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Compilation of 'CALPHAD' formation enthalpy data

Binary intermetallic compounds in the COST 507 Gibbsian database

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Abstract

Calculated values for the enthalpy of formation of all the binary intermetallic compounds described in the COST 507 Thermochemical Database for Light Metal Alloys are compiled. The optimised descriptions of the Gibbs energies of all phases, present in the 44 binary systems stored in this database, were obtained after a Calphad-type assessment. The database contains 171 intermetallic compounds. All the formation enthalpies were calculated at 298.15 K. For compounds stable only at temperatures higher than 298 K, the enthalpies were calculated in the temperature range of the stable existence of the compounds. Some comments concerning enthalpies calculated using CALPHAD methods are presented. © 1998 Elsevier Science B.V.

Keywords: Calculated enthalpy; Calphad; Light alloys; Thermodynamic database

1. Introduction

The scientific and technological importance of enthalpies of formation have provoked a large group of researchers into their determination and another large group of materials manufacturers into their use. Enthalpies are measured, predicted from fundamental theoretical approaches, estimated, calculated and yet, values of enthalpy of formation remain unknown for the majority of the already identified compounds.

Their measurement requires expertise and resources; their prediction at limited temperature from ab initio calculations is in development; there is no general method for estimations. All these reasons make systematic compilations, using any of the approaches, highly desirable.

Calphad-type thermodynamic assessments produce parameters of semi-empirically modelled Gibbs energies for all phases present in a given system. These parameters are determined by least-squares fitting of thermodynamic functions to experimental data and are stored in computer databases which enable the calculation of Gibbs energy data as well as its derivatives, as a function of composition, temperature and pressure. The utilisation of different, but nevertheless correlated experimental data, such as enthalpies, chemical potentials and phase diagram information, can provide thermodynamic descriptions having an extended

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validity, which is more reliable than a description obtained using a single type of experimental observation.

'Gibbsian' databases produced from Calphad assessments are an essential constituent of computational thermodynamics, which can link thermodynamics to other processes in which, for example, time is taken into account (see Refs. [1,2]).

These databases already cover a large number of systems containing assessed properties of intermetallic compounds. The calculated enthalpies of formation for these compounds, using the stored data, are the basis for present 'Calphad' formation enthalpy data compilation.

The production of this compilation was inspired by Miedema's semi-empirical model estimates, so well presented in 'Cohesion in Metals' [3], by the excellent collection of experimental thermodynamic data presented by Colinet and Pasturel [4] for rare earth compounds, by the work of Kubaschewski et al. describing so many estimation methods [5,6] and especially and very recently by the page on the world wide web prepared by Sluiter [7] on Compilation of 'first principles' Formation Enthalpy Data.

This work is restricted to binary systems described in the Cost 507 Thermochemical database for Light Metal Alloys [8,9], which constitute a collection of assessments produced from the collaborative work of several research laboratories.

A future extension of these calculations to higher order compounds and to other kinds of material, e.g. semiconductors and oxides, is in the authors schedule.

2. Determination of enthalpies of formation

It is beyond the scope of this paper to describe the methods for obtaining enthalpies of formation other than those obtained from Calphad assessments. However, some literature is referred to for the other methods, as together they can give an overview of the subject.

2.1. Experimental

Experimental measurement is the most important method of obtaining enthalpies of formation and remains as the ultimate check for any theoretical prediction or estimate.

'Systematic Aspects of the High-temperature Thermochemistry of Binary Alloys and Related Compounds', by Kleppa [10] describes not only the different calorimetric techniques relevant for the kind of systems presented in this compilation, but also makes a comparison with other types of thermodynamic measurements where enthalpies can be indirectly obtained.

The experimental data used for the assessment of the binary systems in the COST 507 database can be obtained from the references quoted in [8]. In the case of unpublished work, the name of the assessor is also reported, which enables to trace the experimental information used.

