

A Thermodynamic Description of the Al-Cr-Si System

Yu Liang, Cuiping Guo, Changrong Li, and Zhenmin Du

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The Al-Cr-Si system was critically assessed using the CALPHAD technique. The solution phases (liquid, bcc, fcc, and diamond) were described by a substitutional solution model. The compounds CrSi_2 , Cr_3Si , AlCr_2 , $\alpha\text{Al}_8\text{Cr}_5$, $\beta\text{Al}_8\text{Cr}_5$, Al_4Cr , and $\text{Al}_{11}\text{Cr}_2$ in the Al-Cr-Si system were treated with sublattice models $(\text{Cr}, \text{Si})(\text{Al}, \text{Cr}, \text{Si})_2$, $(\text{Cr}, \text{Si})_3(\text{Al}, \text{Cr}, \text{Si})$, $(\text{Al}, \text{Cr}, \text{Si})(\text{Al}, \text{Cr})_2$, $\alpha(\text{Al}, \text{Cr}, \text{Si})_8(\text{Al}, \text{Cr}, \text{Si})_5$, $\beta(\text{Al}, \text{Cr}, \text{Si})_8(\text{Al}, \text{Cr}, \text{Si})_5$, $(\text{Al}, \text{Si})_4(\text{Al}, \text{Cr})$, and $(\text{Al}, \text{Si})_{11}(\text{Al}, \text{Cr})_2$, respectively. The ternary intermetallic compounds τ_1 , τ_2 , and τ_3 were treated as the formulae $\text{Al}_{13}\text{Cr}_4\text{Si}_4$, $\text{Al}_9\text{Cr}_3\text{Si}$, and $(\text{Al}, \text{Si})_{11}\text{Cr}_4$, respectively. A set of self-consistent thermodynamic description of the Al-Cr-Si system was obtained.

Keywords metals and alloys, phase diagram, CALPHAD technique, thermodynamic properties, thermodynamic modeling

1. Introduction

Al-Cr-Si alloys show good oxidation resistance with no mass loss after oxidation in air during the melting process.^[1] They might be used as promising coating materials for carbon/carbon composites for application at high temperatures.^[2] Knowledge of phase equilibria is significant for the optimization of alloy compositions and heat-treatment conditions. The CALPHAD technique^[3] was used to analyze the thermodynamic properties of the system in this study.

Robinson^[4,5] determined the crystal structure of the τ_1 phase in the Al-Cr-Si system, which is a ternary compound $\alpha(\text{AlCrSi})$ in the early studies carried out by Pratt and Raynor.^[6,7] Subsequently, Esslinger et al.^[8] investigated the phase equilibria in the Al-rich corner of the Al-Cr-Si system and confirmed that the composition of the τ_1 phase is $\text{Al}_{13}\text{Cr}_4\text{Si}_4$. Another ternary compound $\beta(\text{AlCrSi})$ reported by Pratt and Raynor^[6] and Mondolfo^[9] turned out to be a

solid solution of Al in the binary compound CrSi_2 .^[5] The investigation of Brukl et al.^[10] also indicated that $\beta(\text{AlCrSi})$ was the binary intermetallic CrSi_2 with extended solubility of Al up to 25 at.% Al with Al replacing Si in the sublattice of the intermetallic compound. The AlCr_2 phase was reported to have a solubility of 3 at.% Si at with Si replacing Al.^[11] The Cr_3Si phase was reported to have a solid solubility of ~ 12.5 at.% Al in the Al-Cr-Si system.^[9] The intermetallic compounds Al_8Cr_5 , Al_4Cr , and $\text{Al}_{11}\text{Cr}_2$ all had Si solubilities in the Al-Cr-Si system.^[12]

A series of isothermal sections at 1073, 1173, 1273, and 1373 K over the entire composition range in the Al-Cr-Si system were presented by Gupta.^[13] The ternary compound τ_1 was reported to exist only below 983 K.

Subsequently, Weitzer et al.^[14] reported a new ternary phase $\tau_3\text{-(Al,Si)}_{11}\text{Cr}_4$ which is isostructural to $\text{Mn}_4\text{Al}_{11}$.^[15] Chen et al.^[16] reinvestigated the isothermal section at 1073 K in the Al-Cr-Si system. Three ternary compounds $\tau_1\text{-Al}_{13}\text{Cr}_4\text{Si}_4$, $\tau_2\text{-Al}_9\text{Cr}_3\text{Si}$, and $\tau_3\text{-(Al,Si)}_{11}\text{Cr}_4$ were confirmed to be stable at 1073 K. The observation of the τ_1 phase at 1073 K is inconsistent with the experimental results of Esslinger et al.^[8] and Gupta.^[13] Since Esslinger et al.^[8] determined the stability limit for τ_1 from cooling curves, the occurrence of metastable solidification may be the cause for this discrepancy.^[16] Chen et al.^[16] observed maximum Al solubility in Cr_3Si of 4.1 at.% Al, maximum Si solubility in AlCr_2 of 1.7 at.% Si, Al_8Cr_5 with 5.6 at.% Si, and Al_4Cr with 10.4 at.% Si in the Al-Cr-Si system. Meanwhile, Chen^[17] has also reported a ternary compound τ_4 , which exists in the temperature range from 1381 to 1278 K and predicted the reaction scheme in the Al-Cr-Si system.

2. Thermodynamic Models

In order to obtain the thermodynamic description of the Al-Cr-Si system, the thermodynamic parameters of three binary Al-Cr, Al-Si and Cr-Si systems are necessary. The thermodynamic descriptions of the Al-Si system assessed by Gröbner et al.^[18] are adopted in this study. Coughanowr and

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Yu Liang, Cuiping Guo, Changrong Li, and Zhenmin Du, Department of Materials Science and Engineering, University of Science and Technology, Beijing 100083, P.R. China. Contact e-mail: zmd2@hotmail.com.

Ansara^[19] carried out a thermodynamic evaluation of the Cr-Si system. Recently, a new description based on latest experimental investigation was carried out by Chen et al.^[20] The Al-Cr system was first optimized by Saunders,^[21] and later reoptimized by Liang et al.^[22] according to the experimental results reported by Mahdouk and Gachon^[23] and Grushko et al.^[24] The thermodynamic parameters of the Cr-Si system were reported by Chen et al.^[20] and for the Al-Cr system reported by Liang et al.^[22] and these are adopted in this study. The models employed to describe the ternary phases are presented in Table 1.

2.1 Solution Phases

There are four solution phases: liquid, fcc (Al), bcc (Cr), and diamond (Si) in the Al-Cr-Si system. Their Gibbs energies are described by the following expression:

$$G_m^\phi(T) = x_{Al}G_{Al}^\phi(T) + x_{Cr}G_{Cr}^\phi(T) + x_{Si}G_{Si}^\phi(T) + RT(x_{Al} \ln x_{Al} + x_{Cr} \ln x_{Cr} + x_{Si} \ln x_{Si}) + {}^E G_m^\phi \quad (\text{Eq 1})$$

where x_{Al} , x_{Cr} , and x_{Si} are mole fraction of the pure elements Al, Cr, and Si, respectively; the Gibbs energy function $G_i^\phi(T) = {}^0G_i^\phi(T) - H_i^{\text{SER}}$ (298.15 K) for the element i ($i = \text{Al, Cr, Si}$) in the solution phase ϕ ($\phi = \text{liquid, fcc (Al), bcc (Cr), and diamond (Si)}$) is described by an equation of the following form:

$$G_i^\phi(T) = a + bT + cT \ln T + dT^2 + eT^3 + fT^{-1} + gT^7 + hT^{-9} \quad (\text{Eq 2})$$

where H_i^{SER} (298.15 K) is the molar enthalpy of the element i at 298.15 K in its standard element reference (SER) state, fcc for Al, bcc for Cr, and diamond for Si. The Gibbs energy of the element i , $G_i^\phi(T)$, in its SER state, is denoted by GHSEr_i , i.e.,

$$\text{GHSEr}_i = {}^0G_i^{\text{SER}}(T) - H_i^{\text{SER}} \quad (298.15 \text{ K}) \quad (\text{Eq 3})$$

In this study, the Gibbs energy functions for the element i ($i = \text{Al, Cr, Si}$) are taken from the SGTE compilation of Dinsdale.^[25]

${}^E G_m^\phi$ is the excess Gibbs energy, expressed by the Redlich-Kister polynomial,^[26]

$${}^E G_m^\phi = x_{Al}x_{Cr} \sum_j {}^j L_{Al,Cr}^\phi (x_{Al} - x_{Cr})^j + x_{Cr}x_{Si} \sum_j {}^j L_{Cr,Si}^\phi (x_{Cr} - x_{Si})^j + x_{Al}x_{Si} \sum_j {}^j L_{Al,Si}^\phi (x_{Al} - x_{Si})^j + x_{Al}x_{Si}x_{Cr} L_{Al,Cr,Si}^\phi \quad (\text{Eq 4})$$

where ${}^j L_{Al,Cr}^\phi$, ${}^j L_{Cr,Si}^\phi$, and ${}^j L_{Al,Si}^\phi$ are the interaction parameters between elements Al and Cr, Cr and Si, and Al and Si, respectively. $L_{Al,Cr,Si}^\phi$ is a ternary interaction parameter.

2.2 Intermetallic Compounds

2.2.1 Intermetallic Compounds CrSi₂ and Cr₃Si. The line compound CrSi₂ was reported to have a solubility extending up to 20 at.% Al at 1073 K, 22.80 at.% Al at 1173 K, and 19.27 at.% Al at 1273 K^[13] in the Al-Cr-Si system. A maximum of 25 at.% Al solubility with Al replacing Si in CrSi₂ at 1073 K is observed by Chen et al.^[16] The compound Cr₃Si was reported to have a solubility of approximately 12.5 at.% Al^[9] and 4.1 at.% Al at 1073 K^[16] in the Al-Cr-Si system. These two compounds are treated using two-sublattice models^[27-29] (Cr, Si)(Al, Cr, Si)₂ and (Cr, Si)₃(Al, Cr, Si), respectively. The Gibbs energy per mole of formula unit Cr_mSi_n (CrSi₂ and Cr₃Si) is expressed as follows:

$$G^{\text{Cr}_m\text{Si}_n} = y'_{Cr}y''_{Cr} G_{Cr:Cr}^{\text{Cr}_m\text{Si}_n} + y'_{Cr}y''_{Si} G_{Cr:Si}^{\text{Cr}_m\text{Si}_n} + y'_{Cr}y''_{Al} G_{Cr:Al}^{\text{Cr}_m\text{Si}_n} + y'_{Si}y''_{Cr} G_{Si:Cr}^{\text{Cr}_m\text{Si}_n} + y'_{Si}y''_{Si} G_{Si:Si}^{\text{Cr}_m\text{Si}_n} + y'_{Si}y''_{Al} G_{Si:Al}^{\text{Cr}_m\text{Si}_n} + nRT(y''_{Cr} \ln y''_{Cr} + y''_{Si} \ln y''_{Si} + y''_{Al} \ln y''_{Al}) + mRT(y'_{Cr} \ln y'_{Cr} + y'_{Si} \ln y'_{Si}) + y'_{Cr} \left[y'_{Cr}y'_{Si} \sum_j {}^j L_{Cr,Si:Cr}^{\text{Cr}_m\text{Si}_n} (y'_{Cr} - y'_{Si})^j \right] + y'_{Si} \left[y'_{Cr}y'_{Si} \sum_j {}^j L_{Cr,Si:Si}^{\text{Cr}_m\text{Si}_n} (y'_{Cr} - y'_{Si})^j \right] + y'_{Al} \left[y'_{Cr}y'_{Si} \sum_j {}^j L_{Cr,Si:Al}^{\text{Cr}_m\text{Si}_n} (y'_{Cr} - y'_{Si})^j \right] + y'_{Cr} \left[y''_{Cr}y''_{Si} \sum_j {}^j L_{Cr:Cr,Si}^{\text{Cr}_m\text{Si}_n} (y''_{Cr} - y''_{Si})^j + y''_{Cr}y''_{Al} \sum_j {}^j L_{Cr:Cr,Al}^{\text{Cr}_m\text{Si}_n} (y''_{Cr} - y''_{Al})^j + y''_{Si}y''_{Al} \sum_j {}^j L_{Cr:Si,Al}^{\text{Cr}_m\text{Si}_n} (y''_{Si} - y''_{Al})^j \right] + y'_{Si} \left[y''_{Cr}y''_{Si} \sum_j {}^j L_{Si:Cr,Si}^{\text{Cr}_m\text{Si}_n} (y''_{Cr} - y''_{Si})^j + y''_{Cr}y''_{Al} \sum_j {}^j L_{Si:Cr,Al}^{\text{Cr}_m\text{Si}_n} (y''_{Cr} - y''_{Al})^j + y''_{Si}y''_{Al} \sum_j {}^j L_{Si:Si,Al}^{\text{Cr}_m\text{Si}_n} (y''_{Si} - y''_{Al})^j + y''_{Cr}y''_{Si}y''_{Al} \sum_j {}^j L_{Si:Cr,Si,Al}^{\text{Cr}_m\text{Si}_n} \right] \quad (\text{Eq 5})$$

2.2.2 Intermetallic Compound AlCr₂. The compound AlCr₂ was reported to have a solubility of 3 at.% Si for Al at 973 K^[11] and 1.7 at.% Si at 1073 K.^[16] It was treated with a two-sublattice model (Al, Cr, Si)(Al, Cr)₂.

