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NSWC TR 86-242

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CALCULATION OF MULTICOMPONENT REFRACTORY COMPOSITE PHASE DIAGRAMS

AD-A192 293

BY L. KAUFMAN (MANLABS, INC.)

FOR NAVAL SURFACE WEAPONS CENTER
STRATEGIC SYSTEMS DEPARTMENT

1 JUNE 1986

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Coupled phase diagram/thermochemical description of the Hf-B, Hf-C, Zr-B, and Zr-C binary systems have been developed and combined with previously derived descriptions of the B-C, Zr-Si, Hf-Si, Si-B, and Si-C binary systems in order to calculate the temperatures at which melting first occurs in the composition ranges between C-ZrC-ZrB_2-B_4C, C-HfC-HfB_2-B_4C, HfC-SiC, ZrB_2-SiC, and HfB_2-SiC. These systems are being investigated for advanced applications for use at temperatures as high as 5000°F.

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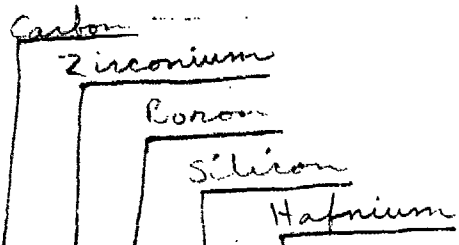
FOREWORD

This work was performed for and funded by the Surface Launched Weaponry Materials Technology (SURFMAT) Program which has focused on the development of materials for use at temperatures as high as 5000°F. The calculation of temperatures at which melting first occurs provides a guide to the limitation of such materials. The current work shows that HfB_2-HfC composites begin melting above 3413K (5683F), ZrB_2-ZrC above 3090K (5102F), HfC-SiC above 2910K (4778F), ZrC-SiC above 2685K (4373F), HfB_2-SiC above 2620K (4256F), and ZrB_2-SiC above 2408K (4004F). These results provide a guide for the development of materials which might be used in advanced high-temperature systems.

Approved by:

D. B. COLBY, Head
Strategic Systems Department



PREFACE

Candidate materials are being studied which can be used at temperatures as high as 5000°F. In order to attain this goal a series of refractory compounds are being considered which can be used as composites. These composites are based on combinations between (C), (Zr), (B) and (Si) or C, (Hf), B and Si. In order to investigate where melting can be expected in the candidate composite systems, coupled phase diagram/thermochemical descriptions of the Hf-B, Hf-C, Zr-B and Zr-C binary systems have been developed and combined with previously derived description of the B-C, Zr-Si, Hf-Si, Si-B and Si-C binary systems in order to calculate the temperatures at which melting occurs in the composition ranges between C-ZrC-ZrB_2-B_4C, C-HfC-HfB_2-B_4C, HfC-SiC, ZrB_2-SiC and HfB_2-SiC.

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ILLUSTRATIONS (Cont.)

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CHAPTER 1

INTRODUCTION

Candidate materials for advanced, high-temperature applications are being studied that are based on combinations of C, B and Si with Zr or Hf for use at temperatures as high as 5000°F. In order to further these studies coupled themochemical calculations of phase diagrams[1-5] have been applied to calculate the temperature at which melting first occurs in such systems.

BACKGROUND

In order to determine the conditions where melting can occur in a multicomponent system such as the five compoent Zr-Mo-Si-B-C example shown in Figure 1, coupled phase diagrams/thermochemical descriptions of the Hf-B, Hf-C, Zr-B, and Zr-C binary systems have been developed and combined with previously derived description of the B-C, Zr-Si, Hf-Si, Si-B, and Si-C binary systems. These descriptions were applied to calculate the temperatures at which melting occurs in the composition ranges between C-ZrC-ZrB_2-B_4C, C-HfC-HfB_2-B_4C, HfC-SiC, ZrB_2-SiC, and HfB_2-SiC. Identification of these melting temperatures define the highest temperatures at which such compositions would be effective.