2.2. First principles

In recent years, there has been a striking increase in ab initio quantum mechanical electron band structure calculations of total energy of compounds at zero temperature (see Ref. [7]). The linking of such calculations to statistical mechanics made it possible to predict thermodynamic properties at limited temperatures [11], thus opening up the possibility for a 'first principles' approach for real materials.

An overview of the evolution as well as a description of the techniques used are given in an accessible way in Ref. [12]. The connection and possible use with semi-empirical treatments like the one used in Calphad-type modelling is discussed.

2.3. Estimates

Estimates are always necessary as it is not possible to cover all the experimental gaps. Frequently, the necessary experiments cannot be performed due to the adverse conditions necessary, for example, very high temperatures.

The state of the art of first principles theoretical predictions, although showing progressive success, is still far from providing values for the large spectra of real materials.

Estimates used in combination with Calphad-type assessments can make the method very powerful and unique for solving applied science problems.

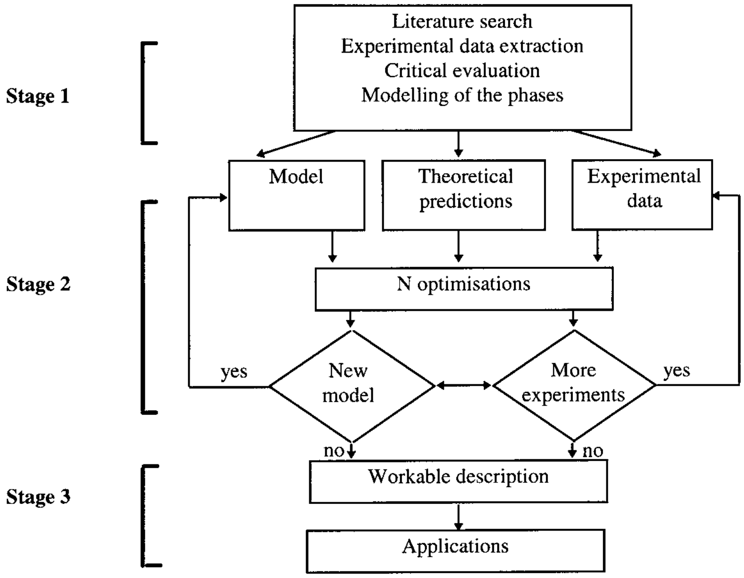

Fig. 1. Assessment procedure.

An overview and update of estimation methods is presented in this issue by Spencer.

2.4. *Calphad assessment*

The standard methodology in the Calphad-type assessment is illustrated in Fig. 1. The procedure defines three different stages: the first one where the literature is critically evaluated and models are proposed for the different existing phases. In the second stage, the determination of a complete set of the Gibbs energies of all phases, appearing in the system, is carried out and it can be improved by new data or new modelling. The process reaches the third stage when a workable description is obtained such that it satisfies the application requirements.

The COST 507 database was produced using the least-squares optimizer programs *Parrot*, developed by Jansson [13] and contained in the *Thermo-Calc* package (see http://www.met.kth.se/~mickus/tc2.html) [14] and Bingss written by Lukas [15,16], that is freely available from the author (lukas@aldix.mpi-stuttgart.mpg.de).

The temperature-dependent Gibbs energy data for the elements, published by Dinsdale [17] on behalf of the Scientific Group Thermodata Europe, *SGTE*, are the standard reference values used in Calphad assessments. These unary data can be freely obtained at ftp://ftp.met.se/thermo/thermo/SGTE.

The optimizer programs make use of experimental thermodynamic and phase diagram data, which are fed in as measured values with error limits. Using defined parametric models for the different phases of the system concerned, the best set of model parameters is obtained after the least-squares fitting of the thermodynamic functions to the selected set of experimental data.

An overview of the present status of some of the higher-order systems in the COST 507 database is given in Ref. [18].

3. Calculated enthalpies

Table 1 shows the calculated enthalpies for 177 binary compounds present in the COST 507 Thermochemical Database for Light Metal Alloys [8,9]. The updated systems in Ref. [9] are marked with an asterisk in this table.

