO;0)     298.15  +20077.8; 4000 N !
  PAR L(AL5MO,AL,SI:MO;1)     298.15  -18885.4; 4000 N !


PHASE AL2U  %  2 .667   .333 !
   CONSTITUENT AL2U  :AL,MO : U :  !

  PARAM G(AL2U,AL:U;0)  298.15     -32966.7+3.4167*T+.667*GHSERAL#
+.333*GHSERUU#; 4000 N !
  PARAM G(AL2U,MO:U;0)  298.15  +10000+.667*GHSERMO#+.333*GHSERUU#;
4000 N !
  PAR L(AL2U,AL,MO:U;0) 298.15  -39621.9875-1.75*T; 4000 N !


PHASE AL3U  %  2 .75   .25 !
   CONSTITUENT AL3U  :AL : U :  !

  PARAM G(AL3U,AL:U;0)  298.15  -31475+4.5663*T+.75*GHSERAL#
+.25*GHSERUU#; 4000 N !


PHASE AL4U  %  2 .80   .20 !
   CONSTITUENT AL4U  :AL : AL,U :  !

  PARAM G(AL4U,AL:U;0)  298.15  -25275+3.5022*T+.80*GHSERAL#
+.20*GHSERUU#; 4000 N !


TYPE_DEFINITION & GES A_P_D BCC_A2 MAGNETIC  -1.0    4.00000E-01 !
PHASE BCC_A2  %&  2 1   3 !
   CONSTITUENT BCC_A2  :AL,MO,SI,U : VA% :  !

  PARAM G(BCC_A2,AL:VA;0) 298.15       +GBCCAL#; 2900 N REF1 !
  PARAM G(BCC_A2,MO:VA;0) 298.15      +GHSERMO#; 6000 N REF1 !
  PARAM G(BCC_A2,SI:VA;0) 298.15       +GBCCSI#; 3600 N REF1 !
  PARAM G(BCC_A2,U:VA;0)  298.15       +GBCCUU#; 3000 N REF1 !
  PAR L(BCC_A2,AL,MO:VA;0)    298.15  -75938.8+10.8187*T; 6000 N !
  PAR L(BCC_A2,AL,MO:VA;1)    298.15  -44502.8+21.6488*T; 6000 N !
  PAR L(BCC_A2,AL,MO:VA;2)    298.15            -22927.1; 6000 N !
  PAR L(BCC_A2,AL,U:VA;0)     298.15      -19247+6.023*T; 4000 N !
  PAR L(BCC_A2,MO,SI:VA;0)    298.15 -103304.7+16.0464*T; 6000 N !
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```
  PAR L(BCC_A2,MO,U:VA;0)     298.15        +26180-9.2*T; 4000 N !
  PAR L(BCC_A2,MO,U:VA;1)     298.15        +28370+2.2*T; 4000 N !
  PAR L(BCC_A2,MO,U:VA;2)     298.15         +47200-25*T; 4000 N !
  PAR L(BCC_A2,SI,U:VA;0)     298.15              -96137; 6000 N !
  PAR L(BCC_A2,AL,MO,SI:VA;0) 298.15                   0; 4000 N !
  PAR L(BCC_A2,AL,MO,SI:VA;1) 298.15             -150000; 4000 N !
  PAR L(BCC_A2,AL,MO,SI:VA;2) 298.15                   0; 4000 N !
  PAR L(BCC_A2,AL,MO,U:VA;0)  298.15             -180000; 4000 N !


PHASE B27 %  2 3.45  3.40 !
   CONSTITUENT B27  :SI : U :  !

  PARAM G(B27,SI:U;0) 298.15 -282080-34.99*T+3.45*GHSERSI#
 +3.40*GHSERUU#; 6000 N !


PHASE C11B  %  2 2   1 !
   CONSTITUENT C11B  :AL,SI,U : MO :  !