Section I: Basic and Applied Research

Table 1 Thermodynamic parameters of the Al-Cr-Si system(a)

Phase	Thermodynamic parameters	Reference
Pure elements	GHSER _{Al} = 298.1-700.0 K: $-7976.15 + 137.093038T - 24.3671976T\ln(T) - 0.001884662T^2 - 8.77664 \times 10^{-7}T^3 + 74092T^{-1}$ 700.0-933.5 K: $-11276.24 + 223.048446T - 38.5844296T\ln(T) + 0.018531982T^2 - 5.764227 \times 10^{-6}T^3 + 74092T^{-1}$ 700.0-2900.0 K: $-11278.378 + 188.684153T - 31.748192T\ln(T) - 1.230524 \times 10^{28}T^{-9}$	[25]
	GHSER _{Cr} = 298.1-2180.0 K: $-8856.94 + 157.48T - 26.908T\ln(T) + 0.00189435T^2 - 1.47721 \times 10^{-6}T^3 + 139250T^{-1}$ 2180.0-6000.0 K: $-34869.344 + 344.18T - 50T\ln(T) - 2.88526 \times 10^{32}T^{-9}$	[25]
	GHSER _{Si} = 298.1-1687.0 K: $-8162.609 + 137.236859T - 22.8317533T\ln(T) - 0.001912904T^2 - 3.552 \times 10^{-9}T^3 + 176667T^{-1}$ 1687.0-3600.0 K: $-9457.642 + 167.281367T - 27.196T\ln(T) - 4.20369 \times 10^{30}T^{-9}$	[25]
	Model (Al, Cr, Si) ₁	[25]
	G(liq., Al) = 298.1-700.0 K: $+3028.879 + 125.251171T - 24.3671976T\ln(T) - 0.001884662T^2 - 8.77664 \times 10^{-7}T^3 + 74092T^{-1} + 7.9337 \times 10^{-20}T^7$ 700.0-933.5 K: $-271.21 + 211.206579T - 38.5844296T\ln(T) + 0.018531982T^2 - 5.764227 \times 10^{-6}T^3 + 74092T^{-1} + 7.9337 \times 10^{-20}T^7$ 933.5-2900.0 K: $-795.996 + 177.430178T - 31.748192T\ln(T)$	[25]
	G(liq., Cr) = 298.1-2180.0 K: $+15483.015 + 146.059775T - 26.908T\ln(T) + 0.0018943T^2 - 1.47721 \times 10^{-6}T^3 + 139250T^{-1} + 2.37615 \times 10^{-21}T^7$ 2180.0-6000.0 K: $-16459.984 + 335.616316T - 50T\ln(T)$	[25]
	G(liq., Si) = 298.1-1687.0 K: $+42533.751 + 107.13742T - 22.8317533T\ln(T) - 0.001912904T^2 - 3.552 \times 10^{-9}T^3 + 176667T^{-1} + 2.09307 \times 10^{-21}T^7$ 1687.0-3600.0 K: $+40370.523 + 137.722298T - 27.196T\ln(T)$	[25]
	${}^0L_{Al, Si}^{liq.} = -11340.1 - 1.23394T$	[18]
	${}^1L_{Al, Si}^{liq.} = -3530.93 + 1.35993T$	[18]
	${}^2L_{Al, Si}^{liq.} = +2265.39$	[18]
Liquid	${}^0L_{Cr, Si}^{liq.} = -128000.0 + 21.23883T$	[20]
	${}^1L_{Cr, Si}^{liq.} = -50016.61 + 14.31913T$	[20]
	${}^0L_{Al, Cr}^{liq.} = -37139.1 + 2.0110T$	[22]
	${}^1L_{Al, Cr}^{liq.} = -15698.7 + 7.4555T$	[22]
	${}^0L_{Al, Cr, Si}^{liq.} = -73008.0 + 47.5147T$	This work
	${}^1L_{Al, Cr, Si}^{liq.} = +12338.1$	This work
	Model (Al, Cr, Si) ₁	[25]
	G(fcc, Al) = +GHSER _{Al}	[25]
	G(fcc, Cr) = 298.1-2180.0 K: $-1572.94 + 157.643T - 26.908T\ln(T) + 0.00189435T^2 - 1.47721 \times 10^{-6}T^3 + 139250T^{-1}$ 2180.0-6000.0 K: $-27585.344 + 344.343T - 50T\ln(T) - 2.88526 \times 10^{32}T^{-9}$	[25]
	Tc(fcc, Cr) = -1109	
β(fcc, Cr) = -2.46	[25]	
G(fcc, Si) = 298.1-1687.0 K: $+42837.391 + 115.436859T - 22.8317533T\ln(T) - 0.001912904T^2 - 3.552 \times 10^{-9}T^3 + 176667T^{-1}$ 1687.0-3600.0 K: $+41542.358 + 145.481367T - 27.196T\ln(T) - 4.20369 \times 10^{30}T^{-9}$	[18]	
${}^0L_{Al, Si}^{fcc} = -3143.78 + 0.39297T$	[22]	
${}^0L_{Al, Cr}^{fcc} = -30946.0 + 8.3017T$	[22]	
${}^0L_{Al, Cr, Si}^{fcc} = +680751.6$	This work	
Fcc	Model (Al, Cr, Si) ₁	[25]
	G(bcc, Al) = 298.1-700.0 K: $+2106.85 + 132.280038T - 24.3671976T\ln(T) - 0.001884662T^2 - 8.77664 \times 10^{-7}T^3 + 74092T^{-1}$ 700.0-933.5 K: $-1193.24 + 218.235446T - 38.5844296T\ln(T) + 0.018531982T^2 - 5.764227 \times 10^{-6}T^3 + 74092T^{-1}$ 933.5-2900.0 K: $-1195.378 + 183.871153T - 31.748192T\ln(T) - 1.230524 \times 10^{28}T^{-9}$	[25]
	G(bcc, Cr) = +GHSER _{Cr}	[25]
	Tc(bcc, Cr) = -311.5	
	β(bcc, Cr) = -0.008	
Bcc	Model (Al, Cr, Si) ₁	[25]

Table 1 continued

Phase	Thermodynamic parameters	Reference
diamond	$G(\text{bcc, Si}) =$ 298.1-1687.0 K: $+38837.391 + 114.736859T - 22.8317533T\ln(T) - 0.001912904T^2 - 3.552 \times 10^{-9}T^3 + 176667T^{-1}$ 1687-3600.0 K: $+37542.358 + 144.781367T - 27.196T\ln(T) - 4.20369 \times 10^{30}T^{-9}$	[25]
	${}^0L_{\text{Al,Cr}}^{\text{bcc}} = -58257.5 + 8.4407T$	[22]
	${}^0L_{\text{Cr,Si}}^{\text{bcc}} = -77309.9324 - 2.3832T$	[20]
	${}^1L_{\text{Cr,Si}}^{\text{bcc}} = -53247.5616 + 13.58981T$	[20]
	${}^0L_{\text{Al,Cr,Si}}^{\text{bcc}} = +630000.0$	This work
	${}^1L_{\text{Al,Cr,Si}}^{\text{bcc}} = +127000.0 + 21.0000T$	This work
	Model (Al, Cr, Si) ₁	
	$G(\text{diamond, Al}) =$ 298.1-700.0 K: $-7976.15 + 167.093038T - 24.3671976T\ln(T) - 0.001884662T^2 - 8.77664 \times 10^{-7}T^3 + 74092T^{-1}$ 700.0-933.5 K: $-11276.24 + 253.048446T - 38.5844296T\ln(T) + 0.018531982T^2 - 5.764227 \times 10^{-6}T^3 + 74092T^{-1}$ 933.5-2900.0 K: $-11278.378 + 218.684153T - 31.748192T\ln(T) - 1.230524 \times 10^{28}T^{-9}$	[25]
	$G(\text{diamond, Si}) = +\text{GHSE}_{\text{Si}}$	[25]
	$G(\text{diamond, Cr}) = +\text{GHSE}_{\text{Cr}} + 5000.0$	This work
${}^0L_{\text{Al,Si}}^{\text{diamond}} = +113246.16 - 47.5551T$	[18]	
CrSi ₂	Model (Cr, Si)(Cr, Si, Al) ₂	
	$G_{\text{Cr:Al}}^{\text{CrSi}_2} = \frac{1}{6}G_{\text{Al:Cr}}^{\alpha\text{Al}_8\text{Cr}_5} + \frac{1}{6}G_{\text{Al:Cr}}^{\text{Al}_4\text{Cr}} + 30000.0$	This work
	$G_{\text{Cr:Cr}}^{\text{CrSi}_2} = +3\text{GHSE}_{\text{Cr}} + 10000.0 - 1.0000T$	[20]
	$G_{\text{Cr:Si}}^{\text{CrSi}_2} = -100597.117 + 336.62707T - 57.86T\ln(T) - 0.01323T^2 - 0.000000432T^3$	[20]
	$G_{\text{Si:Al}}^{\text{CrSi}_2} = +\text{GHSE}_{\text{Si}} + 2\text{GHSE}_{\text{Al}} + 15000.0$	This work
	$G_{\text{Si:Cr}}^{\text{CrSi}_2} = +\text{GHSE}_{\text{Si}} + 2\text{GHSE}_{\text{Cr}} + 224822.024 - 27.60473T$	[20]
	$G_{\text{Si:Si}}^{\text{CrSi}_2} = +3\text{GHSE}_{\text{Si}} + 84524.9887 - 26.27506T$	[20]
	${}^0L_{\text{Cr,Si:Cr}}^{\text{CrSi}_2} = {}^0L_{\text{Cr,Si:Si}}^{\text{CrSi}_2} = +1535.4469$	[20]
	${}^0L_{\text{Cr,Al,Si}}^{\text{CrSi}_2} = -80594.2 + 31.1515T$	This work
	${}^1L_{\text{Cr,Al,Si}}^{\text{CrSi}_2} = +107670.6 - 33.3699T$	This work
$\alpha\text{Cr}_5\text{Si}_3$	Model Cr ₅ Si ₃	
	$G_{\text{Cr:Si}}^{\alpha\text{Cr}_5\text{Si}_3} = -329102.726 + 1077.75585T - 182.578184T\ln(T) - 0.023919688T^2 - 0.00000231728T^3$	[20]
$\beta\text{Cr}_5\text{Si}_3$	Model Cr ₅ (Cr, Si) ₃	
	$G_{\text{Cr:Cr}}^{\beta\text{Cr}_5\text{Si}_3} = +8\text{GHSE}_{\text{Cr}} + 40000$	[20]
	$G_{\text{Cr:Si}}^{\beta\text{Cr}_5\text{Si}_3} = -277240.64 + 1048.67176T - 182.578184T\ln(T) - 0.023919688T^2 - 0.00000231728T^3$	[20]
${}^0L_{\text{Cr:Cr,Si}}^{\beta\text{Cr}_5\text{Si}_3} = -4697.84363$	[20]	
CrSi	Model (Cr) ₁ (Al, Si) ₁	
	$G_{\text{Cr:Si}}^{\text{CrSi}} = -83545.088 + 315.0993T - 51.62865T\ln(T) - 0.00447355T^2 + 391330T^{-1}$	[20]
	$G_{\text{Cr:Al}}^{\text{CrSi}} = \text{GHSE}_{\text{Cr}} + \text{GHSE}_{\text{Si}}$	This work
${}^0L_{\text{Cr:Al,Si}}^{\text{CrSi}} = -43606.3$	This work	
Cr ₃ Si	Model (Cr, Si) ₃ (Cr, Si, Al)	
	$G_{\text{Cr:Al}}^{\text{Cr}_3\text{Si}} = +\text{GHSE}_{\text{Cr}} + G_{\text{Al:Cr}}^{\text{AlCr}_2} + 6623.6$	This work
	$G_{\text{Cr:Cr}}^{\text{Cr}_3\text{Si}} = +4\text{GHSE}_{\text{Cr}} + 20000.0 + 10.0000T$	[20]
	$G_{\text{Cr:Si}}^{\text{Cr}_3\text{Si}} = +3\text{GHSE}_{\text{Cr}} + \text{GHSE}_{\text{Si}} - 125904.402 + 5.14171T$	[20]
	$G_{\text{Si:Al}}^{\text{Cr}_3\text{Si}} = +3\text{GHSE}_{\text{Si}} + \text{GHSE}_{\text{Al}} + 20000.0$	This work
	$G_{\text{Si:Cr}}^{\text{Cr}_3\text{Si}} = +3\text{GHSE}_{\text{Si}} + \text{GHSE}_{\text{Cr}} + 561830.369 - 61.07749T$	[20]
	$G_{\text{Si:Si}}^{\text{Cr}_3\text{Si}} = +4\text{GHSE}_{\text{Si}} + 415925.967 - 65.93576T$	[20]
	${}^0L_{\text{Cr,Si:Cr}}^{\text{Cr}_3\text{Si}} = {}^0L_{\text{Cr,Si:Si}}^{\text{Cr}_3\text{Si}} = -391881.445$	[20]
	Model (Al, Cr, Si) ₈ (Al, Cr, Si) ₅	
	$G_{\text{Al:Al}}^{\alpha\text{Al}_8\text{Cr}_5} = +13\text{GHSE}_{\text{Al}} + 40000.0$	[22]
$G_{\text{Al:Cr}}^{\alpha\text{Al}_8\text{Cr}_5} = +8\text{GHSE}_{\text{Al}} + 5\text{GHSE}_{\text{Cr}} - 252507.8 + 10.3963T$	[22]	
$G_{\text{Al:Si}}^{\alpha\text{Al}_8\text{Cr}_5} = +8\text{GHSE}_{\text{Al}} + 5\text{GHSE}_{\text{Si}} + 65000.0$	This work	
$G_{\text{Cr:Al}}^{\alpha\text{Al}_8\text{Cr}_5} = +8\text{GHSE}_{\text{Cr}} + 5\text{GHSE}_{\text{Al}} + 332507.8 - 10.3963T$	[22]	
$G_{\text{Cr:Cr}}^{\alpha\text{Al}_8\text{Cr}_5} = +13\text{GHSE}_{\text{Cr}} + 40000.0$	[22]	
$G_{\text{Cr:Si}}^{\alpha\text{Al}_8\text{Cr}_5} = +8\text{GHSE}_{\text{Cr}} + 5\text{GHSE}_{\text{Si}} + 65000.0$	This work	
$G_{\text{Si:Al}}^{\alpha\text{Al}_8\text{Cr}_5} = +8\text{GHSE}_{\text{Si}} + 5\text{GHSE}_{\text{Al}} + 150134.2$	This work	
$G_{\text{Si:Cr}}^{\alpha\text{Al}_8\text{Cr}_5} = +8\text{GHSE}_{\text{Si}} + 5\text{GHSE}_{\text{Cr}}$	This work	
$G_{\text{Si:Si}}^{\alpha\text{Al}_8\text{Cr}_5} = +13\text{GHSE}_{\text{Si}} + 65000.0$	This work	
${}^0L_{\text{Al,Cr:Al}}^{\alpha\text{Al}_8\text{Cr}_5} = {}^0L_{\text{Al,Cr:Cr}}^{\alpha\text{Al}_8\text{Cr}_5} = +140019.3 + 2.7138T$	[22]	