Table 1
Enthalpy of formation of the binary compounds

System	Compound	Pearson symbol	Enthalpy of formation (J/mol)	Temperature ranges (K)
Al–B	AlB_{12}-α	*oP*384	−15253.1	
	AlB_{12}-β	*tP*216	−5791.7	
			31785.8/47048.1	1826–2336
	AlB_2	*hP*3	−28602.9	
Al–C [a]	Al_4C_3	*hR*7	−32051.6	
Al–Ce	$Al_{11}Ce_3$	*tI*10	−41000.0	
	Al_3Ce	*hP*8	−44000.0	
	Al_2Ce	*cF*24	−50000.0	
	AlCe	*oC*16	−46000.0	
	$AlCe_3$	*cP*4	−27000.0	
Al–Cr	Al_8Cr_5	*hR*26	−17651.3	
	Al_9Cr_4	*cI*52	−17747.0	
	$Al_{11}Cr_2$	*mP*48	−13498.5	
	$Al_{13}Cr_2$	*mC*104	−11625.7	
	Al_4Cr	*mP*180	−17803.1	
	$AlCr_2$	*tI*6	−10893.5	
Al–Cu	Al_2Cu_3-δ	hR^{*}	−21340.0	
	AlCu-η	*mC*20	−20280.0	
	Al_2Cu-θ	*tI*12	−15535.9	
	AlCu-ε	*hP*4	−18488.0	
			−3430.8/4901.23	852–1124
	Al_4Cu_9-$\gamma(D8_3)$	*cP*52	−20384.4	
	Al_4Cu_9-γ(H)		−15420.0	
			5500.2/12686.2	1054–1293
	Al_9Cu_{11}-ζ	*hP*42	−21000.0	
Al–Fe	Al_5Fe_4	oC^{*}	−19958.0	
			12551.5/16834.5	1369–1495
	Al_3Fe	*mC*102	−28573.3	
	Al_2Fe	$\alpha P18$	−29649.2	
	Al_5Fe_2	oC^{*}	−30039.6	
Al–Li	AlLi	*cF*16	−20648.6	
	Al_2Li_3	*hR*15	−17928.0	
	Al_4Li_9	*mC*26	−14250.0	
Al–Mg [a]	$Al_{12}Mg_{17}$	*cI*58	−1086.6	
	Al_3Mg_2	*cF*112	−1075.0	
	$Al_{30}Mg_{23}$	*hR*53	−991.8	
			4589.6/9368.3	523–683
Al–Mn [a]	Al_4Mn	*oP*60	−20000.9	
	Al_6Mn	*oC*28	−17994.9	
	$Al_{10}Mn_3$	*hP*28	−23564.7	
	$Al_{11}Mn_4$	$\alpha P30$	−23645.9	
	$Al_{12}Mn$	*cI*26	−9671.51	

Table 1 (*continued*)