  PARAM G(C11B,SI:MO;0)  298.15    -114762.8-12.8821*T+GHSERMO#
 +2*GHSERSI#; 4000 N !
  PARAM G(C11B,AL:MO;0)  298.15       +52118.2+0.2380952*GA8M3#
 +0.0952381*GA15AM#; 4000 N !
  PARAM G(C11B,U:MO;0)   298.15 -20000+20*T+GHSERMO#+2*GHSERUU#;
 4000 N !
  PAR L(C11B,AL,SI:MO;0) 298.15         -50000; 4000 N !
  PAR L(C11B,AL,SI:MO;1) 298.15        +100000; 4000 N !


PHASE C14 %  2 .333  .667 !
   CONSTITUENT C14  :AL,MO,U : AL,MO,U :  !

  PARAM G(C14,AL:AL;0) 298.15 +50000+GHSERAL#; 6000 N !
  PARAM G(C14,MO:MO;0) 298.15 +50000+GHSERMO#; 6000 N !
  PARAM G(C14,U:U;0)   298.15 +50000+GHSERUU#; 6000 N !
  PARAM G(C14,AL:U;0)  298.15 +50000+.333*GHSERAL#+.667*GHSERUU#;
 6000 N !
  PARAM G(C14,U:AL;0)  298.15 -19695.1375-0.75*T+.667*GHSERAL#
 +.333*GHSERUU#; 6000 N !
  PARAM G(C14,AL:MO;0) 298.15 +50000+.333*GHSERAL#+.667*GHSERMO#;
 6000 N !
  PARAM G(C14,MO:AL;0) 298.15 +50000+.667*GHSERAL#+.333*GHSERMO#;
 6000 N !
  PARAM G(C14,MO:U;0)  298.15 +50000+.333*GHSERMO#+.333*GHSERUU#;
 6000 N !
  PARAM G(C14,U:MO;0)   298.15 +48400-2.9*T+.667*GHSERAL#
 +.333*GHSERUU#; 6000 N !
 PAR L(C14,U:AL,U;0)  298.15   +5000; 4000 N !
 PAR L(C14,U:MO,U;0)  298.15   +5000; 4000 N !
 PAR L(C14,AL:AL,U;0) 298.15   +5000; 4000 N !
 PAR L(C14,AL:MO,U;0) 298.15   +5000; 4000 N !
 PAR L(C14,MO:AL,U;0) 298.15   +5000; 4000 N !
 PAR L(C14,MO:MO,U;0) 298.15   +5000; 4000 N !
 PAR L(C14,AL,U:U;0)  298.15   +5000; 4000 N !
 PAR L(C14,MO,U:U;0)  298.15   +5000; 4000 N !
 PAR L(C14,AL,U:MO;0) 298.15   +5000; 4000 N !
 PAR L(C14,MO,U:MO;0) 298.15   +5000; 4000 N !
 PAR L(C14,AL,U:AL;0) 298.15   +5000; 4000 N !
 PAR L(C14,MO,U:AL;0) 298.15   +5000; 4000 N !
 PAR L(C14,AL,MO:U;0)  298.15 +20000; 4000 N !
 PAR L(C14,AL,MO:MO;0) 298.15 +20000; 4000 N !
 PAR L(C14,AL,MO:AL;0) 298.15 +20000; 4000 N !
 PAR L(C14,U:AL,MO;0)  298.15 -138500+14.6*T; 4000 N !
 PAR L(C14,MO:AL,MO;0) 298.15 -138500+14.6*T; 4000 N !
 PAR L(C14,AL:AL,MO;0) 298.15 -138500+14.6*T; 4000 N !


PHASE C32 %  2 5  3 !
   CONSTITUENT C32  :SI : U :  !
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  PARAM G(C32,SI:U;0) 298.15 -343192-31.62*T+5*GHSERSI#+3*GHSERUU#;
 6000 N !


PHASE C40  %  2 2   1 !
   CONSTITUENT C40  :AL,SI : MO :  !