Table 1 continued

Phase	Thermodynamic parameters	Reference
$\beta\text{Al}_8\text{Cr}_5$	${}^1L_{\text{Al:Cr:Al}}^{\alpha\text{Al}_8\text{Cr}_5} = {}^1L_{\text{Al:Cr:Cr}}^{\alpha\text{Al}_8\text{Cr}_5} = -298819.0 + 92.86567T$	[22]
	${}^0L_{\text{Al:Al:Cr}}^{\alpha\text{Al}_8\text{Cr}_5} = {}^0L_{\text{Cr:Al:Cr}}^{\alpha\text{Al}_8\text{Cr}_5} = -302291.9 + 156.94097T$	[22]
	${}^1L_{\text{Al:Al:Cr}}^{\alpha\text{Al}_8\text{Cr}_5} = {}^1L_{\text{Cr:Al:Cr}}^{\alpha\text{Al}_8\text{Cr}_5} = -84584.3$	[22]
	${}^0L_{\text{Al:Si:Cr}}^{\alpha\text{Al}_8\text{Cr}_5} = -241956.1$	This work
	${}^1L_{\text{Al:Si:Cr}}^{\alpha\text{Al}_8\text{Cr}_5} = -95286.9$	This work
	Model $(\text{Al}, \text{Cr}, \text{Si})_8(\text{Al}, \text{Cr}, \text{Si})_5$	
	$G_{\text{Al:Al}}^{\beta\text{Al}_8\text{Cr}_5} = +13\text{GHSE}_{\text{RAl}} + 40000.0$	[22]
	$G_{\text{Al:Cr}}^{\beta\text{Al}_8\text{Cr}_5} = +8\text{GHSE}_{\text{RAl}} + 5\text{GHSE}_{\text{RCr}} - 238114.8$	[22]
	$G_{\text{Al:Si}}^{\beta\text{Al}_8\text{Cr}_5} = +8\text{GHSE}_{\text{RAl}} + 5\text{GHSE}_{\text{RSi}} + 65000.0$	This work
	$G_{\text{Cr:Al}}^{\beta\text{Al}_8\text{Cr}_5} = +8\text{GHSE}_{\text{RCr}} + 5\text{GHSE}_{\text{RAl}} + 318114.8$	[22]
$G_{\text{Cr:Cr}}^{\beta\text{Al}_8\text{Cr}_5} = +13\text{GHSE}_{\text{RCr}} + 40000.0$	[22]	
$G_{\text{Cr:Si}}^{\beta\text{Al}_8\text{Cr}_5} = +8\text{GHSE}_{\text{RCr}} + 5\text{GHSE}_{\text{RSi}} + 65000.0$	This work	
$G_{\text{Si:Al}}^{\beta\text{Al}_8\text{Cr}_5} = +8\text{GHSE}_{\text{RSi}} + 5\text{GHSE}_{\text{RAl}} + 112155.5$	This work	
$G_{\text{Si:Cr}}^{\beta\text{Al}_8\text{Cr}_5} = +8\text{GHSE}_{\text{RSi}} + 5\text{GHSE}_{\text{RCr}}$	This work	
$G_{\text{Si:Si}}^{\beta\text{Al}_8\text{Cr}_5} = +13\text{GHSE}_{\text{RSi}} + 65000.0$	This work	
${}^0L_{\text{Al:Cr:Al}}^{\beta\text{Al}_8\text{Cr}_5} = {}^0L_{\text{Al:Cr:Cr}}^{\beta\text{Al}_8\text{Cr}_5} = +194038.6 - 57.0982T$	[22]	
${}^1L_{\text{Al:Cr:Al}}^{\beta\text{Al}_8\text{Cr}_5} = {}^1L_{\text{Al:Cr:Cr}}^{\beta\text{Al}_8\text{Cr}_5} = +16289.5 - 99.3751T$	[22]	
${}^0L_{\text{Al:Al:Cr}}^{\beta\text{Al}_8\text{Cr}_5} = {}^0L_{\text{Cr:Al:Cr}}^{\beta\text{Al}_8\text{Cr}_5} = +198488.0 - 236.4091T$	[22]	
${}^1L_{\text{Al:Al:Cr}}^{\beta\text{Al}_8\text{Cr}_5} = {}^1L_{\text{Cr:Al:Cr}}^{\beta\text{Al}_8\text{Cr}_5} = -254728.3 + 98.3046T$	[22]	
${}^0L_{\text{Al:Si:Cr}}^{\beta\text{Al}_8\text{Cr}_5} = -218309.8 - 29.8816T$	This work	
${}^1L_{\text{Al:Si:Cr}}^{\beta\text{Al}_8\text{Cr}_5} = -74357.3$	This work	
Al_7Cr	Model $\text{Al}_7(\text{Al}, \text{Cr})$	
$G_{\text{Al:Cr}}^{\text{Al}_7\text{Cr}} = +7\text{GHSE}_{\text{RAl}} + \text{GHSE}_{\text{RCr}} - 100970 + 23.5612T$	[22]	
$G_{\text{Al:Al}}^{\text{Al}_7\text{Cr}} = +8\text{GHSE}_{\text{RAl}} + 24074.5$	[22]	
${}^0L_{\text{Al:Al:Cr}}^{\text{Al}_7\text{Cr}} = -21094.1 + 12.6986T$	[22]	
Al_4Cr	Model $(\text{Al}, \text{Si})_4(\text{Al}, \text{Cr})$	
$G_{\text{Al:Al}}^{\text{Al}_4\text{Cr}} = +5\text{GHSE}_{\text{RAl}} + 25868.2$	[22]	
$G_{\text{Al:Cr}}^{\text{Al}_4\text{Cr}} = +4\text{GHSE}_{\text{RAl}} + \text{GHSE}_{\text{RCr}} - 79750.0 + 9.8532T$	[22]	
$G_{\text{Si:Al}}^{\text{Al}_4\text{Cr}} = +4\text{GHSE}_{\text{RSi}} + \text{GHSE}_{\text{RAl}} + 50000.0$	This work	
$G_{\text{Si:Cr}}^{\text{Al}_4\text{Cr}} = +4\text{GHSE}_{\text{RSi}} + \text{GHSE}_{\text{RCr}}$	This work	
${}^0L_{\text{Al:Si:Cr}}^{\text{Al}_4\text{Cr}} = -76324.1 + 6.0128T$	This work	
${}^1L_{\text{Al:Si:Cr}}^{\text{Al}_4\text{Cr}} = -1530.8 - 10.1702T$	This work	
${}^0L_{\text{Al:Al:Cr}}^{\text{Al}_4\text{Cr}} = -71625.0 + 53.0030T$	[22]	
$\text{Al}_{11}\text{Cr}_2$	Model $(\text{Al}, \text{Si})_{11}(\text{Al}, \text{Cr})_2$	
$G_{\text{Al:Al}}^{\text{Al}_{11}\text{Cr}_2} = +13\text{GHSE}_{\text{RAl}} + 30000.0$	[22]	
$G_{\text{Al:Cr}}^{\text{Al}_{11}\text{Cr}_2} = +11\text{GHSE}_{\text{RAl}} + 2\text{GHSE}_{\text{RCr}} - 145700.9$	[22]	
$G_{\text{Si:Al}}^{\text{Al}_{11}\text{Cr}_2} = +11\text{GHSE}_{\text{RSi}} + 2\text{GHSE}_{\text{RAl}} + 90985.5$	This work	
$G_{\text{Si:Cr}}^{\text{Al}_{11}\text{Cr}_2} = +11\text{GHSE}_{\text{RSi}} + 2\text{GHSE}_{\text{RCr}} + 65000.0$	This work	
${}^0L_{\text{Al:Si:Cr}}^{\text{Al}_{11}\text{Cr}_2} = -67755.9 + 180.7592T$	This work	
${}^1L_{\text{Al:Si:Cr}}^{\text{Al}_{11}\text{Cr}_2} = -55861.3 + 203.3824T$	This work	
${}^0L_{\text{Al:Al:Cr}}^{\text{Al}_{11}\text{Cr}_2} = +199602.3 - 186.4713T$	[22]	
AlCr_2	Model $(\text{Al}, \text{Cr}, \text{Si})(\text{Al}, \text{Cr})_2$	
$G_{\text{Al:Al}}^{\text{AlCr}_2} = +3\text{GHSE}_{\text{RAl}} + 15000$	[22]	
$G_{\text{Al:Cr}}^{\text{AlCr}_2} = +\text{GHSE}_{\text{RAl}} + 2\text{GHSE}_{\text{RCr}} - 45279.2$	[22]	
$G_{\text{Cr:Al}}^{\text{AlCr}_2} = +\text{GHSE}_{\text{RCr}} + 2\text{GHSE}_{\text{RAl}} + 75279.2$	[22]	
$G_{\text{Cr:Cr}}^{\text{AlCr}_2} = +3\text{GHSE}_{\text{RCr}} + 15000.0$	[22]	
$G_{\text{Si:Al}}^{\text{AlCr}_2} = +\text{GHSE}_{\text{RSi}} + 2\text{GHSE}_{\text{RAl}} + 15000.0$	This work	
$G_{\text{Si:Cr}}^{\text{AlCr}_2} = +\text{GHSE}_{\text{RSi}} + 2\text{GHSE}_{\text{RCr}} + 15000.0$	This work	
${}^0L_{\text{Al:Al:Cr}}^{\text{AlCr}_2} = {}^0L_{\text{Cr:Al:Cr}}^{\text{AlCr}_2} = -31502.4 + 5.7033T$	[22]	
${}^0L_{\text{Al:Cr:Al}}^{\text{AlCr}_2} = {}^0L_{\text{Al:Cr:Cr}}^{\text{AlCr}_2} = -11282.4 - 6.3700T$	[22]	
${}^0L_{\text{Al:Si:Cr}}^{\text{AlCr}_2} = -109098.9 + 5.5894T$	This work	
τ_1	Model $\text{Al}_{13}\text{Cr}_4\text{Si}_4$	
$G_{\text{Al:Cr:Si}}^{\tau_1} = +4\text{GHSE}_{\text{RCr}} + 13\text{GHSE}_{\text{RAl}} + 4\text{GHSE}_{\text{RSi}} - 437554.6 + 69.7236T$	This work	
τ_2	Model $\text{Al}_9\text{Cr}_3\text{Si}$	
$G_{\text{Al:Cr:Si}}^{\tau_2} = +3\text{GHSE}_{\text{RCr}} + 9\text{GHSE}_{\text{RAl}} + \text{GHSE}_{\text{RSi}} - 258834.9 + 25.6494T$	This work	