SUMMARY

The current work shows the ZrB_2-ZrC composites begin melting above 3090K (5102F), HfB_2-HfC above 3413K (5683F), ZrC-SiC above 2685K (4373F), HfC-SiC above 2910K (4778F), ZrB_2-SiC above 2480K (4004F), and HfB_2-SiC above 2620K (4256F). These results provide a guide for the development of advanced high-temperature materials.

CHAPTER 2

TECHNICAL DESCRIPTION

PURE COMPONENTS AND BINARY SYSTEMS

Table 1 shows the current values of the lattice stability of B, C, Zr and Hf.[1-5] These values were used to define the Gibbs energies of the solution and compound phases of interest. Table 2 and Figure 2 show the description of the B-C system[3] while Tables 3 through 6 and Figures 3 through 6 show the thermochemical description and phase diagrams calculated for the Zr-C, Hf-C, Zr-B, and Hf-B derived here. Relevant data on Zr-Si, Hf-Si, Si-B, and Si-C were taken from earlier studies.[3-5]

It would be noted that the thermochemical description of the liquid and solid phases contained in Tables 1 through 6 can be employed to compute the binary and ternary phase diagrams as well as the various thermochemical properties of all components in these systems. The thermochemical properties include: activity and activity coefficients, heats of fusion and mixing, etc.

TERNARY SYSTEMS

The Gibbs energy of ternary liquid was modeled by employing Kohler's equation shown at the bottom of Table 4 for the B-C-Hf system. All of the binary parameters, i.e., LBBCC, LCCBB, LBBHF, LHFBB, LCCHF, and LHFCC are defined form Tables 2 to 6 and the previous work. As a first approximation the ternary interaction parameter TRNL can be set equal to zero. In the B-C-Zr case illustrated by Figures 7 to 10, this procedure was followed as a first approximation. Figure 8 shows the result obtained in the calculation of the ZrB_2-ZrC eutectic temperature which was calculated at 3250K (5408^{o}F) as compared with the experimental value of 3090K (5102^{o}F)

reported by Rudy.[6] By means of iterative adjustments it was found a value of TRNL = -125520 Joules/g.at. was necessary to reduce the eutectic temperature to 3090K (5102°F) in agreement with the experimental results. Figures 8 through 15 show the present B-C-Zr calculation while Figures 16 through 24 show the B-C-Hf calculations.

In the latter case a much smaller ternary liquid interaction parameter, TRNL = -12552, was found to provide an accurate reproduction of the HfB_2-HfC eutectic at 3413K (5683°F) as shown in Figure 17. Figure 8 shows the ZrB_2-C join where the calculated eutectic is 2700K (4400°F) and the result proposed by Rudy[6] is 2663K (4333°F). In Figure 10 the calculated eutectic on the ZrB_2-B_4C join is 2493K (4027°F). Figures 11 through 15 show the isothermal sections computed at 3273K (5431°F), 3073K (5071°F), 2873K (4711°F), 2673K (4351°F), and 2573K (4171°F) with TRNL = -125520 and those proposed by Rudy.[6] The general level of agreement is seen to be quite good.

Figure 16 presents the isothermal calculations to be performed in the B-C-Hf system with reference to the component binary systems. As indicated above, a value of TRNL much nearer to zero, i.e., -12520 J/g.at. is required (to provide agreement with Rudy's proposal[6]) than in the B-C-Zr case. This is illustrated in Figures 17 through 19 where the calculated and observed HfB_2-HFC, HfB_2-C, and HfB_2-B_4C are displayed at 3413K (5683°F), 2823K (4621°F) calculated and 2788K (4558°F) experimental and 2603K (4225°F), respectively. Thus with TRNL = -12552 for B-C-Hf good agreement is attained between experimental and calculated eutectic temperatures. Similarly, good agreement is displayed in Figures 20 through 24 at 3473K (5791°F), 3373K (5611°F), 3073K (5071°F), 2673K (4351°F), and 2573K (4171°F).