  PARAM G(C40,SI:MO;0) 298.15  +3300+GMOSI2#; 4000 N !
  PARAM G(C40,AL:MO;0) 298.15  +45583.5+0.2380952*GA8M3#
 +0.0952381*GA15AM#; 4000 N !
  PAR L(C40,AL,SI:MO;0)    298.15 -188552.1+22.1039*T; 4000 N !
  PAR L(C40,AL,SI:MO;1)    298.15   +5754.8+26.1722*T; 4000 N !


PHASE C54  %  2 2   1 !
   CONSTITUENT C54  :AL,SI : MO :  !

  PARAM G(C54,SI:MO;0)  298.15   +2500+GMOSI2#; 4000 N !
  PARAM G(C54,AL:MO;0)  298.15   +15335.2+0.2380952*GA8M3#
 +0.0952381*GA15AM#; 4000 N REF63 !
  PAR L(C54,AL,SI:MO;0)  298.15   -101026.3+7.4496*T; 4000 N !
  PAR L(C54,AL,SI:MO;1)  298.15   +70467.2-19.6436*T; 4000 N !


PHASE SI2U %  2 2  1 !
   CONSTITUENT SI2U  :SI : U :  !

  PARAM G(SI2U,SI:U;0) 298.15 -125979-7.77*T+2*GHSERSI#+GHSERUU#;
 6000 N !


PHASE Cc %  2 1.88  1 !
   CONSTITUENT Cc  :SI : U :  !

  PARAM G(Cc,SI:U;0) 298.15 -124792-8.06*T+1.88*GHSERSI#+GHSERUU#;
 6000 N !


PHASE D8M  %  3 .5 .125   .375 !
   CONSTITUENT D8M  :MO : MO,SI : AL,MO,SI :  !

  PARAM G(D8M,MO:MO:AL;0) 298.15 .1845238*GA15AM#+0.0238095*GA8M3#
 +5000; 4000 N !
  PARAM G(D8M,MO:SI:AL;0) 298.15 +10000+.375*GHSERAL#+.5*GHSERMO#
 +.125*GHSERSI#; 4000 N !
  PARAM G(D8M,MO:MO:MO;0) 298.15  +25434.5+0.5439*T+GHSERMO#;
 4000 N !
  PARAM G(D8M,MO:SI:MO;0) 298.15  +17425.8+1.0128*T+.875*GHSERMO#
 +.125*GHSERSI#; 4000 N !
  PARAM G(D8M,MO:MO:SI;0) 298.15  -38980-3.5536*T+.625*GHSERMO#
 +.375*GHSERSI#; 4000 N !
  PARAM G(D8M,MO:SI:SI;0) 298.15  -25000+2.0000*T+.5*GHSERMO#
 +.5*GHSERSI#; 4000 N !
  PAR L(D8M,MO:MO,SI:AL;0) 298.15      -14000-11*T; 4000 N !
  PAR L(D8M,MO:MO,SI:MO;0) 298.15      -14000-11*T; 4000 N !
  PAR L(D8M,MO:MO,SI:SI;0) 298.15      -14000-11*T; 4000 N !
  PAR L(D8M,MO:MO:MO,SI;0) 298.15 -29000+13.1599*T; 4000 N !
  PAR L(D8M,MO:SI:MO,SI;0) 298.15 -29000+13.1599*T; 4000 N !
  PAR L(D8M,MO:MO:AL,SI;0) 298.15            -5000; 4000 N !
  PAR L(D8M,MO:SI:AL,SI;0) 298.15            -5000; 4000 N !
  PAR L(D8M,MO:MO:AL,SI;1) 298.15            +6000; 4000 N !
  PAR L(D8M,MO:SI:AL,SI;1) 298.15            +6000; 4000 N !


PHASE DIAMOND_A4  %  1  1.0  !
   CONSTITUENT DIAMOND_A4  :AL,SI% :  !