Table 1 continued

Phase	Thermodynamic parameters	Reference
τ_3	Model (Al,Si) ₁₁ Cr ₄	
	$G_{Cr:Al}^{\tau_3} = \frac{5}{12}G_{Al:Cr}^{\alpha Al_8Cr_5} + \frac{23}{12}G_{Al:Cr}^{Al_4Cr} + 18470.7$	This work
	$G_{Cr:Si}^{\tau_3} = +4GHSE_{Cr} + 11GHSE_{Si} - 20732.1$	This work
	${}^0L_{Cr:Al:Si}^{\tau_3} = -473921.1 + 230.4174T$	This work
	${}^1L_{Cr:Al:Si}^{\tau_3} = -559720.9 + 90.6686T$	This work
τ_4	Model Al ₅₈ Cr ₃₁ Si ₁₁	
	$G_{Al:Cr:Si}^{\tau_4} = +58GHSE_{Al} + 31GHSE_{Cr} + 11GHSE_{Si} - 1560841.1 - 388.2631T$	This work

(a) In J/mol of the formula units

Table 2 Calculated invariant reactions in the Al-Cr-Si system

Reactions	Present work		Experimental data	
	Type	T, K	Ref 8	Ref 17
liq. + $\beta Cr_5Si_3 \rightarrow Cr_3Si + \alpha Cr_5Si_3$	U1	1774
liq. + CrSi $\rightarrow CrSi_2 + \alpha Cr_5Si_3$	U2	1633	...	1633
liq. + bcc $\rightarrow Cr_3Si + \beta Al_8Cr_5$	U3	1538	...	1571
liq. + Cr ₃ Si $\rightarrow \alpha Cr_5Si_3 + \beta Al_8Cr_5$	U4	1467	...	1462
liq. + $\alpha Cr_5Si_3 \rightarrow CrSi_2 + \beta Al_8Cr_5$	U5	1381
liq. + CrSi ₂ + $\beta Al_8Cr_5 \rightarrow \tau_4$	P1	1380	...	1381
$\beta Al_8Cr_5 + \tau_4 \rightarrow \alpha Al_8Cr_5 + liq.$	U6	1356
liq. + $\alpha Al_8Cr_5 + \tau_4 \rightarrow \tau_3$	P2	1331	...	1320
liq. + $\tau_4 \rightarrow \tau_3 + CrSi_2$	U7	1326	...	1314
liq. + $\alpha Al_8Cr_5 \rightarrow Al_4Cr + \tau_3$	U8	1308	...	1309
liq. + $\tau_3 \rightarrow Al_4Cr + CrSi_2$	U9	1264	...	1256
liq. + $Al_4Cr + CrSi_2 \rightarrow \tau_1(a)$	P3	1081	> 1073(b)	1079
liq. + $Al_4Cr \rightarrow Al_{11}Cr_2 + \tau_1(a)$	U10	988	953-983(a)	1058
liq. + $Al_{11}Cr_2 \rightarrow Al_7Cr + \tau_1$	U11	966	953	1045
liq. + $Al_7Cr \rightarrow \tau_1 + fcc$	U12	908	898	907
liq. + CrSi ₂ $\rightarrow diamond + \tau_1$	U13	881	863	847-868
liq. $\rightarrow diamond + fcc + \tau_1$	E1	850	848	847
bcc + $\beta Al_8Cr_5 \rightarrow \alpha Al_8Cr_5 + Cr_3Si$	U14	1412
$\beta Al_8Cr_5 + Cr_3Si \rightarrow \alpha Al_8Cr_5 + \alpha Cr_5Si_3$	U15	1386
$\alpha Cr_5Si_3 + \beta Al_8Cr_5 \rightarrow CrSi_2 + \alpha Al_8Cr_5$	U16	1363
$\beta Al_8Cr_5 + CrSi_2 \rightarrow \alpha Al_8Cr_5 + \tau_4$	U17	1362
$\tau_4 \rightarrow \tau_3 + CrSi_2 + \alpha Al_8Cr_5$	E2	1278	...	1278
$Al_4Cr + \tau_3 \rightarrow CrSi_2 + \tau_2$	U18	1230	...	1230
bcc + $Cr_3Si \rightarrow \alpha Al_8Cr_5 + AlCr_2$	U19	1185	...	1158
$\alpha Al_8Cr_5 + CrSi_2 \rightarrow \tau_3 + \alpha Cr_5Si_3$	U20	1074
$CrSi_2 + Al_4Cr \rightarrow \tau_1 + \tau_2$	U21	1012
$Al_4Cr + \tau_3 \rightarrow \alpha Al_8Cr_5 + \tau_2$	U22	1006
$Al_{11}Cr_2 \rightarrow Al_4Cr + \tau_1 + Al_7Cr$	E3	961
$\tau_1 + Al_4Cr \rightarrow \tau_2 + Al_7Cr$	U23	821

(a) Reported by Gupta^[13] and (b) Reported by Chen et al.^[16]

2.2.3 Intermetallic Compounds Al₄Cr, Al₁₁Cr₂, αAl_8Cr_5 , and βAl_8Cr_5 . The compound Al₄Cr has an extended solubility of ~10.4 at.% Si^[16] and Al₁₁Cr₂ also has an appreciable Si solubility.^[12] They are treated using

two-sublattice models (Al, Si)₄(Al, Cr) and (Al, Si)₁₁(Al, Cr)₂. The Gibbs energy per mole of formula unit Al_mCr_n (Al₄Cr and Al₁₁Cr₂) is expressed as follows:

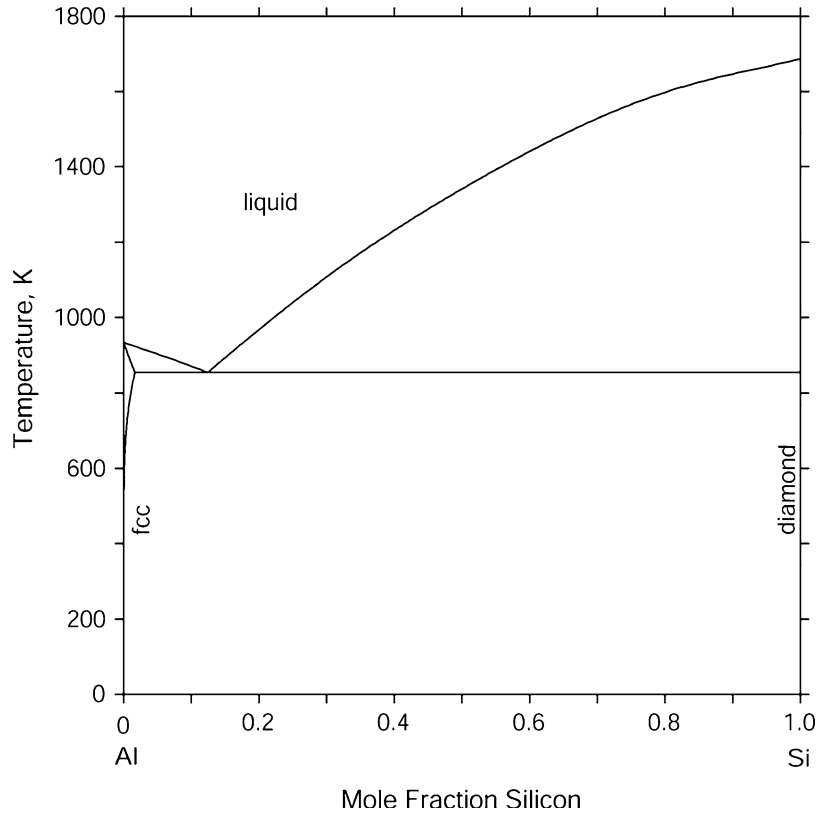


Fig. 1 Al-Si phase diagram optimized by Gröbner et al.^[18]

$$\begin{aligned}
 G^{Al_mCr_n} = & y'_{Al}y''_{Al}G_{Al:Al}^{Al_mCr_n} + y'_{Al}y''_{Cr}G_{Al:Cr}^{Al_mCr_n} + y'_{Si}y''_{Al}G_{Si:Al}^{Al_mCr_n} \\
 & + y'_{Si}y''_{Cr}G_{Si:Cr}^{Al_mCr_n} + mRT(y'_{Al} \ln y'_{Al} + y'_{Si} \ln y'_{Si}) \\
 & + nRT(y''_{Al} \ln y''_{Al} + y''_{Cr} \ln y''_{Cr}) \\
 & + y'_{Al} \left[y''_{Al}y''_{Cr} \sum_j^j L_{Al:Al,Cr}^{Al_mCr_n} (y''_{Al} - y''_{Cr})^j \right] \\
 & + y'_{Si} \left[y''_{Al}y''_{Cr} \sum_j^j L_{Si:Al,Cr}^{Al_mCr_n} (y''_{Al} - y''_{Cr})^j \right] \\
 & + y'_{Al} \left[y'_{Al}y'_{Si} \sum_j^j L_{Al:Si,Al}^{Al_mCr_n} (y'_{Al} - y'_{Si})^j \right] \\
 & + y'_{Cr} \left[y'_{Al}y'_{Si} \sum_j^j L_{Al:Si,Cr}^{Al_mCr_n} (y'_{Al} - y'_{Si})^j \right] \quad (Eq 6)
 \end{aligned}$$

The compounds αAl_8Cr_5 and βAl_8Cr_5 have solubility of ~ 5.6 at.% Si,^[16] and are treated as a two-sublattice model (Al, Cr, Si)₈(Al, Cr, Si)₅.

2.2.4 Intermetallic Compounds τ_1 , τ_2 , τ_3 , and τ_4 . The Gibbs energy per mole of formula unit $Al_lCr_mSi_n$ for the intermetallic compounds τ_1 - $Al_{13}Cr_4Si_4$, τ_2 - Al_9Cr_3Si , and τ_4 - $Al_{58}Cr_{31}Si_{11}$ is expressed as follows:

$$\begin{aligned}
 G_m^{Al_lCr_mSi_n} = & lGHSER_{Al} + mGHSER_{Cr} + nGHSER_{Si} \\
 & + \Delta G_f^{Al_lCr_mSi_n} \quad (Eq 7)
 \end{aligned}$$

where $\Delta G_f^{Al_lCr_mSi_n}$ is the Gibbs energy of formation per mole of formula unit $Al_lCr_mSi_n$. Due to lack of experimental

measurements, and it is assumed that the Neumann-Kopp rule applies to the heat capacity, i.e. $\Delta Cp_f = 0$. Thus, $\Delta G_f^{Al_lCr_mSi_n}$ can be given by the following expression:

$$\Delta G_f^{Al_lCr_mSi_n} = a + bT \quad (Eq 8)$$

where the parameters a and b were evaluated in this study.

In the Al-Cr-Si system, the intermetallic compound τ_3 , which varies in composition ranges from $Al_{65}Cr_{27}Si_8$ (coexisting with Al_8Cr_5 and Cr_5Si_3) to $Al_{60}Cr_{27}Si_{13}$ (coexisting with Cr_5Si_3 and $CrSi_2$),^[16] was treated using a two-sublattice model $(Al,Si)_{11}Cr_4$ with Al and Si on the first sublattice, and Cr on the second one. The Gibbs energy per mole of formula unit $(Al,Si)_{11}Cr_4$ is expressed as follows:

$$\begin{aligned}
 G_m^{(Al,Si)_{11}Cr_4} = & y_{Al}G_{Al:Cr}^{(Al,Si)_{11}Cr_4} + y_{Si}G_{Si:Cr}^{(Al,Si)_{11}Cr_4} \\
 & + 11RT(y_{Al} \ln y_{Al} + y_{Si} \ln y_{Si}) \\
 & + y_{Al}y_{Si} \sum_j^j L_{Al:Si,Cr}^{(Al,Si)_{11}Cr_4} (y_{Al} - y_{Si})^j \quad (Eq 9)
 \end{aligned}$$

3. Assessment Procedure

The thermodynamic parameters of the Al-Cr-Si system were optimized on the basis of the experimental information

