

Ge-Au-Sb

3D ternary phase diagram

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<3D Ternary diagram 그리기>

1. 각 compound(Ge, Au, Sb, AuSb₂)의 열역학적 데이터(깁스에너지)를 수집한다.
2. 1에서 얻은 열역학적 데이터를 이용해서 isothermal에서의 ternary diagram을 구한다. 200-1060°C 범위에서 20°C 간격으로 phase diagram을 구하고, 온도변화에 따라 생성되는 compound들을 확인하였다. 이를 3D-ternary diagram과 비교하였다.

(본 활동은 Factsage에서 데이터를 얻고, Factsage를 통해 isothermal-ternary diagram을 확인하였다.)

Ge

	G(T)			T(K)
S1	-9486.15300	+165.635573 T	+5.568297000E-03 T ²	298 - 900
	+163298.000 T ⁻¹	-1.513694000E-06 T ³	-29.5337682 T ln(T)	
S1	-5689.24027	+102.860870 T	-3.672527000E-03 T ²	900 - 1211
	-19.8536239 T ln(T)			
S1	-9548.20480	+156.708024 T	-8.598090000E+28 T ⁻⁹	1211 - 3200
	-27.6144000 T ln(T)			
S2	26513.8470	+143.335573 T	+5.568297000E-03 T ²	298 - 900
	+163298.000 T ⁻¹	-1.513694000E-06 T ³	-29.5337682 T ln(T)	
S2	30310.7597	+80.5608701 T	-3.672527000E-03 T ²	900 - 1211
	-19.8536239 T ln(T)			
S2	26451.7952	+134.408024 T	-8.598090000E+28 T ⁻⁹	1211 - 3200
	-27.6144000 T ln(T)			
S3	24613.8470	+142.135573 T	+5.568297000E-03 T ²	298 - 900
	+163298.000 T ⁻¹	-1.513694000E-06 T ³	-29.5337682 T ln(T)	
S3	28410.7598	+79.3608701 T	-3.672527000E-03 T ²	900 - 1211
	-19.8536239 T ln(T)			
S3	24551.7952	+133.208024 T	-8.598090000E+28 T ⁻⁹	1211 - 3200
	-27.6144000 T ln(T)			
L1	27655.3370	+134.948530 T	+5.568297000E-03 T ²	298 - 900
	+163298.000 T ⁻¹	-1.513694000E-06 T ³	+8.566320000E-21 T ⁷	
	-29.5337682 T ln(T)			
L1	31452.2497	+72.1738271 T	-3.672527000E-03 T ²	900 - 1211
	+8.566320000E-21 T ⁷	-19.8536239 T ln(T)		
L1	27243.4722	+126.324187 T	-27.6144000 T ln(T)	1211 - 3200

Sb

	G(T)			T(K)
S1	-9242.85800	+156.154689 T	+7.748768000E-03 T ²	298 - 904
	+100625.000 T ⁻¹	-3.003415000E-06 T ³	-30.5130752 T ln(T)	
S1	-11738.6702	+169.485713 T	+1.610442000E+27 T ⁻⁹	904 - 2000
	-31.3800000 T ln(T)			
S2	10631.1420	+142.454689 T	+7.748768000E-03 T ²	298 - 904
	+100625.000 T ⁻¹	-3.003415000E-06 T ³	-30.5130752 T ln(T)	
S2	8135.17067	+155.785872 T	+1.616849014E+27 T ⁻⁹	904 - 2000
	-31.3800000 T ln(T)			
S3	10631.1429	+141.054689 T	+7.748768000E-03 T ²	298 - 904
	+100625.000 T ⁻¹	-3.003415000E-06 T ³	-30.5130752 T ln(T)	
S3	8135.33066	+154.385713 T	+1.610442000E+27 T ⁻⁹	904 - 2000
	-31.3800000 T ln(T)			
L1	10579.7420	+134.234089 T	+7.748768000E-03 T ²	298 - 903
	+100625.000 T ⁻¹	-3.003415000E-06 T ³	-1.737850000E-20 T ⁷	
	-30.5130752 T ln(T)			
L1	10671.1316	+134.127928 T	+7.748768000E-03 T ²	903 - 904
	+100625.000 T ⁻¹	-3.003415000E-06 T ³	-1.610440000E+27 T ⁻⁹	
	-30.5130752 T ln(T)			
L1	8175.31944	+147.458952 T	+2.000000000E+21 T ⁻⁹	904 - 2000
	-31.3800000 T ln(T)			

Au

	G(T)			T(K)
S1	-6938.85579	+106.830098 T	-3.859240000E-03 T ²	298 - 929
	-25097.0000 T ⁻¹	+3.796250000E-07 T ³	-22.7545500 T ln(T)	
S1	-93586.4769	+1021.69539 T	+8.756015000E-02 T ²	929 - 1337
	+10637210.0 T ⁻¹	-1.151871300E-05 T ³	-155.706740 T ln(T)	
S1	314067.820	-2016.37825 T	-0.118216830 T ²	1337 - 1736
	-67999830.0 T ⁻¹	+8.923844000E-06 T ³	+263.252260 T ln(T)	
S1	-12133.7820	+165.272523 T	-30.9616000 T ln(T)	1736 - 3200
	-2688.85571	+105.730098 T	-3.859240000E-03 T ²	
S2	-25097.0000 T ⁻¹	+3.796250000E-07 T ³	-22.7545500 T ln(T)	298 - 929
	-89336.4769	+1020.59539 T	+8.756015000E-02 T ²	
S2	+10637210.0 T ⁻¹	-1.151871300E-05 T ³	-155.706740 T ln(T)	929 - 1337
	318317.820	-2017.47825 T	-0.118216830 T ²	
S2	-67999830.0 T ⁻¹	+8.923844000E-06 T ³	+263.252260 T ln(T)	1337 - 1736
	-7883.78186	+164.172523 T	-30.9616000 T ln(T)	
L1	5613.14421	+97.4442318 T	-3.859240000E-03 T ²	298 - 929
	-25097.0000 T ⁻¹	+3.796250000E-07 T ³	-22.7545500 T ln(T)	
L1	-81034.4769	+1012.30952 T	+8.756015000E-02 T ²	929 - 1337
	+10637210.0 T ⁻¹	-1.151871300E-05 T ³	-155.706740 T ln(T)	
L1	326619.820	-2025.76412 T	-0.118216830 T ²	1337 - 1736
	-67999830.0 T ⁻¹	+8.923844000E-06 T ³	+263.252260 T ln(T)	
L1	418.218046	+155.886657 T	-30.9616000 T ln(T)	1736 - 3200

AuSb2

	G(T)			T(K)
S1	-41674.9861	+366.293601 T	-9.706880000E-03 T ²	298 - 628
	-71.6300800 T ln(T)			

<각 component의 G data>

Ge(s), Ge(s2), Ge(s3) / Au(s), Au(s2) / Sb(s),
Sb(s2), Sb(s3) : factsage의 Ftlite
AuSb2 : factsage의 FactPS