  PARAM G(DIAMOND_A4,AL;0) 298.15               +GDIAAL#; 2900 N REF1 !
  PARAM G(DIAMOND_A4,MO;0) 298.15         +5000+GHSERMO#; 4000 N !
  PARAM G(DIAMOND_A4,SI;0) 298.15              +GHSERSI#; 3600 N REF1 !
  PAR L(DIAMOND_A4,AL,SI;0)  298.15  +113246.2-47.5551*T; 4000 N !
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PHASE DOC %  2 1  3 !
   CONSTITUENT DOC  :SI : U :  !

  PARAM G(DOC,SI:U;0) 298.15 -99727-11.1*T+GHSERSI#+3*GHSERUU#;
 6000 N !


PHASE D5A %  2 2  3 !
   CONSTITUENT D5A  :SI : U :  !

  PARAM G(D5A,SI:U;0) 298.15 -171618-41.84*T+2*GHSERSI#+3*GHSERUU#;
 6000 N !


TYPE_DEFINITION ( GES A_P_D FCC_A1 MAGNETIC  -3.0    2.80000E-01 !
PHASE FCC_A1  %(  2 1   1 !
   CONSTITUENT FCC_A1  :AL%,MO,SI,U : VA% :  !

  PARAM G(FCC_A1,AL:VA;0) 298.15  +GHSERAL#; 2900 N REF1 !
  PARAM G(FCC_A1,MO:VA;0) 298.15   +GFCCMO#; 6000 N REF1 !
  PARAM G(FCC_A1,SI:VA;0) 298.15   +GFCCSI#; 3600 N REF1 !
  PARAM G(FCC_A1,U:VA;0)  298.15   +GFCCUU#; 3000 N REF1 !
  PAR L(FCC_A1,AL,MO:VA;0)   298.15    -85300+20.40*T; 6000 N !
  PAR L(FCC_A1,AL,MO:VA;1)   298.15            -10000; 6000 N !
  PAR L(FCC_A1,AL,SI:VA;0)   298.15  -3143.8+0.3930*T; 4000 N !


PHASE FCC_L12 %  2 3  1 !
   CONSTITUENT FCC_L12  :SI : U :  !

  PARAM G(FCC_L12,SI:U;0) 298.15 -131618-11.24*T+3*GHSERSI#+GHSERUU#;
 6000 N !


TYPE_DEFINITION ) GES A_P_D HCP_A3 MAGNETIC  -3.0    2.80000E-01 !
PHASE HCP_A3  %)  2 1   .5 !
   CONSTITUENT HCP_A3  :AL,MO,SI,U : VA% :  !

  PARAM G(HCP_A3,AL:VA;0)  298.15  +GHCPAL#; 2900 N REF1 !
  PARAM G(HCP_A3,MO:VA;0)  298.15  +GHCPMO#; 5000 N REF1 !
  PARAM G(HCP_A3,SI:VA;0)  298.15  +GHCPSI#; 3600 N REF1 !
  PARAM G(HCP_A3,U:VA;0)   298.15  +GHCPUU#; 2500 N REF1 !


PHASE ORTHORHOMBIC_A20  %  1  1.0  !
   CONSTITUENT ORTHORHOMBIC_A20  :AL,MO,U :  !

  PARAM G(ORTHORHOMBIC_A20,AL;0) 298.15 +15000+GHSERAL#; 4000 N !
  PARAM G(ORTHORHOMBIC_A20,MO;0) 298.15 +20000+GHSERMO#; 4000 N !
  PARAM G(ORTHORHOMBIC_A20,U;0)  298.15       +GHSERUU#; 3000 N !
  PAR L(ORTHORHOMBIC_A20,MO,U;0) 298.15    +34180-9.2*T; 4000 N !
  PAR L(ORTHORHOMBIC_A20,MO,U;1) 298.15    +28370+2.2*T; 4000 N !
  PAR L(ORTHORHOMBIC_A20,MO,U;2) 298.15     +47200-25*T; 4000 N !


PHASE TETRAGONAL_U  %  1  1.0  !
   CONSTITUENT TETRAGONAL_U  :AL,MO,SI,U :  !