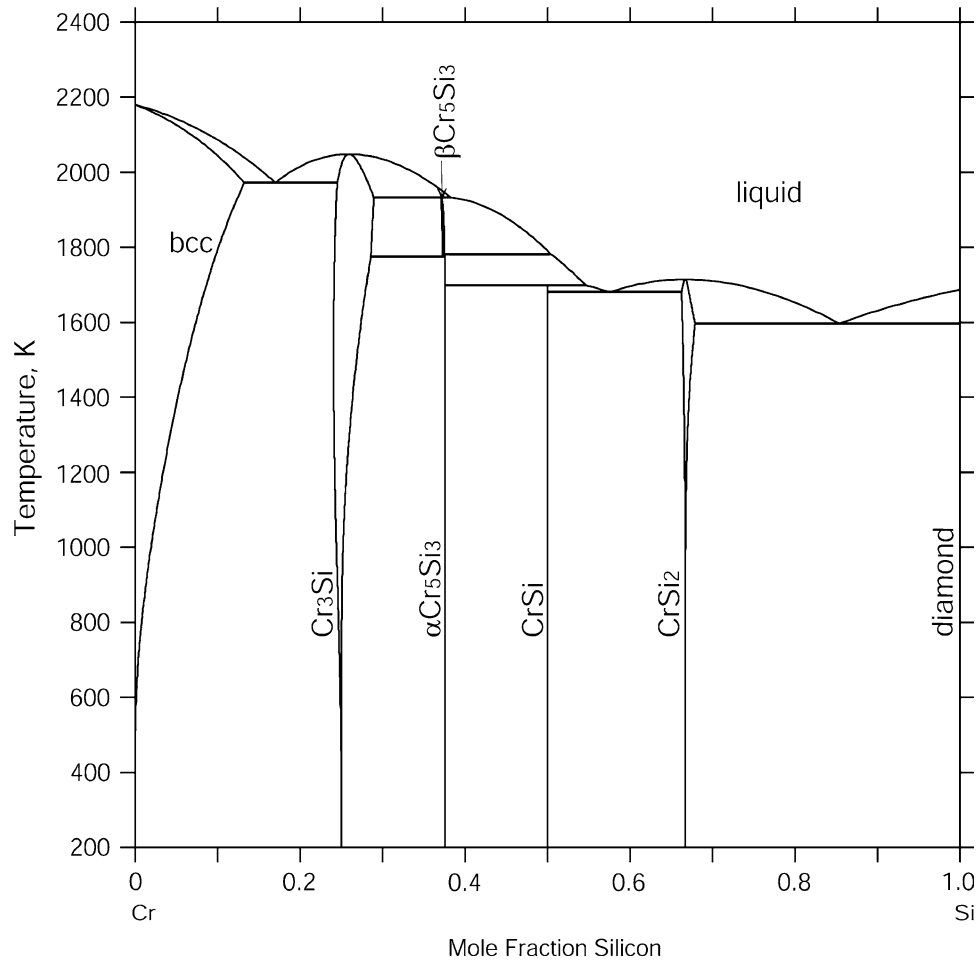


Fig. 2 Cr-Si phase diagram optimized by Chen et al.^[20]

available in the literature.^[8,13,16,17] A general rule for selection of the adjustable parameters is that only those coefficients that can be determined by the experimental values should be adjusted.^[30] The optimization was carried out by means of the optimization module PARROT of the software Thermo-Calc.^[31] The program works by minimizing a squared error sum where each of the selected values is given a certain weight. The weight is chosen by our personal judgment and changed by trial and error during the study until most of the selected experimental information is reproduced within the expected uncertainty limits.

The thermodynamic descriptions of the liquid, fcc, bcc, and diamond phases were obtained by combination of the corresponding Gibbs energy functions from the assessments of binary systems^[18,20,22] using Muggianu interpolation of binary excess terms.^[32] In this study, the coefficients ${}^0L_{Al,Cr,Si}^{liq}$ and ${}^0L_{Al,Cr,Si}^{fcc}$ were optimized based on the experimental data reported by Esslinger et al.^[8] and Gupta.^[13] The diamond structure for pure element Cr is not stable; however, its lattice stability is required for the optimization. According to the estimation of Guillermet and Huang^[33] for

high melting bcc metals V, Nb, and Ta, the following lattice stability was estimated,

$$G(\text{diamond, Cr}) = \text{GHSER}_{Cr} + 5000.0 \quad (\text{Eq 10})$$

The thermodynamic parameters of compounds in the Al-Cr-Si system were optimized on the basis of experimental data and thermodynamic parameters of compounds in the binary systems.

For the compounds CrSi₂ and Cr₃Si, the parameters $G_{Cr:Cr}^{CrSi_2}$, $G_{Cr:Si}^{CrSi_2}$, $G_{Si:Cr}^{CrSi_2}$, $G_{Si:Si}^{CrSi_2}$, ${}^0L_{Cr,Si:Cr}^{CrSi_2}$, and ${}^0L_{Cr,Si:Si}^{CrSi_2}$ of CrSi₂ and $G_{Cr:Cr}^{Cr_3Si}$, $G_{Cr:Si}^{Cr_3Si}$, $G_{Si:Cr}^{Cr_3Si}$, $G_{Si:Si}^{Cr_3Si}$, ${}^0L_{Cr,Si:Cr}^{Cr_3Si}$, ${}^0L_{Cr,Si:Si}^{Cr_3Si}$, ${}^0L_{Cr:Cr,Si}^{Cr_3Si}$, and ${}^0L_{Si:Cr,Si}^{Cr_3Si}$ of Cr₃Si in Eq 5 were derived from the binary Cr-Si system optimized by Chen et al.^[20] $G_{Cr:Al}^{CrSi_2}$ and $G_{Cr:Al}^{Cr_3Si}$ are the Gibbs energy of the hypohetic compounds CrAl₂ and Cr₃Al in the Al-Cr system, respectively, and calculated by the following equation:

$$G_{Cr:Al}^{CrSi_2} = \frac{1}{6}G_{Al:Cr}^{\alpha Al_8Cr_5} + \frac{1}{6}G_{Al:Cr}^{Al_4Cr} + u \quad (\text{Eq 11})$$

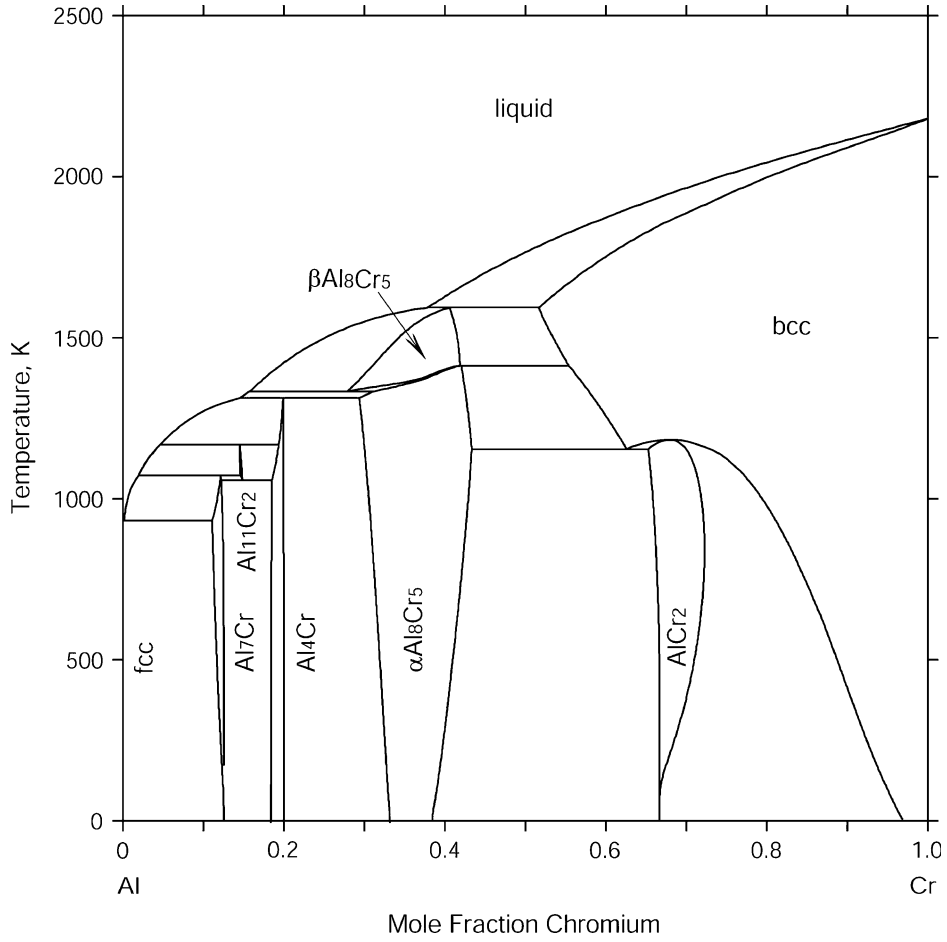


Fig. 3 Al-Cr phase diagram optimized by Liang et al.^[22]

$$G_{Cr:Al}^{Cr_3Si} = +GHSE_{Cr} + G_{Al:Cr}^{AlCr_2} + v \quad (\text{Eq 12})$$

where $G_{Al:Cr}^{\alpha Al_8Cr_5}$, $G_{Al:Cr}^{Al_4Cr}$, and $G_{Al:Cr}^{AlCr_2}$ are the Gibbs energies of the stable compounds in the Al-Cr system. In order to keep $CrAl_2$ and Cr_3Al unstable in the Al-Cr system, u and v must always be positive.

$G_{Si:Al}^{CrSi_2}$ and $G_{Si:Al}^{Cr_3Si}$ describe the Gibbs energies of metastable compounds $SiAl_2$ and Si_3Al in the Al-Si system, respectively. According to the estimation of Guillermet and Huang,^[33] the following lattice stability is estimated:

$$G_{Si:Al}^{CrSi_2} = +GHSE_{Si} + 2GHSE_{Al} + 15000.0 \quad (\text{Eq 13})$$

$$G_{Si:Al}^{Cr_3Si} = +3GHSE_{Si} + GHSE_{Al} + 20000.0 \quad (\text{Eq 14})$$

In this study, the parameters $G_{Cr:Al}^{CrSi_2}$, $G_{Cr:Al}^{Cr_3Si}$, ${}^0L_{Cr:Al,Si}^{CrSi_2}$, and ${}^1L_{Cr:Al,Si}^{CrSi_2}$ are optimized according to the experimental data measured by Gupta^[13] and Chen et al.^[16]

For $AlCr_2$, the parameters $G_{Al:Al}^{AlCr_2}$, $G_{Al:Cr}^{AlCr_2}$, $G_{Cr:Al}^{AlCr_2}$, $G_{Cr:Cr}^{AlCr_2}$, ${}^0L_{Al:Al,Cr}^{AlCr_2}$, ${}^0L_{Cr:Al,Cr}^{AlCr_2}$, ${}^0L_{Al,Cr,Al}^{AlCr_2}$, and ${}^0L_{Al,Cr,Cr}^{AlCr_2}$ were derived

from the binary Al-Cr system optimized by Liang et al.^[22] The following assumptions are made:

$$G_{Si:Al}^{AlCr_2} = +GHSE_{Si} + 2GHSE_{Al} + 15000.0 \quad (\text{Eq 15})$$

$$G_{Si:Cr}^{AlCr_2} = +GHSE_{Si} + 2GHSE_{Cr} + 15000.0 \quad (\text{Eq 16})$$

Only one parameter ${}^0L_{Al,Si,Cr}^{AlCr_2}$ is optimized in this study.

For Al_4Cr and $Al_{11}Cr_2$, the parameters $G_{Al:Al}^{Al_4Cr}$, $G_{Al:Cr}^{Al_4Cr}$, and ${}^0L_{Al:Al,Cr}^{Al_4Cr}$ of Al_4Cr and $G_{Al:Al}^{Al_{11}Cr_2}$, $G_{Al:Cr}^{Al_{11}Cr_2}$, and ${}^0L_{Al:Al,Cr}^{Al_{11}Cr_2}$ of $Al_{11}Cr_2$ in Eq 6 were derived from Liang et al.^[22] $G_{Si:Cr}^{Al_{11}Cr_2}$ is expressed by the following assumption:

$$G_{Si:Cr}^{Al_{11}Cr_2} = +11GHSE_{Si} + 2GHSE_{Cr} + 65000.0 \quad (\text{Eq 17})$$

The parameters $G_{Si:Al}^{Al_4Cr}$, $G_{Si:Al}^{Al_{11}Cr_2}$, ${}^jL_{Al,Si,Cr}^{Al_4Cr}$, and ${}^jL_{Al,Si,Cr}^{Al_{11}Cr_2}$ are optimized in this study based on the experimental results reported by Chen et al.^[16]

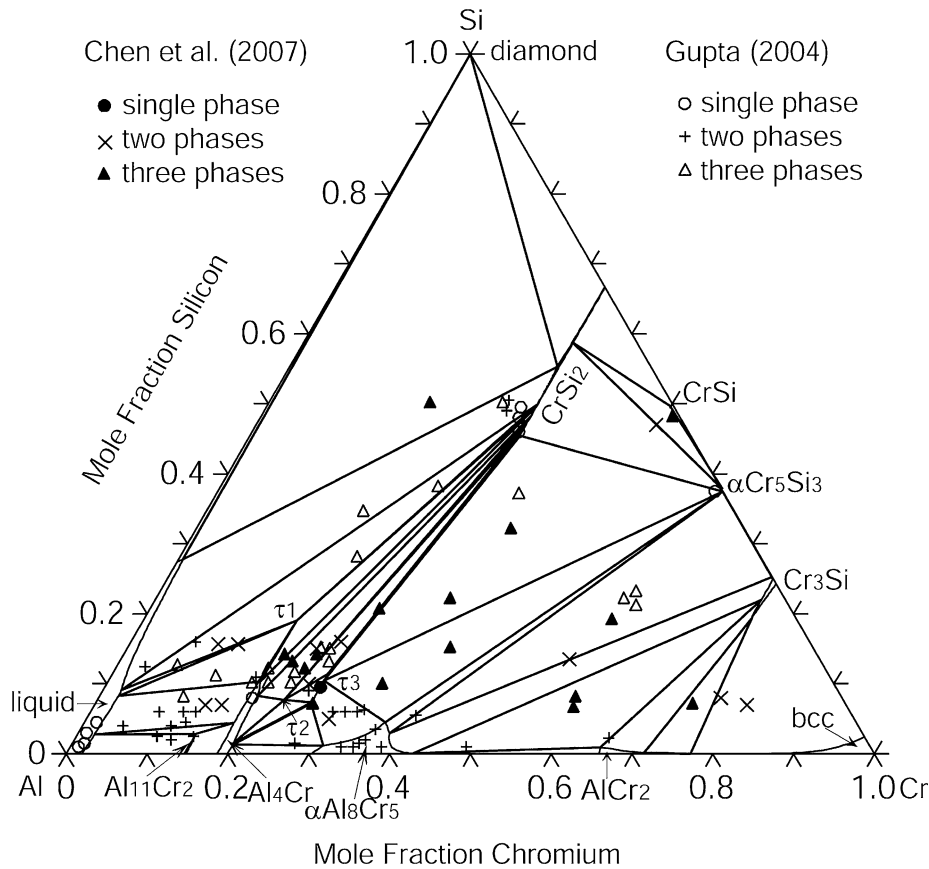


Fig. 4 Calculated isothermal section of the Al-Cr-Si system at 1073 K using the present thermodynamic description with the experimental data^[13,16]