Al–N	AlN	*hP*4	−15899.0	
Al–Nd	$Al_{11}Nd_3$	*tI*28	−41000.0	
	Al_3Nd	*hP*8	−46000.0	
	Al_2Nd	*cF*24	−55133.3	
	AlNd	*oP*16	−49940.0	
	$AlNd_2$	*oP*12	−36180.0	
	$AlNd_3$	*hP*8	−27210.0	
Al–Ti	$AlTi_3$	*hP*8	−27519.9	
	AlTi	*tP*4	−39821.7	
	Al_3Ti	*tI*8	−36148.8	
	Al_2Ti	*tI*24	−40500.0	
	$Al_{11}Ti_5$	*tP*32	−38845.0	
			−9877/2477.1	1260–1628
Al–V	Al_3V	*tI*8	−26077.0	
	Al_8V_5	*cI*52	−22640.0	
	$Al_{21}V_2$	*cF*176	−10111.0	
	$Al_{23}V_4$	*hP*54	−15950.0	
	$Al_{45}V_7$	*mC*104	−13600.0	
Al–Y	Al_3Y	*hP*8	−66865.0	
	Al_2Y	*cF*24	−82006.0	
	AlY	*oC*8	−86905.0	
	Al_2Y_3	*tP*20	−74721.0	
	AlY_2	*oP*12	−63636.0	
	Al_3Y_5	*hP*16	−70559.9	
Al–Zr	AlZr	*oC*8	−44500.0	
	$AlZr_2$	*hP*6	−33375.0	
	$AlZr_3$	*cP*4	−27000.0	
	Al_2Zr	*hP*12	−45810.0	
	Al_2Zr_3	*tP*20	−38427.0	
	Al_3Zr	*tI*16	−40625.0	
	Al_3Zr_2	*oF*40	−46940.0	
	Al_3Zr_5	*tI*32	−36248.0	
			−76117.5/6882.92	1241–1656
	Al_4Zr_5	*hP*18	−41000.0	
B–C [a]	B_4C	*hR*15	−23141.4	
B–N	BN	*hP*4	−125300.0	
B–Si	B_nSi (n=36)	*hR*12	−1819.9	
	B_3Si	*hR*15	−6149.2	
	B_6Si	*oP*280	−4238.3	
B–Ti	BTi	*oP*8	−83098.4	
	B_2Ti	*hP*3	−106248.0	
	B_4Ti_3	*oI*14	−94484.8	
C–Si	CSi-β	*cF*8	−35266.4	
C–Ti	CTi	*cF*8	−93981.3	

Table 1 (*continued*)

System	Compound	Pearson symbol	Enthalpy of formation (J/mol)	Temperature ranges (K)
Ce–Mg	CeMg	*cP*2	−23000.0	
	$CeMg_2$	*cF*24	−17581.5	
			−360.4/4146.2	888–1020
	$CeMg_3$	*cF*16	−19200.0	
	Ce_5Mg_{41}	*tI*92	−12500.0	
	$CeMg_{10.3}$	*hP*38	−11430.0	
			5195.0/5419.8	882–889
	$CeMg_{12}$	*tI*26	−10760.0	
Cr–Mn	Cr_3Mn_5		−9064.9	
	$CrMn_3$	*tP*30	−6271.07	
Cr–Si	CrSi	*cP*8	−30158.2	
	$CrSi_2$	*hP*9	−26081.8	
	Cr_3Si	*cP*8	−31584.9	
	Cr_5Si_3	*tI*32	−32468.5	
Cr–Ti	Cr_2Ti-α	*cF*24	8255.1	
			30749.4/43667.9	1093–1645
	Cr_2Ti-β	*hP*12	12686.4	
Cr–Zn	$CrZn_{13}$		−3178.79	
	$CrZn_{17}$		−3134.05	
Cr–Zr	Cr_2Zr-α	*cF*24	−28597.2	
	Cr_2Zr-β	*hP*24	−22946.9	
			31392.8/33672.1	1857–1900
	Cr_2Zr-γ	*hP*12	−2698.13	
			53253.6/55799.5	1896–1947
Cu–Mg [a]	$CuMg_2$	*oF*48	−9540.0	
	Cu_2Mg	*cF*24	−10909.2	
Cu–Si [a]	$Cu_{87}Si_{13}$-κ	*hP*2	2668.73	
			16440.8/24599.9	827–1117
	Cu_4Si-ε	*cI*76	1550.58	
			12702.3/22741.4	698-1078
	Cu_3Si-δ	*hP*72	2829.77	
			20415.1/24063.6	967–1096
	$Cu_{56}Si_{11}$-γ	*cP*20	1509.25	
			11464.3/21260.0	666-1003
	$Cu_{17}Si_3$-β	*cI*2	4116.35	
			24319.3/29094.0	1058–1124
	$Cu_{19}Si_6$-η	*t* **	2365.03	
Cu–Zn	CuZn	*cI*2	3451.98	
			15374.0/25494.0	741–1082
	CuZn	*cP*2	−9446.99	
	$CuZn_4$	*hP*2	−5720.05	
	Cu_5Zn_8	*cI*52	−11552.0	