Consequently, the forgoing tests of the model parameters in the calculations of the B-C-Zr and B-C-Hf ternary systems in the range of temperature and compositions of interest provide a good measure of confidence in the predictive capability of the computational system and permit consideration of higher order systems.

QUATERNARY SYSTEMS

The extension to higher order systems was performed by expanding the Kohler Model (Table 4) to multicomponent systems. Table 7 shows the description of the partial Gibbs energies for a five component system. Calculation of the SiC-ZrC, SiC-HfC, SiC-ZrB_2, and SiC-HfB_2 joins displayed in Figures 25 through 28 was performed by equilibrating the partial Gibbs energies of the individual components in the liquid and solid phases. The results show a eutectic in SiC-ZrC at 2685K (4373°F), in SiC-HfC at 2910K (4778°F), in SiC-ZrB_2 at 2480K (4004°F), and in SiC-HfB_2 at 2620K (4256°F). These results suggest that the SiC-HfC composite could provide the highest temperature capability before encountering degradation due to melting at 2910K (4778°F).

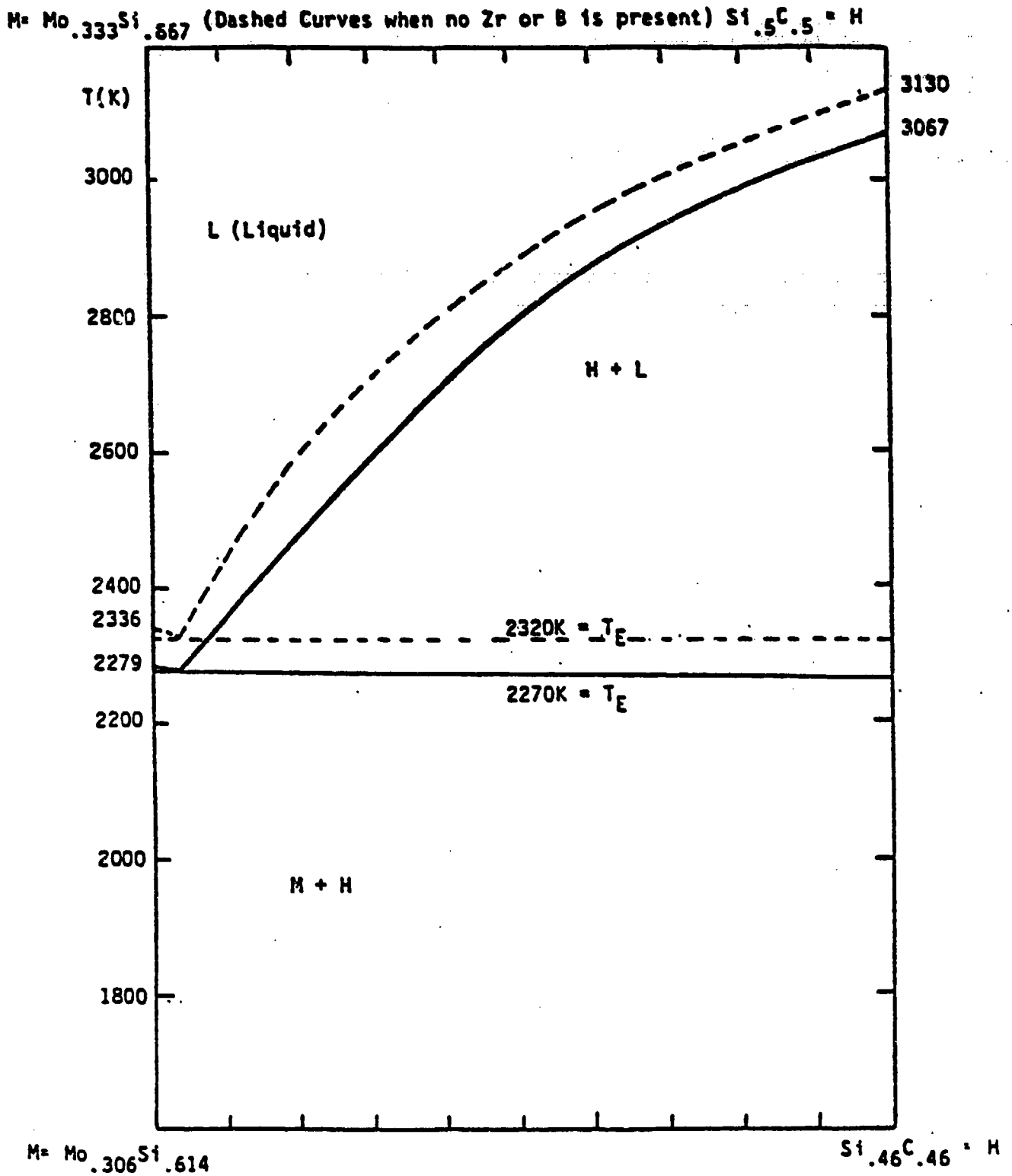

FIGURE 1. CALCULATED QUASI-BINARY JOIN BETWEEN $Mo_{.333}Si_{.667}$ AND $Si_{0.5}C_{0.5}$ WITH THE ADDITION OF .04Zr AND .04B (FULL CURVES) (DASHED CURVES REPRESENT NO Zr OR B)