For the compounds $\alpha\text{Al}_8\text{Cr}_5$ and $\beta\text{Al}_8\text{Cr}_5$, the parameters $G_{\text{Al:Al}}^\phi$, $G_{\text{Al:Cr}}^\phi$, $G_{\text{Cr:Al}}^\phi$, $G_{\text{Cr:Cr}}^\phi$, $jL_{\text{Al:Cr:Al}}^\phi$, $jL_{\text{Al:Cr:Cr}}^\phi$, $jL_{\text{Al:Al:Cr}}^\phi$, and $jL_{\text{Cr:Al:Cr}}^\phi$ ($\phi = \alpha\text{Al}_8\text{Cr}_5$, $\beta\text{Al}_8\text{Cr}_5$) were derived from the binary Al-Cr system.^[22] The parameters $G_{\text{Al:Si}}^\phi$, $G_{\text{Cr:Si}}^\phi$, and $G_{\text{Si:Si}}^\phi$ were assumed as follows:

$$G_{\text{Al:Si}}^\phi = +8\text{GHSE}_{\text{Al}} + 5\text{GHSE}_{\text{Si}} + 65000.0 \quad (\text{Eq 18})$$

$$G_{\text{Cr:Si}}^\phi = +8\text{GHSE}_{\text{Cr}} + 5\text{GHSE}_{\text{Si}} + 65000.0 \quad (\text{Eq 19})$$

$$G_{\text{Si:Si}}^\phi = +13\text{GHSE}_{\text{Si}} + 65000.0 \quad (\text{Eq 20})$$

In this study, the parameters $G_{\text{Si:Al}}^\phi$ and $jL_{\text{Al:Si:Cr}}^\phi$ are optimized from the experimental data of Chen et al.^[16]

For the ternary compound $\tau_3\text{-(Al,Si)}_{11}\text{Cr}_4$, the parameter $G_{\text{Cr:Al}}^{\tau_3}$ in Eq 9 is described as

$$G_{\text{Cr:Al}}^{\tau_3} = \frac{5}{12}G_{\text{Al:Cr}}^{\alpha\text{Al}_8\text{Cr}_5} + \frac{23}{12}G_{\text{Al:Cr}}^{\text{Al}_4\text{Cr}} + w \quad (\text{Eq 21})$$

where w is a positive value. The parameters $G_{\text{Cr:Al}}^{\tau_3}$, ${}^0L_{\text{Cr:Al:Si}}^{\tau_3}$, and ${}^1L_{\text{Cr:Al:Si}}^{\tau_3}$ are optimized in this study.

4. Results and Discussions

A thermodynamic description of the Al-Cr-Si system obtained in this study is shown in Table 1. The calculated invariant equilibria are listed in Table 2. Satisfactory agreement was obtained between the experimental present calculations of this study and the previous experimental results.^[8,13,16,17]

Figures 1 to 3 show the Al-Si phase diagram optimized by Gröbner et al.,^[18] with the Cr-Si phase diagram optimized by Chen et al.^[20] and the Al-Cr phase diagram optimized by Liang et al.,^[22] respectively.

Figure 4 is the calculated isothermal section at 1073 K in comparison with the experimental data.^[13,16] Good agreement was obtained between the calculated and experimental results determined by Chen et al.^[16] The calculated three-phase regions related to the compounds $\alpha\text{Al}_8\text{Cr}_5$, $\text{Al}_{11}\text{Cr}_2$, τ_1 , τ_2 , and τ_3 are inconsistent with the experimental data of Gupta^[13] because τ_1 , τ_2 , and τ_3 exist and Al_8Cr_5 and Al_9Cr_4 are replaced by $\alpha\text{Al}_8\text{Cr}_5$ at 1073 K.^[16]

A series of isothermal sections in the Al-Cr-Si system constructed by Gupta^[13] were based on the binary phase diagram of the Al-Cr system reviewed by Massalski.^[34]

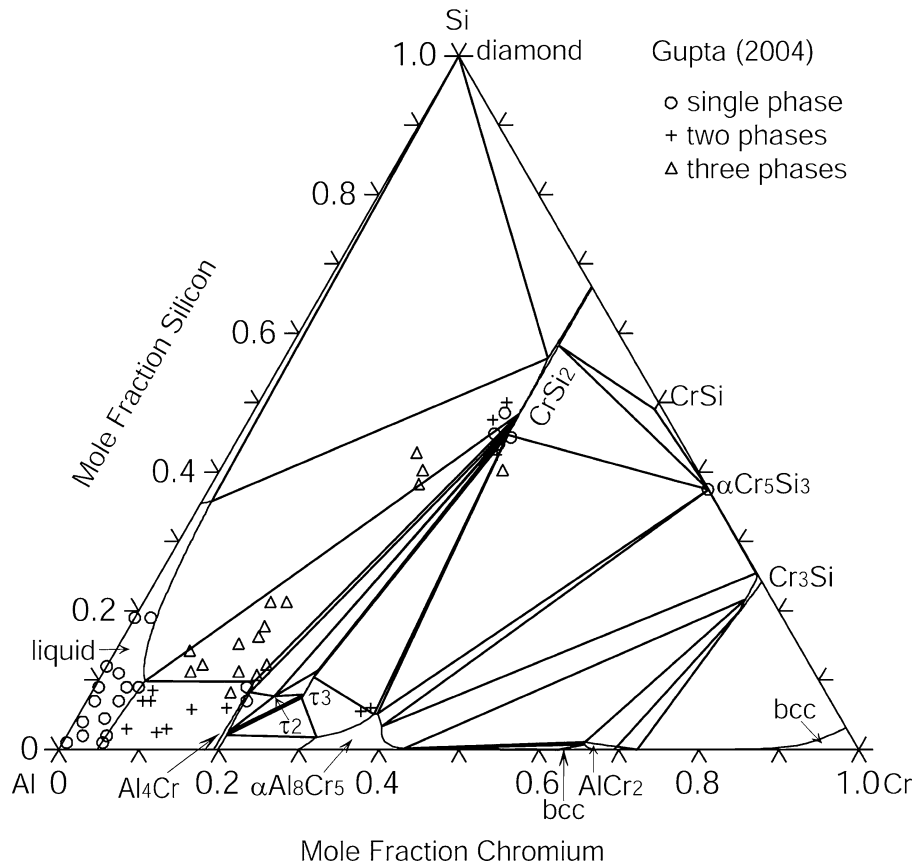


Fig. 5 Calculated isothermal section of the Al-Cr-Si system at 1173 K using the present thermodynamic description in comparison with the experimental data measured by Gupta^[13]

Later, Mahdouk and Gachon^[23] reported the existence of $\text{Al}_{11}\text{Cr}_2$ between 1058 and 1168 K in the Al-Cr system. The experimental results of Grushko et al.^[24] showed that there were one high-temperature phase $\beta\text{Al}_8\text{Cr}_5$ between 1333 and 1593 K and one low-temperature phase $\alpha\text{Al}_8\text{Cr}_5$ below 1413 K in the composition range between 30 and 42 at.% Cr, and Al_9Cr_4 did not exist in the Al-Cr system. These results were accepted in the thermodynamic assessment of binary Al-Cr system.^[22] Accordingly, the phase relationship reported by Gupta^[13] was modified in this study according to the binary phase diagram of the Al-Cr^[22] and the experimental data.^[16]

Figures 5 to 7 are the calculated Al-Cr-Si isothermal sections at 1173, 1273, and 1373 K in comparison with the experimental data.^[13] Satisfactory agreement is obtained between the calculated and experimental results. As shown in Fig. 5, due to the stable existence of $\text{Al}_{11}\text{Cr}_2$ from 1058 to 1168 K and the congruent decomposition of AlCr_2 into the bcc phase at 68.07 at.% Cr and 1183 K in the Al-Cr system,^[22] two three-phase fields $\text{liq.} + \text{CrSi}_2 + \text{Al}_{11}\text{Cr}_2$ and $\text{Al}_4\text{Cr} + \text{CrSi}_2 + \text{Al}_{11}\text{Cr}_2$ reported by Gupta^[13] were replaced by $\text{liq.} + \text{Al}_4\text{Cr} + \text{CrSi}_2$, and two three-phase fields $\alpha\text{Al}_8\text{Cr}_5 + \text{bcc} + \text{AlCr}_2$ and $\text{Cr}_3\text{Si} + \text{bcc} + \text{AlCr}_2$ were added. Because of a low-temperature phase $\alpha\text{Al}_8\text{Cr}_5$ instead

of phases Al_9Cr_4 and Al_8Cr_5 in the binary Al-Cr system,^[22] three-phase fields $\alpha\text{Cr}_5\text{Si}_3 + \text{Cr}_3\text{Si} + \text{Al}_8\text{Cr}_5$, $\text{Cr}_3\text{Si} + \text{AlCr}_2 + \text{Al}_8\text{Cr}_5$, and $\text{CrSi}_2 + \alpha\text{Cr}_5\text{Si}_3 + \text{Al}_9\text{Cr}_4$ ^[13] were replaced by $\alpha\text{Cr}_5\text{Si}_3 + \text{Cr}_3\text{Si} + \alpha\text{Al}_8\text{Cr}_5$, $\text{Cr}_3\text{Si} + \text{AlCr}_2 + \alpha\text{Al}_8\text{Cr}_5$, and $\text{CrSi}_2 + \alpha\text{Cr}_5\text{Si}_3 + \alpha\text{Al}_8\text{Cr}_5$, respectively. And the three-phase field $\alpha\text{Cr}_5\text{Si}_3 + \text{Al}_8\text{Cr}_5 + \text{Al}_9\text{Cr}_4$ ^[13] did not exist. With the existence of τ_2 and τ_3 ,^[16,17] the three-phase field $\text{Al}_4\text{Cr} + \text{CrSi}_2 + \text{Al}_9\text{Cr}_4$ ^[13] was replaced by $\text{Al}_4\text{Cr} + \text{CrSi}_2 + \tau_2$, $\tau_2 + \tau_3 + \text{CrSi}_2$, $\alpha\text{Al}_8\text{Cr}_5 + \text{CrSi}_2 + \tau_3$, $\tau_2 + \tau_3 + \text{Al}_4\text{Cr}$, and $\alpha\text{Al}_8\text{Cr}_5 + \tau_3 + \text{Al}_4\text{Cr}$ in this study. Figures 6 and 7 are similar to Fig. 5; only the three-phase regions related to the compounds $\alpha\text{Al}_8\text{Cr}_5$, $\beta\text{Al}_8\text{Cr}_5$, τ_3 , and τ_4 are in disagreement with the experimental data of Gupta.^[13]

Figures 8 and 9 are the vertical sections of the Al-Cr-Si system at 5 at.% Cr and 4 at.% Si calculated by the present thermodynamic description in comparison with the experimental data.^[8] In the experimental results of Esslinger et al.,^[8] there did not exist the phase regions involving Al_4Cr in the vertical sections of the Al-Cr-Si system at 5 at.% Cr and 4 at.% Si, and τ_1 existed below 983 K with a peritectic reaction $\text{liq.} + \text{CrSi}_2 + \text{Al}_{11}\text{Cr}_2 \rightarrow \tau_1$. These results were inconsistent with recent experimental results,^[13,16] where $\text{liq.} + \text{CrSi}_2 + \text{Al}_{11}\text{Cr}_2 \rightarrow \tau_1$ at 983 K^[8] should be

