Supplementary Information

Theory

The difference of the chemical potentials between liquid and solid is given by

$$\Delta\mu = x\Delta\mu_{AD} + (1-x)\Delta\mu_{BD}, \tag{S1}$$

where the chemical potential differences of AD and BD pairs in the liquid and in the solid state are given by

$$\Delta\mu_{AD} = \mu_A^L + \mu_D^L - \mu_{AD}^s, \tag{S2}$$

$$\Delta\mu_{BD} = \mu_B^L + \mu_D^L - \mu_{BD}^s. \tag{S3}$$

The chemical potentials of the species in the liquid are expressed as $\mu_i^L = \mu_i^0 + k_B T ln(c_i) + \vartheta_i$, namely

$$\begin{aligned}\mu_A^L = \mu_A^0 + k_B T ln(c_A) &+ \omega_{AB}{c_B}^2 + \omega_{AD}{c_D}^2 \\ &+ \omega_{AU}{c_U}^2 \\ &+ (\omega_{AB} + \omega_{AD} - \omega_{BD})c_B c_D \\ &+ (\omega_{AB} + \omega_{AU} - \omega_{BU})c_B c_U \\ &+ (\omega_{AD} + \omega_{AU} - \omega_{DU})c_D c_U \\ &+ (c_B c_D - 2c_A c_B c_D)\omega_{ABD} \\ &+ (c_B c_U - 2c_A c_B c_U)\omega_{ABU} \\ &+ (c_D c_U - 2c_A c_D c_U)\omega_{ADU} \\ &- 2c_B c_D c_U \omega_{BDU} \\ &+ (2c_A c_B - {c_B}^2 - 2c_B {c_A}^2 \\ &+ 2{c_B}^2 c_A)\omega'_{AB} \\ &+ (2c_A c_D - {c_D}^2 - 2c_D {c_A}^2 \\ &+ 2{c_D}^2 c_A)\omega'_{AD} \\ &+ (2c_A c_U - {c_U}^2 - 2c_U {c_A}^2 \\ &+ 2{c_U}^2 c_A)\omega'_{AU} \\ &+ 2(c_B {c_D}^2 - {c_B}^2 c_D)\omega'_{BD} \\ &+ 2(c_B {c_U}^2 - {c_B}^2 c_U)\omega'_{BU} \\ &+ 2(c_D {c_U}^2 - {c_D}^2 c_U)\omega'_{DU},\end{aligned} \tag{S4}$$

$$\begin{aligned}\mu_B^L = \mu_B^0 + k_B T ln(c_B) &+ \omega_{AB}{c_A}^2 + \omega_{BD}{c_D}^2 \\ &+ \omega_{BU}{c_U}^2 \\ &+ (\omega_{AB} + \omega_{BD} - \omega_{AD})c_A c_D \\ &+ (\omega_{AB} + \omega_{BU} - \omega_{AU})c_A c_U \\ &+ (\omega_{BD} + \omega_{BU} - \omega_{DU})c_D c_U \\ &+ (c_A c_D - 2c_A c_B c_D)\omega_{ABD} \\ &+ (c_A c_U - 2c_A c_B c_U)\omega_{ABU} \\ &+ (c_D c_U - 2c_B c_D c_U)\omega_{BDU} \\ &- 2c_A c_D c_U \omega_{ADU} \\ &+ (2c_A c_B - {c_A}^2 - 2c_A {c_B}^2 \\ &+ 2{c_A}^2 c_B)\omega'_{BA} \\ &+ (2c_B c_D - {c_D}^2 - 2c_D {c_B}^2 \\ &+ 2{c_D}^2 c_B)\omega'_{BD} \\ &+ (2c_B c_U - {c_U}^2 - 2c_U {c_B}^2 \\ &+ 2{c_U}^2 c_B)\omega'_{BU} \\ &+ 2(c_A {c_D}^2 - {c_A}^2 c_D)\omega'_{AD} \\ &+ 2(c_A {c_U}^2 - {c_A}^2 c_U)\omega'_{AU} \\ &+ 2(c_D {c_U}^2 - {c_D}^2 c_U)\omega'_{DU},\end{aligned} \tag{S5}$$