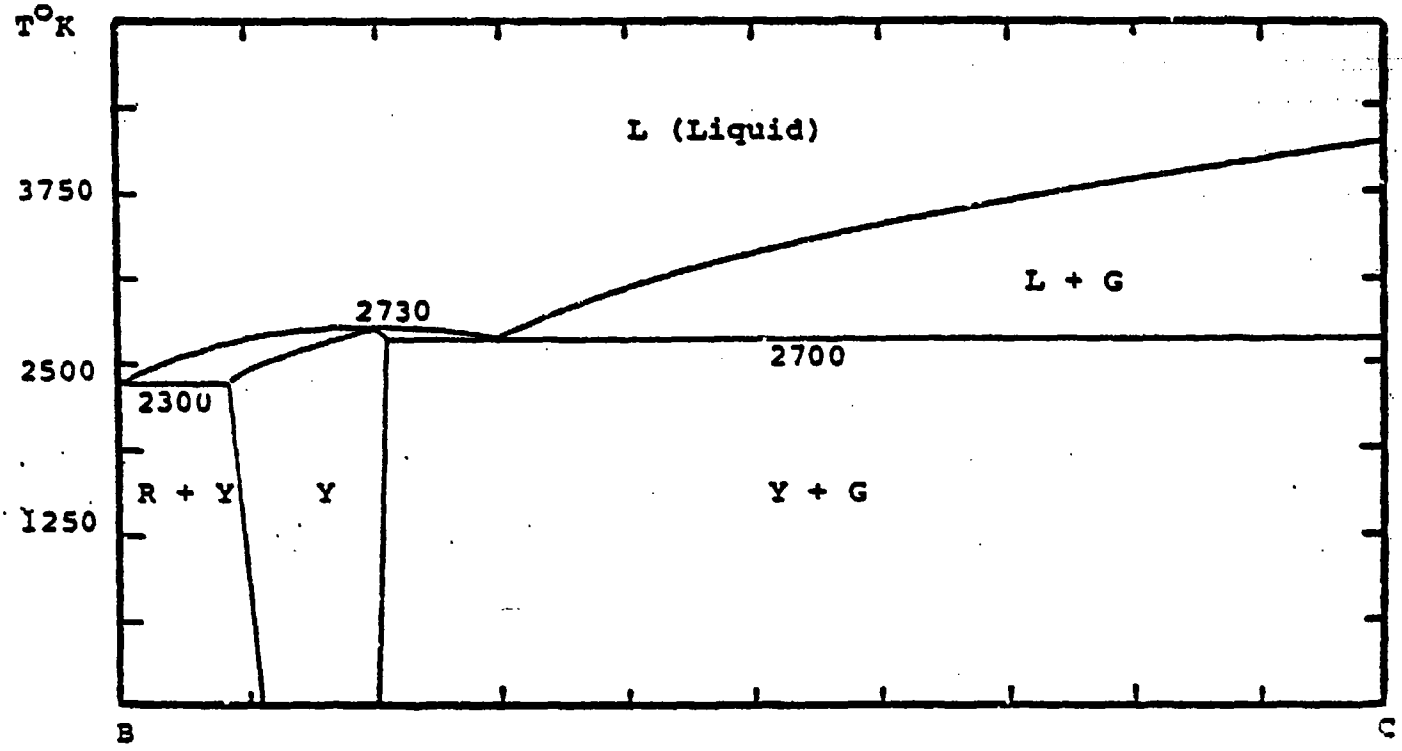

FIGURE 2. CALCULATED B-C PHASE DIAGRAM