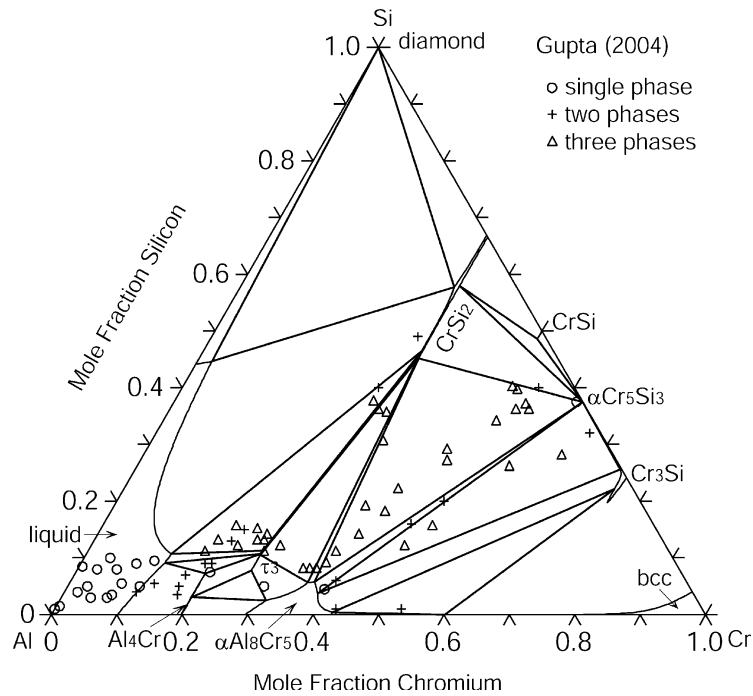


Fig. 6 Calculated isothermal section of the Al-Cr-Si system at 1273 K using the present thermodynamic description in comparison with the experimental data measured by Gupta^[13]

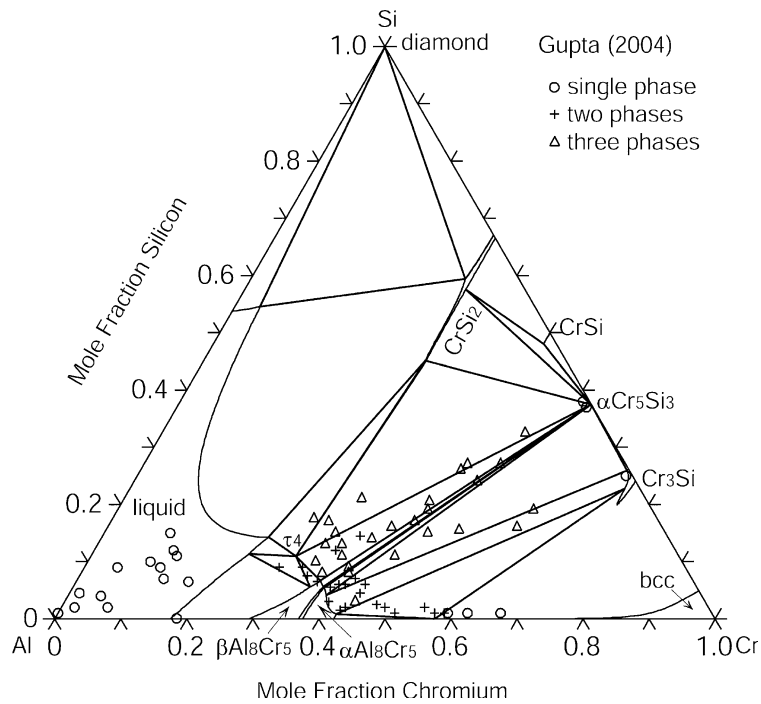


Fig. 7 Calculated isothermal section of the Al-Cr-Si system at 1373 K using the present thermodynamic description in comparison with the experimental data measured by Gupta^[13]

liq. + CrSi₂ + Al₄Cr → τ₁^[13] at higher than 1073 K,^[16] an invariant reaction liq. + Al₄Cr → Al₁₁Cr₂ + τ₁ at 953 to 983 K was reported by Gupta,^[13] and Al₁₁Cr₂ had a

relatively low solubility of silicon.^[16] The discrepancy between the calculated and experimental composition^[8] of the invariant reaction liq. → diamond + fcc + τ₁ (850 K)

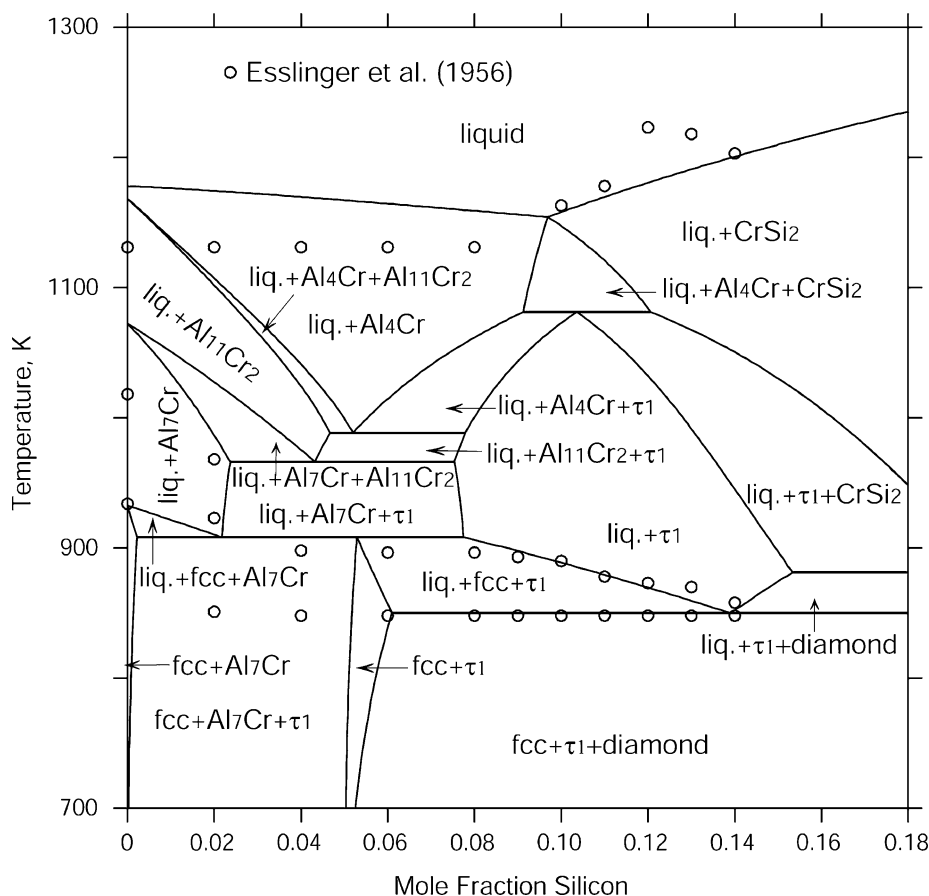


Fig. 8 Calculated vertical section of the Al-Cr-Si system at 5 at.% Cr using the present thermodynamic description in comparison with the experimental data measured by Esslinger et al.^[8]

was mainly caused by the very low solubility of Cr in fcc (Al),^[22] which results in the difference between calculated results and experimental data^[8] at the composition ranges of the three-phase regions fcc + Al₇Cr + τ_1 , liq. + fcc + τ_1 , and fcc + τ_1 + diamond. The calculated Al-rich liquidus temperatures are higher than the experimental data reported by Esslinger et al.^[8] This discrepancy was mainly caused by the higher liquidus in the Al-rich part of the newly assessed the binary Al-Cr system.^[22] And the changing of the liquidus also caused the shrinking of the two-phase region liq. + τ_1 in Fig. 9. In addition, the three-phase regions liq. + Al₁₁Cr₂ + CrSi₂ and liq. + Al₁₁Cr₂ + τ_1 ^[8] were replaced by liq. + Al₄Cr + CrSi₂ and liq. + Al₄Cr + τ_1 , respectively, and two-phase regions liq. + Al₄Cr and liq. + Al₄Cr + Al₁₁Cr₂ were added in Fig. 8, based on the experimental results.^[13,16,22] And three-phase regions liq. + Al₄Cr, liq. + Al₄Cr + Al₁₁Cr₂, and liq. + Al₇Cr + Al₁₁Cr₂ were added in Fig. 9 because of the existence of liq. + Al₄Cr \rightarrow Al₁₁Cr₂ + τ_1 (U10).^[13]

Figure 10(a) is the calculated liquidus projection of the Al-Cr-Si system using the present thermodynamic description. Figure 10(b) is the enlarged section of Fig. 10(a). In the experimental results of Gupta,^[13] a quasi-peritectic

reaction liq. + Al₄Cr \rightarrow Al₁₁Cr₂ + τ_1 (U10) between 953 and 983 K was reported. The reaction temperature ranging from 953 to 983 K,^[13] correspond to the quasi-peritectic reaction liq. + Al₁₁Cr₂ \rightarrow Al₇Cr + τ_1 at 953 K and the peritectic reaction liq. + CrSi₂ + Al₁₁Cr₂ \rightarrow τ_1 at 983 K, respectively, as reported by Esslinger et al.^[8] Gupta^[13] pointed out that the three-phase field liq. + Al₄Cr + Al₁₁Cr₂ of the reaction liq. + Al₄Cr \rightarrow Al₁₁Cr₂ + τ_1 descended from the binary peritectic reaction liq. + Al₄Cr \rightarrow Al₁₁Cr₂ at 1214 K of the Al-Cr system,^[34] another three-phase field liq. + Al₄Cr + τ_1 originated possibly from the peritectic reaction at 983 K. Thus, the peritectic reaction liq. + CrSi₂ + Al₁₁Cr₂ \rightarrow τ_1 at 983 K reported by Esslinger et al.^[8] should be replaced by liq. + CrSi₂ + Al₄Cr \rightarrow τ_1 at 983 K to be consistent with the three-phase fields descending or ascending. Because the compound τ_1 was confirmed to be stable at 1079 K by Chen,^[17] in this study, the reaction temperatures of liq. + CrSi₂ + Al₄Cr \rightarrow τ_1 (P3) and liq. + Al₄Cr \rightarrow Al₁₁Cr₂ + τ_1 (U10) were optimized to be at 1081 and 988 K, respectively. Satisfactory agreement was obtained between the calculated and experimental results.^[13,16] Chen^[17] also predicted the projection of the liquidus surface of the Al-Cr-Si system, in which the

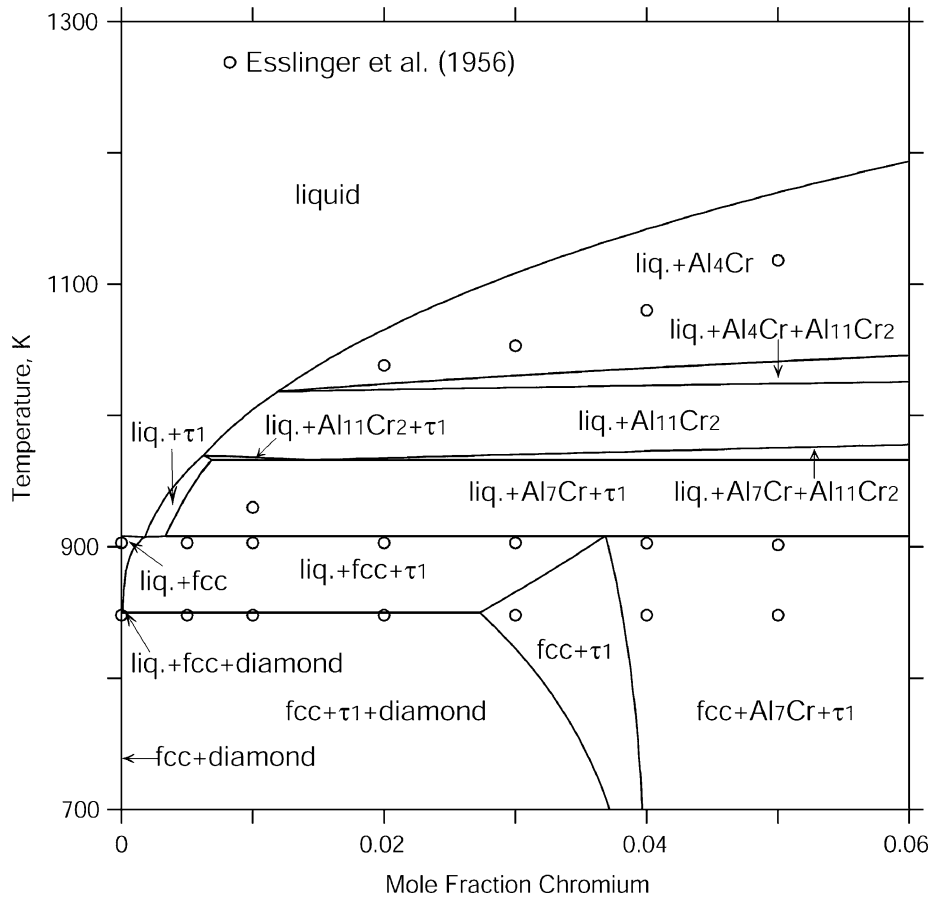


Fig. 9 Calculated vertical section of the Al-Cr-Si system at 4 at.% Si using the present thermodynamic description in comparison with the experimental data measured by Esslinger et al.^[8]

invariant reaction temperature for $\text{liq.} + \text{Al}_8\text{Cr}_5 + \tau_3 \rightarrow \text{Al}_4\text{Cr}$ at 1309 K is nearly same as for $\text{liq.} + \text{Al}_8\text{Cr}_5 \rightarrow \text{Al}_4\text{Cr}$ at 1309 K in the Al-Cr binary system; however, the invariant reaction composition of the liquid phase varies from 0 to ~23.2 at.% Si. In addition, the invariant reaction temperature for $\text{liq.} + \text{Al}_4\text{Cr} \rightarrow \text{Al}_{11}\text{Cr}_2 + \tau_1$ at 1058 K reported by Chen^[17] is consistent with the decomposition temperature of $\text{Al}_{11}\text{Cr}_2$ in the Al-Cr binary system.^[22,23] Therefore, the projection of the liquidus surface at Al-rich corner reported by Chen^[17] is not adopted in this study.