  PARAM G(TETRAGONAL_U,AL;0) 298.15  +15000+GHSERAL#; 4000 N !
  PARAM G(TETRAGONAL_U,MO;0) 298.15  +18400+GHSERMO#; 4000 N !
  PARAM G(TETRAGONAL_U,SI;0) 298.15   +5000+GHSERSI#; 6000 N !
  PARAM G(TETRAGONAL_U,U;0)  298.15         +GTETUU#; 3000 N REF1 !
  PAR L(TETRAGONAL_U,AL,U;0) 298.15      +12438-23.626*T; 4000 N !
  PAR L(TETRAGONAL_U,MO,U;0) 298.15         +20180-9.2*T; 4000 N !
  PAR L(TETRAGONAL_U,MO,U;1) 298.15         +28370+2.2*T; 4000 N !
  PAR L(TETRAGONAL_U,MO,U;2) 298.15          +47200-25*T; 4000 N !
  PAR L(TETRAGONAL_U,SI,U;0) 298.15             -78915.5; 6000 N !
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 PHASE UMO2AL20 %  3  .043  .174  .783 !
    CONSTITUENT UMO2AL20  :U : AL,MO : AL  :  !

   PARAM G(UMO2AL20,U:AL:AL;0)  298.15         +7182.875-2.5*T+0.043*GHSERUU#
  +0.957*GHSERAL#; 4000 N !
   PARAM G(UMO2AL20,U:MO:AL;0)  298.15   -10000+0.043*GHSERUU#+0.174*GHSERMO#
  +0.783*GHSERAL#; 4000 N !
   PAR L(UMO2AL20,U:AL,MO:AL;0) 298.15   -88414.375+12.5*T; 4000 N !


 PHASE U6MO4AL43 %  4  .113  .113  .208  .566 !
    CONSTITUENT U6MO4AL43  :U : AL,MO : AL,MO : AL  :  !

   PARAM G(U6MO4AL43,U:AL:AL:AL;0) 298.15  -2663.425-0.5*T+0.113*GHSERUU#
  +0.887*GHSERAL#; 4000 N !
   PARAM G(U6MO4AL43,U:MO:AL:AL;0) 298.15  -29000+0.113*GHSERUU#
  +0.113*GHSERMO#+0.774*GHSERAL#; 4000 N !
   PARAM G(U6MO4AL43,U:AL:MO:AL;0) 298.15  -243.125+37.5*T+0.113*GHSERUU#
  +0.208*GHSERMO#+0.679*GHSERAL#; 4000 N !
   PARAM G(U6MO4AL43,U:MO:MO:AL;0) 298.15  +36585.625+12.5*T+0.113*GHSERUU#
  +0.321*GHSERMO#+0.566*GHSERAL#; 4000 N !
   PAR L(U6MO4AL43,U:AL,MO:AL:AL;0) 298.15 -43414.375+12.5*T; 4000 N !
   PAR L(U6MO4AL43,U:AL,MO:MO:AL;0) 298.15 -43414.375+12.5*T; 4000 N !
   PAR L(U6MO4AL43,U:AL:AL,MO:AL;0) 298.15   -111828.75+25*T; 4000 N !
   PAR L(U6MO4AL43,U:MO:AL,MO:AL;0) 298.15   -111828.75+25*T; 4000 N !


 LIST_OF_REFERENCES
 NUMBER  SOURCE
   REF1     'PURE4 - SGTE Pure Elements (Unary) Database (Version 4.6),
         developped by SGTE (Scientific Group Thermodata Europe), 1991-2008,
         and provided by TCSAB (January 2008).'
   REF283   'Alan Dinsdale, SGTE Data for Pure Elements, Calphad 15, 317-425
         (1991), also in NPL Report DMA(A)195 Rev. August 1990.'
!