Table 1 (*continued*)

Cu–Zr	CuZr	*cP*2	−10052.1	
			9057.2/16315.9	977–1209
	$CuZr_2$	*tI*6	−14634.7	
	$Cu_{10}Zr_7$	*oC*68	−14220.6	
	Cu_5Zr	*Cf*24	−10299.0	
	$Cu_{51}Zr_{14}$	*hP*65	−12975.6	
	Cu_8Zr_3	*oP*44	−13460.3	
Fe–Si	$FeSi_2$ LT	*tP*3	−24333.2	
	$FeSi_2$ HT	*oC*48	−16904.2	
			7764.1/15312.9	1233–1482
	Fe_2Si	*hP*6	−17652.6	
			9072.7/17312.9	1241–1488
	FeSi	*cP*8	−31805.9	
	Fe_5Si_3	*hP*16	−24424.6	
			−13268.7/6096.3	730–1364
Mg–Ni	$MgNi_2$	*hP*24	−18414.7	
	Mg_2Ni	*hP*18	−17863.7	
Mg–Si [a]	Mg_2Si	*cF*12	−21744.8	
Mg–Y	$Mg_{24x}Y_5$	*cI*58	−7837.3	
	Mg_2Y	*hP*12	−13025.3	
	$Mg_{1x}Y$	*cP*2	−16081.4	
Mg–Zn [a]	$MgZn_2$	*hP*12	−11785.1	
	Mg_2Zn_{11}	*cP*39	−5678.3	
	MgZn		−9479.2	
	Mg_2Zn_3	*mC*110	−10881.1	
	Mg_7Zn_3	*oI*142	−4728.8	
			3266.7/3720.0	599–614
Mn–Si	MnSi	*cP*8	−28006.4	
	Mn_3Si-β	*cF*16	−18280.4	
	$Mn_{11}Si_{19}$	*tP*120	−18280.4	
	$Mn_{44}Si_9$	*hR*53	−20411.5	
	Mn_5Si_3	*hP*16	−12199.5	
	Mn_9Si_2	*mC*110	−13675.2	
Mn–Ti	MnTi-α	t^{*}58	−5738.83	
	MnTi-β	*tP*30	−5539.82	
			18784.1/35549.3	1071–1500
	Mn_3Ti		−4637.74	
			26134.9/38764.7	1222–1524
	Mn_2Ti	*hP*12	−8799.77	
	Mn_4Ti	*hR*53	−2444.72	
			27592.9/40389.8	1198–1503
N–Ti	NTi_2	*tP*6	−133308.0	
Si–Ti	$TiSi_2$	*oF*24	−58346.2	
	TiSi	*oP*8	−77530.9	
	Ti_3Si	*tP*32	−50000.0	
	Ti_5Si_3	*hP*16	−72945.5	
	Ti_5Si_4	*tP*36	−79000.0	

Table 1 (*continued*)

System	Compound	Pearson symbol	Enthalpy of formation (J/mol)	Temperature ranges (K)
Si–V	SiV_3	*cP*8	−46409.1	
	Si_2V	*hP*9	−40021.7	
	Si_3V_5	*tI*32	−53643.0	
	Si_5V_6	*oI*44	−49216.1	
			−18872.7/−3834.6	1435–1943
Si–Y	Si_2Y-α	*hP*3	−73067.0	
	Si_2Y-β	*oI*12	−71544.0	
			−380665/−29587.0	1523–1793
	Si_3Y_5	*hP*16	−73500.0	
	Si_4Y_5	*tP*36	−77550.0	
	Si_5Y_3-α	*hP*3	−75919.5	
	Si_5Y_3-β		−75196.5	
			−64599.2/−28983.3	723–1915
	SiY	*oC*8	−80350.0	
Si–Zr	SiZr-β	*oC*8	−83672.1	
	$SiZr_2$	*tI*12	−77059.6	
	$SiZr_3$	*tP*32	−60955.0	
	Si_2Zr	*oC*12	−56292.8	
	Si_2Zr_3	*tP*10	−88812.4	
	Si_3Zr_5	*hP*16	−78175.1	
			−38499.9/−25104.4	1752–2182
	Si_4Zr_5-β		−88301.5	
Sn–Ti	Sn_5Ti_6-β	*hP*22	−37920.7	
	Sn_3Ti_5	*hP*16	−39465.5	
	$SnTi_2$	*hP*6	−40403.3	
	$SnTi_3$	*hP*8	−37445.6	