Figure 11 is the calculated reaction scheme of the Al-Cr-Si system. The compounds τ_1 , τ_3 , and τ_4 are formed by the peritectic reactions $\text{liq.} + \text{Al}_4\text{Cr} + \text{CrSi}_2 \rightarrow \tau_1$ at 1081 K, which are in agreement with the experimental results

determined by Gupta^[13] and Chen et al.,^[16] $\text{liq.} + \alpha\text{Al}_8\text{Cr}_5 + \tau_4 \rightarrow \tau_3$ at 1331 K, and $\text{liq.} + \text{CrSi}_2 + \beta\text{Al}_8\text{Cr}_5 \rightarrow \tau_4$ at 1380 K, respectively.

5. Summary

The phase relationships and a thermodynamic description in the Al-Cr-Si system were critically evaluated from the experimental information available in the literature. A set of self-consistent thermodynamic parameters was derived. With the thermodynamic description available, one can now make various calculations of practical interest.

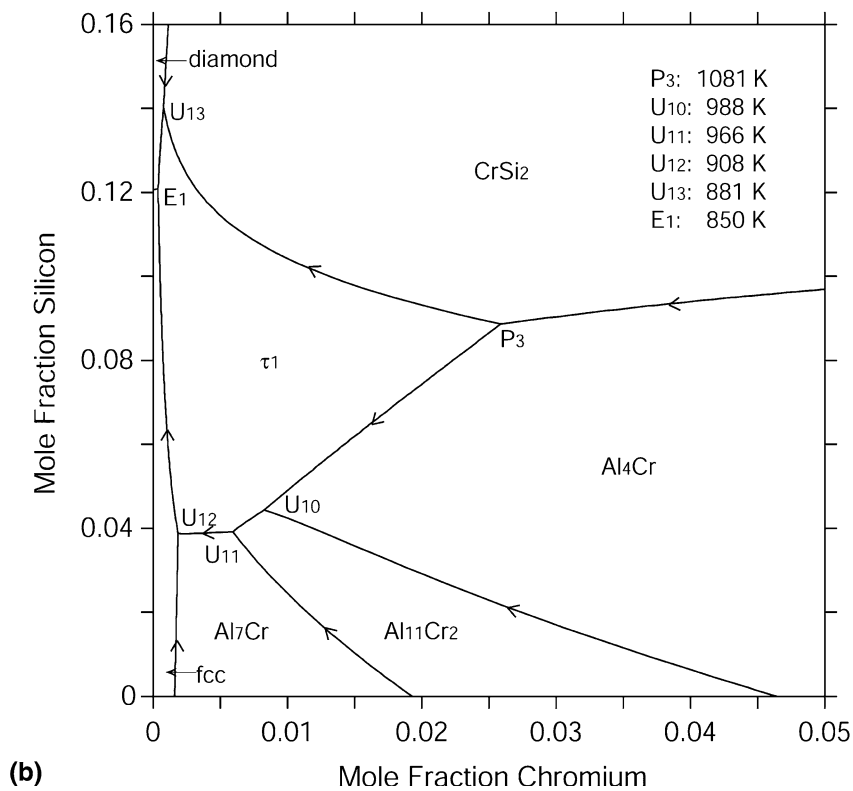
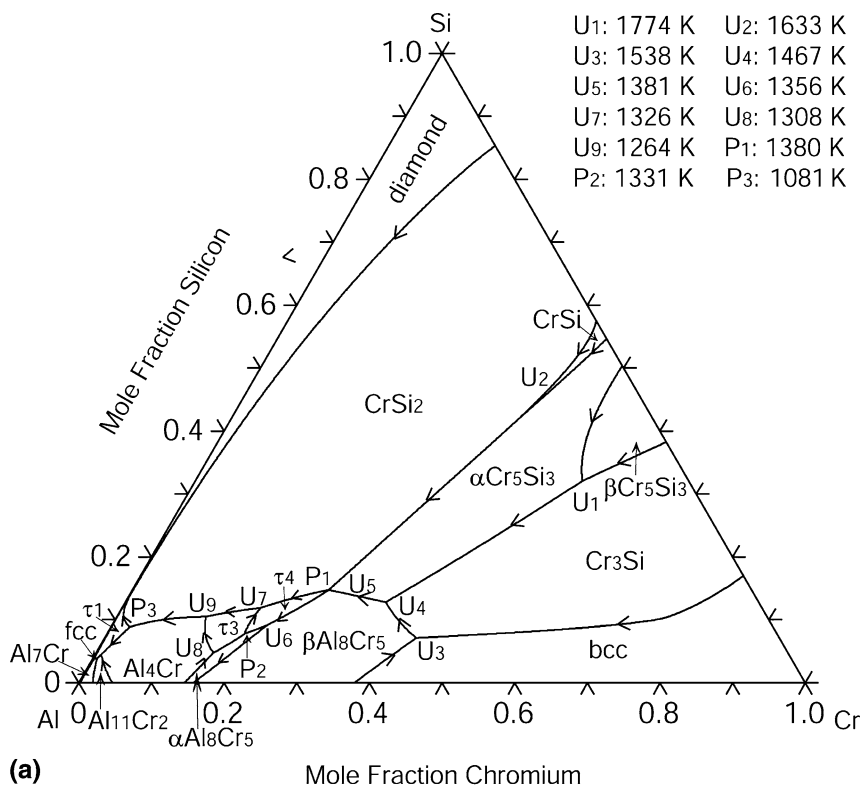
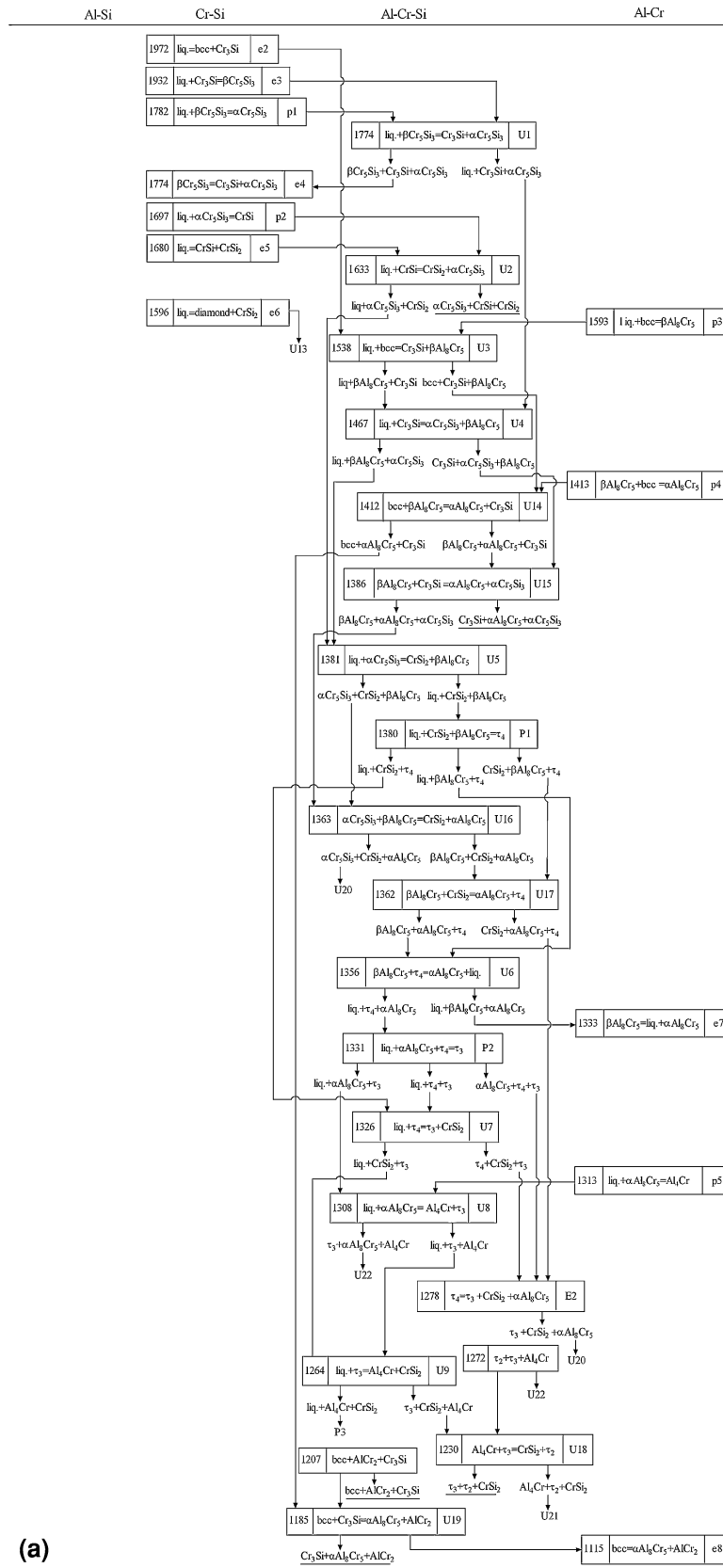
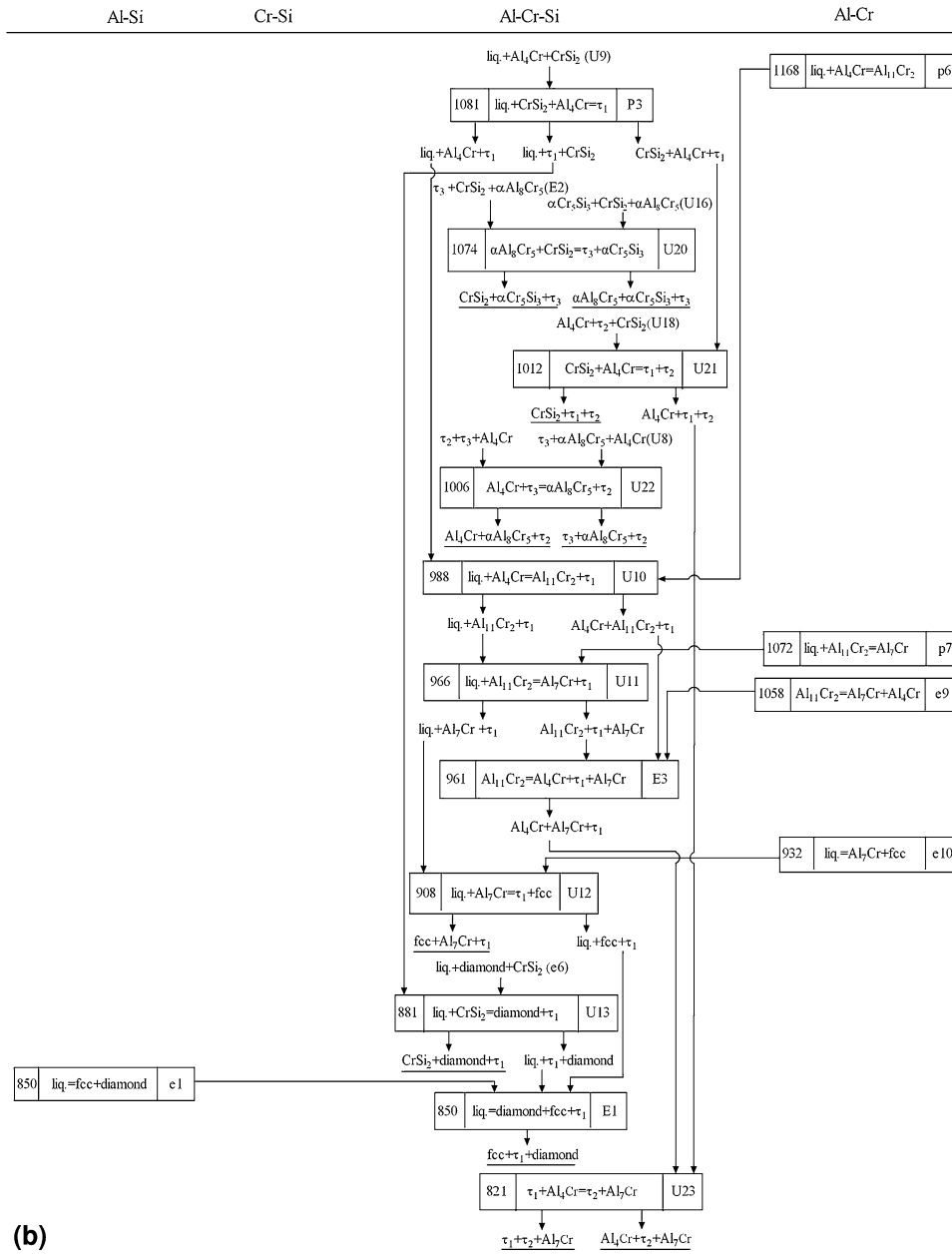


Fig. 10 (a) Calculated liquidus projection of the Al-Cr-Si system using the present thermodynamic description. (b) Enlarged section of Fig. 10(a)



(a)

Fig. 11 Calculated reaction scheme of the Al-Cr-Si system



(b)

Fig. 11 continued

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