$$\mu_D^L = \mu_D^0 + k_B T ln(c_D) + \omega_{AD} {c_A}^2 + \omega_{BD} {c_B}^2 + \omega_{DU} {c_U}^2 + (\omega_{AD} + \omega_{BD} - \omega_{AB}) c_A c_B + (\omega_{AD} + \omega_{DU} - \omega_{AU}) c_A c_U + (\omega_{BD} + \omega_{DU} - \omega_{BU}) c_B c_U + (c_A c_B - 2 c_A c_B c_D) \omega_{ABD} + (c_A c_U - 2 c_A c_D c_U) \omega_{ADU} + (c_B c_U - 2 c_B c_D c_U) \omega_{BDU} - 2 c_A c_B c_U \omega_{ABU} + (2 c_A c_D - {c_A}^2 - 2 c_A {c_D}^2 + 2 {c_A}^2 c_D) \omega'_{DA} + (2 c_B c_D - {c_B}^2 - 2 c_B {c_D}^2 + 2 {c_B}^2 c_D) \omega'_{DB} + (2 c_D c_U - {c_U}^2 - 2 c_U {c_D}^2 + 2 {c_U}^2 c_D) \omega'_{DU} + 2 (c_A {c_B}^2 - {c_A}^2 c_B) \omega'_{AB} + 2 (c_A {c_U}^2 - {c_A}^2 c_U) \omega'_{AU} + 2 (c_B {c_U}^2 - {c_B}^2 c_U) \omega'_{BU}. \quad \text{(S6)}$$

Here μ^0 is the Gibbs free energy of the corresponding pure element, ω_{ij} and ω_{ijk} are the binary and ternary interaction parameters.

The chemical potentials in the solid of AD and BD binary species are given by

$$\mu_{AD}^S = \mu_{AD}^0 + k_B T ln x + (1-x)^2 [\omega_S + (4x-1)\omega'_S], \quad \text{(S7)}$$

$$\mu_{BD}^S = \mu_{BD}^0 + k_B T ln(1-x) + x^2 [\omega_S + (4x-3)\omega'_S]. \quad \text{(S8)}$$

Here ω_S and ω'_S are the temperature dependent interaction parameters of zeroth and first order, and μ^0 is the Gibbs free energy of the corresponding binary compound.

The parameter b is given by [1]

$$b = \alpha - 6 c_{tot}^2 \omega'_{AB} - 2 c_{tot} [\omega_{AB} - 3 c_{tot} \omega'_{AB} - c_D (\omega'_{AD} + \omega'_{BD}) - c_U (\omega'_{AU} + \omega'_{BU}) + c_D \omega_{ABD} + c_U \omega_{ABU}] \quad \text{(S9)}$$

with

$$\alpha = \Delta\mu_{AD}^0 - \Delta\mu_{BD}^0 + (\omega_{AB} - c_{tot} \omega'_{AB} - 2 c_D \omega'_{BD} - 2 c_U \omega'_{BU} + c_D \omega_{ABD} + c_U \omega_{ABU}) c_{tot} + (\omega_{AD} - \omega_{BD}) c_D + (\omega_{AU} - \omega_{BU}) c_U - (\omega'_{AD} - \omega'_{BD}) c_D^2 - (\omega'_{AU} - \omega'_{BU}) c_U^2 + (\omega_{ADU} - \omega_{BDU}) c_D c_U. \quad \text{(S10)}$$

The parameter b_D is given by

$$b_D = \mu_{AD}^0 - \mu_A^0 - \mu_D^0 - \vartheta_A - \vartheta_D. \quad \text{(S11)}$$

Parameters for As-Ga-In, In-Ga-Sb and Al-Ga-As material systems

Table S1. Ternary interaction parameters of the As-Au-Ga-In-Sb system. The energy values are in J/mole and the temperature is in K.

Ternary System	ω_{ijk}	ω_s	Refs.
Al-As-Ga	-55508.5 + 33.2087·T	2187	[2]
Ga-In-Sb	-5072.76 - 10.8842·T	9093 - 2.8698·T	[3]
In-Ga-As	-12889.5	19698.8 - 7.51693·T	[4]
In-Ga-Au	20500		[5]
Au-In-Sb	1129.0976 - 16.232·T		[6]

Table S2. Binary interaction parameters of the As-Au-Ga-In-Sb system. The energy values are in J/mole and the temperature is in K.

Binary Systems	ω_{ij}	ω'_{ij}	Refs.
Al-Ga	2613.3 - 2.94533·T	692.4 - 0.09271·T	[7]
Al-As	-15693 - 34.163·T		[7]
As-Ga	-25503.6 - 4.3109·T	-5174.7	[7]
Ga-Sb	-13953.8 + 71.07866·T - 9.6232·T·ln(T)	1722.9 - 1.92588·T	[7]
As-In	-15851 - 11.27053·T	-1219.5	[7]
In-Sb	-25631.2 + 102.9324·T - 13.45816·T·ln(T)	-2115.4 - 1.31907·T	[7]
Ga-In	4450 + 1.19185·T	0.25943	[8]
Al-Au	-131996.19 + 36.42·T	40781.83 - 1.896·T	[9]
Au-Sb	-10288.0428 - 14.7865028·T	-2901.66787 - 7.2503632·T	[10]
As-Au	18160.759 - 14.327686·T	-13132.906 + 13.229781·T	[11]
Au-In	-76196.19 + 64.2914·T - 6.6375·T·ln(T)	-31134.02 + 81.3582·T - 8.5134·T·ln(T)	[12]
Au-Ga	-71830.123 + 42.286·T - 4.289·T·ln(T)	-22892.323 + 5.069·T	[13]

Table S3. The chemical potentials of the species in the solid. The energy values are in J/mole and the temperature is in K.