[a] Indicates the updated in [9] systems.

4. Discussion

Calculated enthalpies using thermodynamic optimised descriptions have certain characteristics peculiar to this method:

4.1. *Calphad values supplementing experiments: Cr–Si*

The least-squares fitting technique requires that the experimental data set, describing the same property, lies inside the gaussian distribution determined by the experimental error. Experimental data that do not obey this assumption should not be used together in the optimisation, because they contradict each other. This requirement obliges the assessor to make a selection between data sets which belong to non-overlapping gaussian distributions, although describing the same observable.

The decision as to which set should be taken into account can be facilitated by combination and comparison with different best related experimental data.

The assessment reported in Ref. [19] illustrates this situation. A complete set of formation enthalpies for all the compounds in the Cr–Si system [20,21] was published by the same author. For one of the compounds, however, the enthalpy of formation has also been reported by another author [21], but with a considerably less negative value than that included in the other data set [20]. The less negative value was found to correspond better with other thermodynamic data and was therefore used in an optimisation. The enthalpies of formation for other compounds were obtained from this optimisation which incorpo-

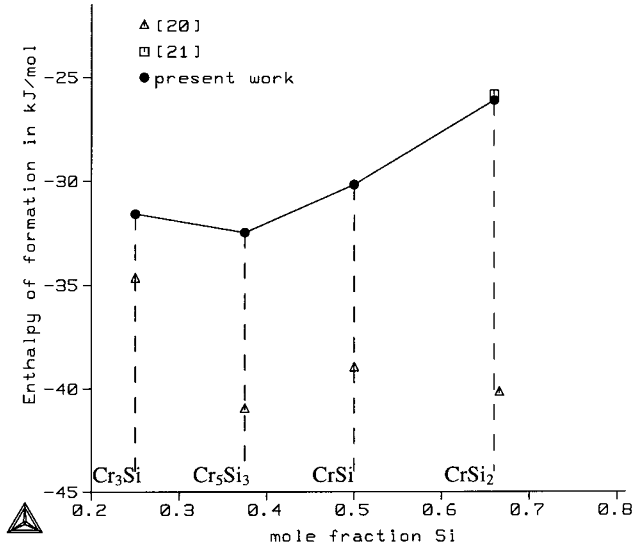

Fig. 2. Enthalpy of formation of the compounds in the Cr–Si system compared with experimental data [20,21].

rated a complete set of compatible experimental data. In this case, the optimisation method resolved the conflict between different experimental data and provided guidance for further experimental investigations.

Fig. 2 shows the calculated enthalpies of formation for all the compounds in the Cr–Si system compared to the experimental values determined [20,21]. The calculated values provide the best estimate for the formation enthalpies of these compounds.