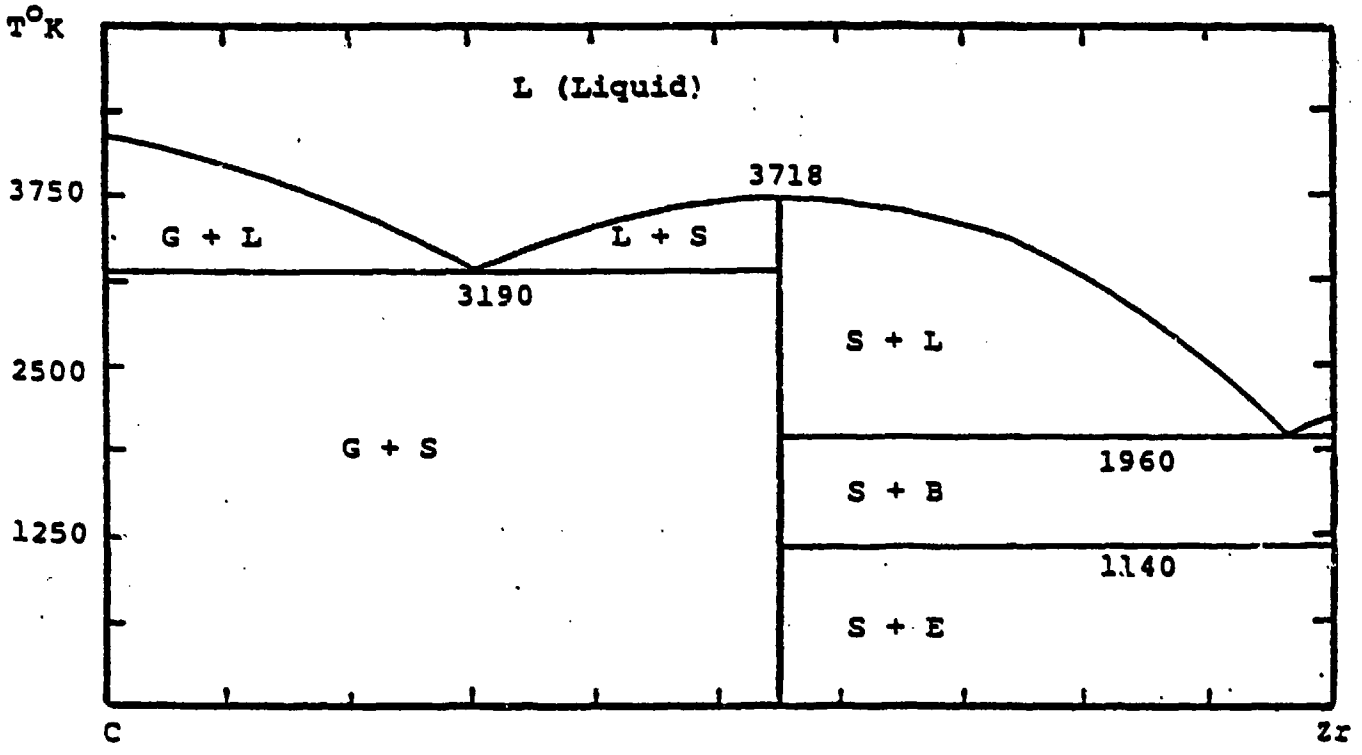

FIGURE 3. CALCULATED C-Zr PHASE DIAGRAM