$*********************************************************************
$
$            Database file *** MoPu.TDB *** described by P.E.A. Turchi
$
$                              *** {Mo,Pu} ***
$
$ With data for the pure elements from the PURE4 database.
$
$*********************************************************************

$ From database: SSOL4
 ELEMENT /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00!
 ELEMENT VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00!
 ELEMENT MO   BCC_A2                    9.5940E+01  4.5890E+03  2.8560E+01!
 ELEMENT PU   ALPHA_PU                  2.4406E+02  0.0000E+00  0.0000E+00!


 FUNCTION GHSERMO  298.15  -7746.302+131.9197*T-23.56414*T*LN(T)
 -.003443396*T**2+5.66283E-07*T**3+65812*T**(-1)-1.30927E-10*T**4; 2896 Y
  -30556.41+283.559746*T-42.63829*T*LN(T)-4.849317E+33*T**(-9); 5000  N !
 FUNCTION GHSERPU  298.15  -7396.309+80.301382*T-18.1258*T*LN(T)
 -.02241*T**2; 400 Y
  -16605.962+236.786603*T-42.4187*T*LN(T)-.00134493*T**2+2.63443E-07*T**3
 +579325*T**(-1); 944 Y
  -14462.156+232.961553*T-42.248*T*LN(T); 4000 N !
 FUNCTION GLIQMO  298.15  +34085.045+117.224788*T-23.56414*T*LN(T)
 -.003443396*T**2+5.66283E-07*T**3+65812*T**(-1)-1.30927E-10*T**4
 +4.24519E-22*T**7; 2896 Y
  +3538.963+271.6697*T-42.63829*T*LN(T); 5000 N REF2 !
 FUNCTION GLIQPU  298.15  -788.209+67.788082*T-18.1258*T*LN(T)
 -.02241*T**2; 400 Y
  -9997.862+224.273303*T-42.4187*T*LN(T)-.00134493*T**2+2.63443E-07*T**3
 +579325*T**(-1); 944 Y
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 -7854.056+220.448253*T-42.248*T*LN(T); 3000 N REF2 !
FUNCTION GBCCPU  298.15  -1358.984+116.603882*T-27.094*T*LN(T)
-.009105*T**2+2.061667E-06*T**3+20863*T**(-1); 745 Y
 -2890.817+156.878957*T-33.72*T*LN(T); 956 Y
 +29313.619-132.788248*T+6.921*T*LN(T)-.02023305*T**2+1.426922E-06*T**3
-4469245*T**(-1); 2071 Y
 -15400.585+227.421855*T-42.248*T*LN(T); 3000 N !
FUNCTION GFCCMO  298.15  +15200+.63*T+GHSERMO#; 4000 N !
FUNCTION GFCCPU  298.15  -3920.781+127.586536*T-28.4781*T*LN(T)
-.0054035*T**2; 990 Y
 +3528.208+41.52572*T-15.7351*T*LN(T)-.0154772*T**2+1.524942E-06*T**3
-864940*T**(-1); 1464 Y
 -12865.948+226.18075*T-42.248*T*LN(T); 4000 N !
FUNCTION GBETPU  2.98.15  -4873.654+123.249151*T-27.416*T*LN(T)
-.00653*T**2; 679.5 Y
 +2435.094+43.566585*T-15.7351*T*LN(T)-.0154772*T**2+1.524942E-06*T**3
-864940*T**(-1); 1464 Y
 -13959.062+228.221615*T-42.248*T*LN(T); 4000 N !
FUNCTION GGAMPU  298.15  -16766.303+419.402655*T-77.5802*T*LN(T)
+.0816415*T**2-2.8103833E-05*T**3+574825*T**(-1); 487.9 Y
 -2942.77+88.325069*T-22.0233*T*LN(T)-.0114795*T**2;  5.93900E+02  Y
 -9336.967+160.314641*T-32.3405*T*LN(T)-.0070383*T**2+6.92887E-07*T**3
+630600*T**(-1); 1179 Y
 -12435.75+226.131617*T-42.248*T*LN(T); 4000 N !
FUNCTION GTETPU  298.15  -496.178+54.586547*T-16.43*T*LN(T)
-.024006*T**2+5.166667E-06*T**3-158470*T**(-1); 736 Y
 -6122.307+173.35008*T-35.56*T*LN(T); 757 Y
 +3982.078+63.890352*T-19.756*T*LN(T)-.00937295*T**2+6.59882E-07*T**3
-1112565*T**(-1); 2157 Y
 -15200.539+228.05641*T-42.248*T*LN(T); 4000 N !
FUNCTION UN_ASS 298.15 0; 300 N !