4.2. Calphad assessment demanding further experiments: Cu–Si

In the Cu–Si system there are six compounds ($Cu_{85}Si_{15}$-β, $Cu_{19}Si_6$-η, $Cu_{33}Si_7$-δ, Cu_4Si-ε,

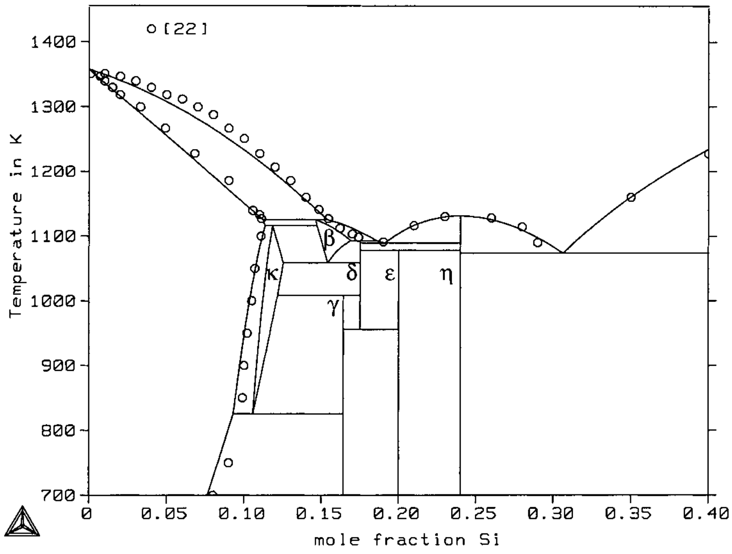

Fig. 3. Calculated Cu–Si phase diagram compared with experimental data [22].

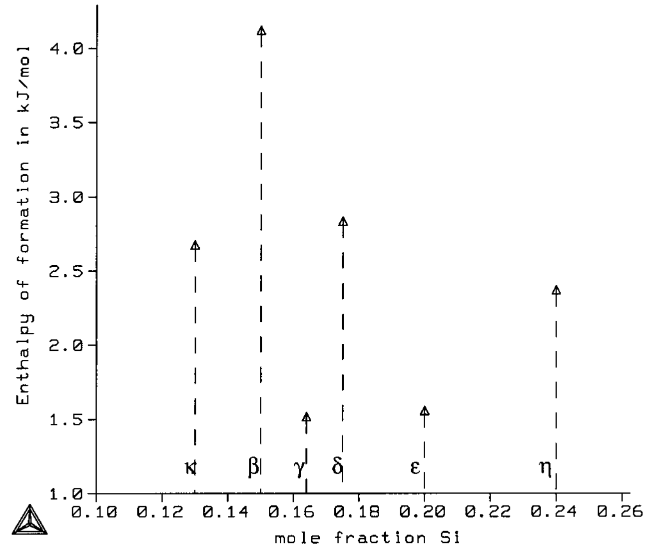

Fig. 4. Enthalpy of formation of the compounds in the Cu–Si system.

$Cu_{56}Si_{11}$-γ, $Cu_{87}Si_{13}$-κ), for which only invariant equilibria and solubility ranges are known. Fig. 3 shows the calculated phase diagram compared with experimental data [22]; above 673 K the calculated and experimental data are in good agreement.

However, the present evaluation of the system does not describe the stability of all phases at room temperature: the Cu_4Si-ε and $Cu_{56}Si_{11}$-γ phases are not stable. The main problem in the assessed description is the lack of calorimetric information for each compound, in particular, because the Gibbs energy cannot be estimated reliably from the phase diagram invariant temperatures alone.

Fig. 4 shows the calculated molar enthalpies for all the phases present in the system. It is important to note here that they are all positive, which results in the predicted decomposition at low temperature. There is no experimental evidence for this behaviour.

The assessment clearly reveals the need for experimental calorimetric data to obtain a reliable description of the Cu–Si binary system.

4.3. Calphad assessment selecting experimental data for theoretical comparison

Just as in case (a), the comparison of scattered experimental data with distinct, but nevertheless related, experimental values can clarify which values within a scattered set of measurements of the same type are more reliable. Although not directly comparable to the values predicted at zero temperature, the Calphad calculated enthalpies of formation at 298.15 K can give indication concerning trends and order of magnitude of actual values, which can be used to evaluate the exactness of first principles predictions when experimental data is scattered or unknown.

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