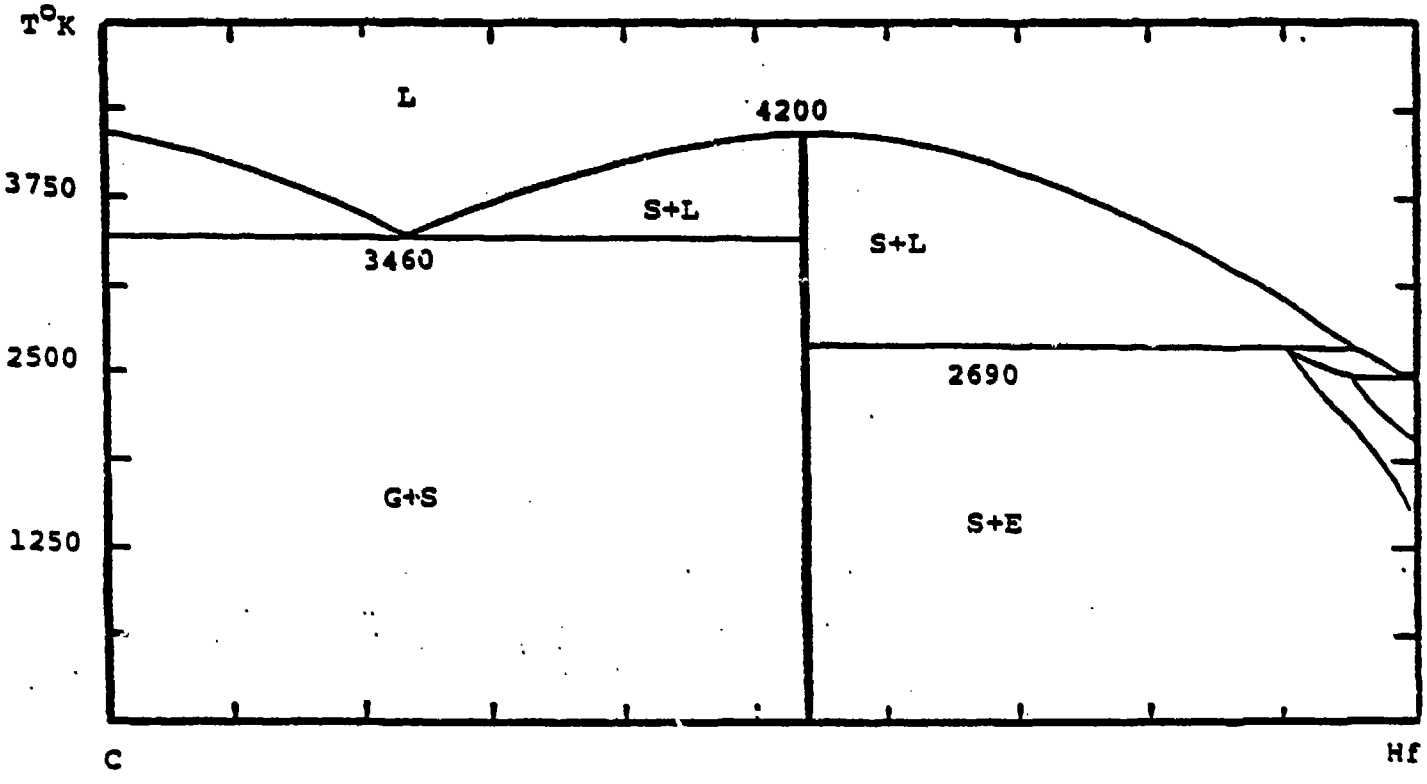

FIGURE 4. CALCULATED C-Hf PHASE DIAGRAM