TYPE_DEFINITION % SEQ *!
DEFINE_SYSTEM_DEFAULT ELEMENT 2 !
DEFAULT_COMMAND DEF_SYS_ELEMENT VA /- !


PHASE LIQUID:L %  1  1.0  !
   CONSTITUENT LIQUID:L :MO,PU :  !

  PARAMETER G(LIQUID,MO;0)  298.15     +GLIQMO#; 5000 N REF2 !
  PARAMETER G(LIQUID,PU;0)  298.15     +GLIQPU#; 3000 N REF2 !
  PAR L(LIQUID,MO,PU;0)  298.15  49161-12.908*T; 4000 N !
  PAR L(LIQUID,MO,PU;1)  298.15  43496-11.056*T; 4000 N !


PHASE ALPHA_PU  %  1  1.0  !
   CONSTITUENT ALPHA_PU  :MO,PU :  !

  PARA G(ALPHA_PU,MO;0) 298.15 20000; 6000 N!
  PARAMETER G(ALPHA_PU,PU;0)  298.15    +GHSERPU#; 4000 N !


TYPE_DEFINITION & GES A_P_D BCC_A2 MAGNETIC  -1.0    4.00000E-01 !
PHASE BCC_A2  %&  2 1   3 !
   CONSTITUENT BCC_A2  :MO%,PU : VA% :  !

  PARAMETER G(BCC_A2,MO:VA;0)  298.15   +GHSERMO#; 5000 N !
  PARAMETER G(BCC_A2,PU:VA;0)  298.15    +GBCCPU#; 3000 N !
  PAR L(BCC_A2,MO,PU:VA;0)  298.15  79958-4.441*T; 4000 N !
  PAR L(BCC_A2,MO,PU:VA;1)  298.15  32449-3.236*T; 4000 N !


PHASE BETA_PU  %  1  1.0  !
   CONSTITUENT BETA_PU  :MO,PU :  !

  PARA G(BETA_PU,MO;0) 298.15 20000; 6000 N!
  PARAMETER G(BETA_PU,PU;0)  2.98.15     +GBETPU#; 4000 N !


PHASE FCC_A1  %  1  1.0  !
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```
   CONSTITUENT FCC_A1  :MO,PU :  !

  PARAMETER G(FCC_A1,MO;0)  298.15       +GFCCMO#; 4000 N !
  PARAMETER G(FCC_A1,PU;0)  298.15       +GFCCPU#; 4000 N !
  PAR   L(FCC_A1,MO,PU;0)   298.15         +25000; 4000 N !


PHASE GAMMA_PU  %  1  1.0  !
   CONSTITUENT GAMMA_PU  :MO,PU :  !

  PARA G(GAMMA_PU,MO;0) 298.15 20000; 6000 N!
  PARAMETER G(GAMMA_PU,PU;0)  298.15     +GGAMPU#; 4000 N !


PHASE TETRAGONAL_A6  %  1  1.0  !
   CONSTITUENT TETRAGONAL_A6  :MO,PU :  !

  PARA G(TETRAGONAL_A6,MO;0) 298.15 20000; 6000 N!
  PARAMETER G(TETRAGONAL_A6,PU;0)  298.15 +GTETPU#; 4000 N !


LIST_OF_REFERENCES
NUMBER  SOURCE
  REF2   'SSOL4.9 (2004-2008): The SGTE General Alloy Solutions Database,
         V4.9f, developed by SGTE (Scientific Group Thermodata Europe), and
         provided by Thermo-Calc Software. '
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$*********************************************************************
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