Binary Systems	μ_{ij}^0	Refs.
Al-As	-117130+7.78·T + $GHSER_{Al}$ + $GHSER_{As}$	[7]
Ga-As	-104352 + 265.43256·T - 48.681258·T·ln(T) - 11.158E-04·T^2 + 127670·T^{-1} - 7.1378E-07·T^3 (2)	[7]
In-As	-73057.2 + 230.91896·T - 45.187942·T·ln(T) - 0.00773·T^2 + 69438·T^{-1} + 14.18E-08·T^3	[7]
Ga-Sb	-43476.2 - 21.07528·T + 5.385752·T·ln(T) - 0.00275582·T^2 + $GHSER_{Ga}$ + $GHSER_{Sb}$	[7]
In-Sb	-31698.6 + 0.586278·T + 2.587162·T·ln (T) + $GHSER_{In}$ + $GHSER_{Sb}$	[7]

Table S4. The chemical potentials of the species in the liquid. The energy values are in J/mole and the temperature is in K.

Systems	μ_i^0	Refs.
Al	(298.15<T<700) 3028.879 + 125.251171·T - 24.3671976·T·ln(T) - 0.001884662·T^2 - 8.77664E-07·T^3 + 74092·T^{-1} + 7.9337E-20·T^7 (700<T<933.47) - 271.21 + 211.206579·T - 38.5844296·T·ln(T) + 0.018531982·T^2 - 5.764227E-06·T^3 + 74092·T^{-1} + 7.9337E-20·T^7	[14]
As	(298.15<T<1200) 24442.9 - 22.424679·T + $GHSER_{As}$	[14]
Ga	(200<T<302.91) 5491.298-18.073995·T + $GHSER_{Ga}$ - 7.0171E-17·T^7 (302.91<T<4000) 5666.455-18.681147·T + $GHSER_{Ga}$ - 1.64547E+23·T^{-9}	[14]
In	(298.15<T<429.75) -3696.798 + 84.701255·T - 21.8386·T·ln(T) - 0.00572566·T^2 - 2.120321E-06·T^3 - 22906·T^{-1} - 5.59058E-20·T^7 (429.75<T<3800) - 3749.81 + 116.835784·T - 27.4562·T·ln(T) + 5.4607E-04·T^2 - 8.367E-08·T^3 - 211708·T^{-1}	[14]
Sb	(298.15<T<903.78) 19822.328 - 21.923164·T + $GHSER_{Sb}$ - 1.74847E-20·T^7 (903.78<T<2000) 8175.359 + 147.455986·T - 31.38·T·ln(T)	[14]

Table S5. GHSER. The energy values are in J/mole and the temperature is in K.

Systems	$GHSER_i$	Refs.
Al	(298.15<T<700) -7976.15 + 137.093038·T - 24.3671976·T·ln(T) - 0.001884662·T^2 - 8.77664E-07·T^3 + 74092·T^{-1} (700<T<933.47) -11276.24 + 223.048446·T - 8.5844296·T·ln(T) + 0.018531982·T^2 - 5.764227E-06·T^3 + 74092·T^{-1}	[14]
As	(298.15<T<1090) -7270.447 + 122.211069·T - 23.3144·T·ln(T) - 0.00271613·T^2 + 11600·T^{-1} (1090<T<1200) -10454.913 + 163.457433·T - 29.216037·T·ln(T)	[14]
Ga	(298.15<T<302.91) -21312.331 + 585.263691·T - 108.228783·T·ln(T) + 0.227155636·T^2 - 1.18575257E-04·T^3 + 439954·T^{-1} (302.91<T<4000) -7055.643 + 132.73019·T - 26.0692906·T·ln(T) + 1.506E-04·T^2 - 4.0173E-08·T^3 - 118332·T^{-1} + 1.64547E+23·T^{-9}	[14]
In	(298.15<T<429.75) -6978.89 + 92.338115·T - 21.8386·T·ln(T) - 0.00572566·T^2 - 2.120321E-06·T^3 - 22906·T^{-1} (429.75<T<3800) -7033.516 + 124.476588·T - 27.4562·T·ln(T) + 5.4607E-04·T^2 - 8.367E-08·T^3 - 211708·T^{-1} + 3.53116E+22·T^{-9}	[14]
Sb	(298.15<T<903.78) -9242.858 + 156.154689·T - 30.5130752·T·ln(T) + 0.007748768·T^2 - 3.003415E-06·T^3 + 100625·T^{-1} (903.78<T<2000) -11738.83 + 169.485872·T - 31.38·T·ln(T) + 1.616849E+27·T^{-9}	[14]

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