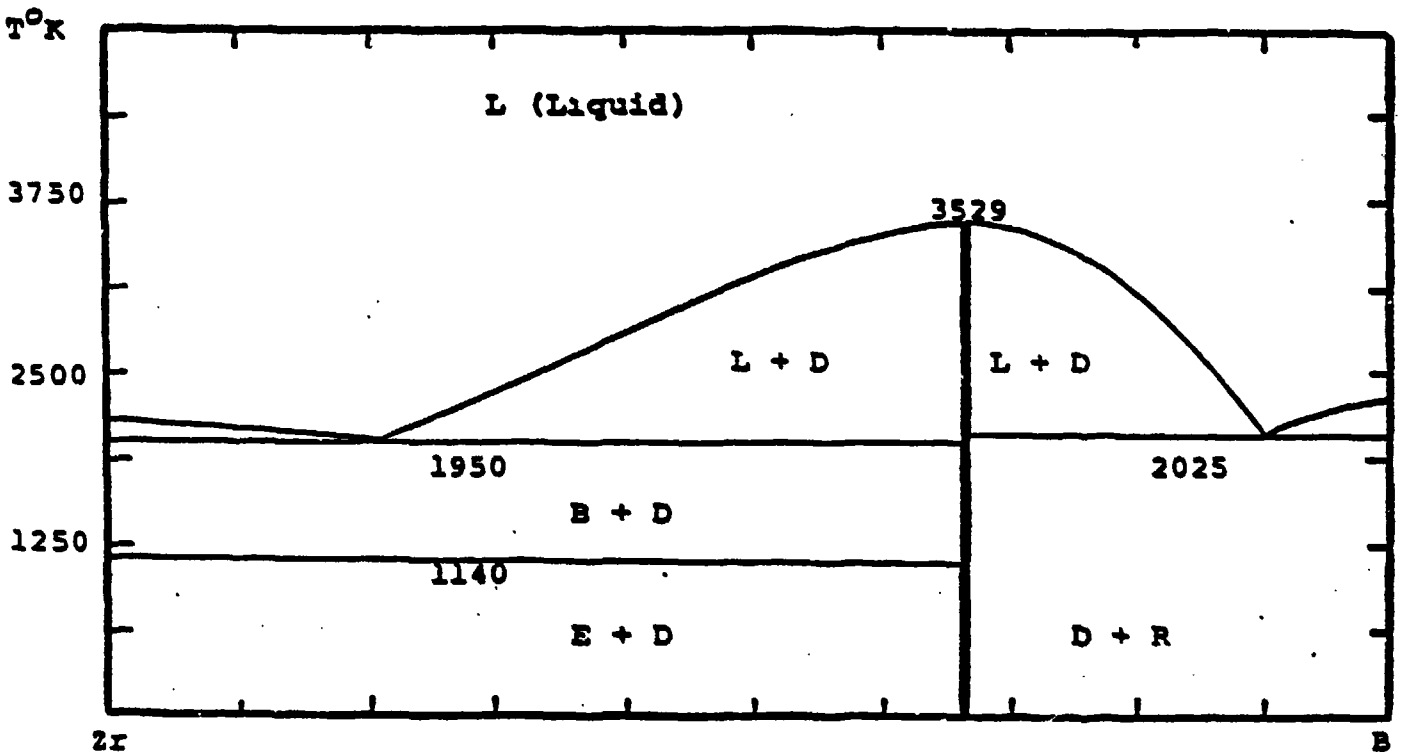

FIGURE 5. CALCULATED Zr-B PHASE DIAGRAM

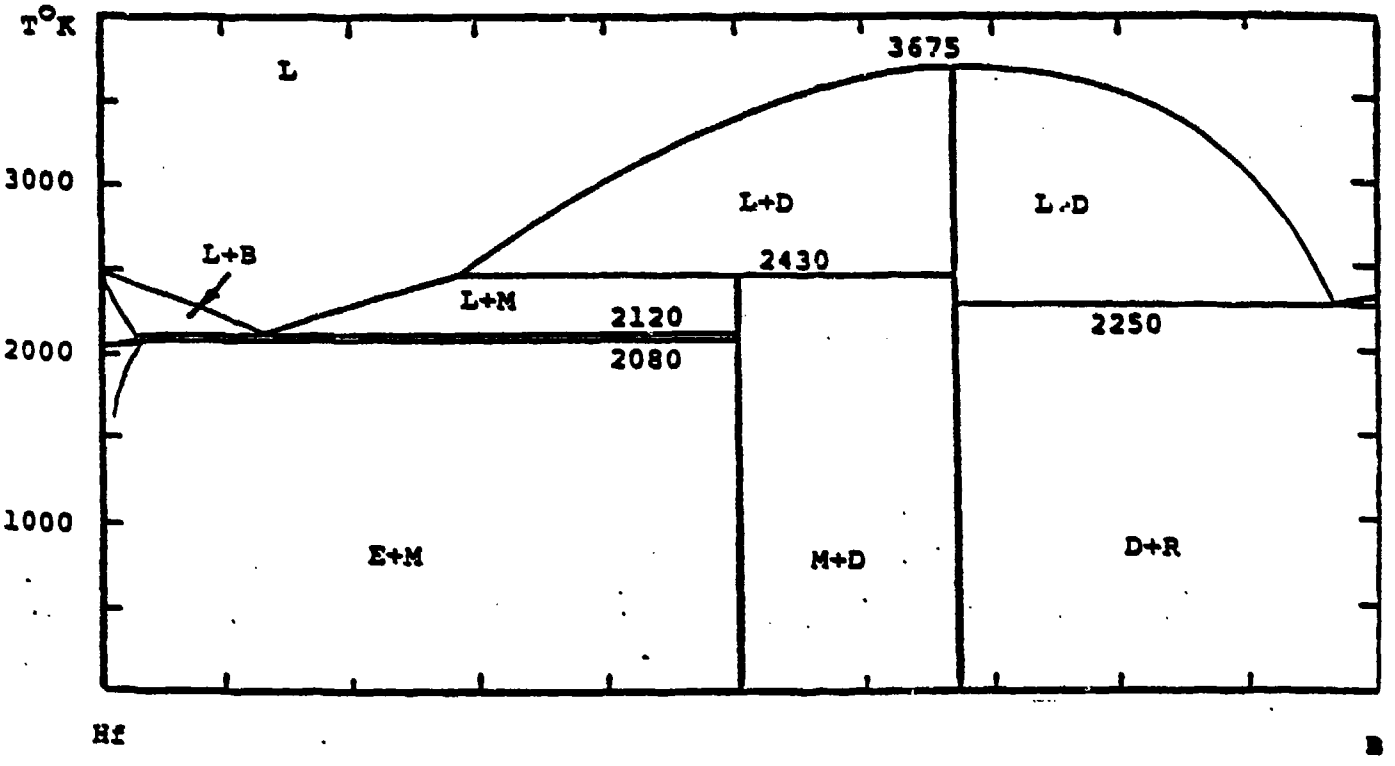

FIGURE 6. CALCULATED Hf-B PHASE DIAGRAM

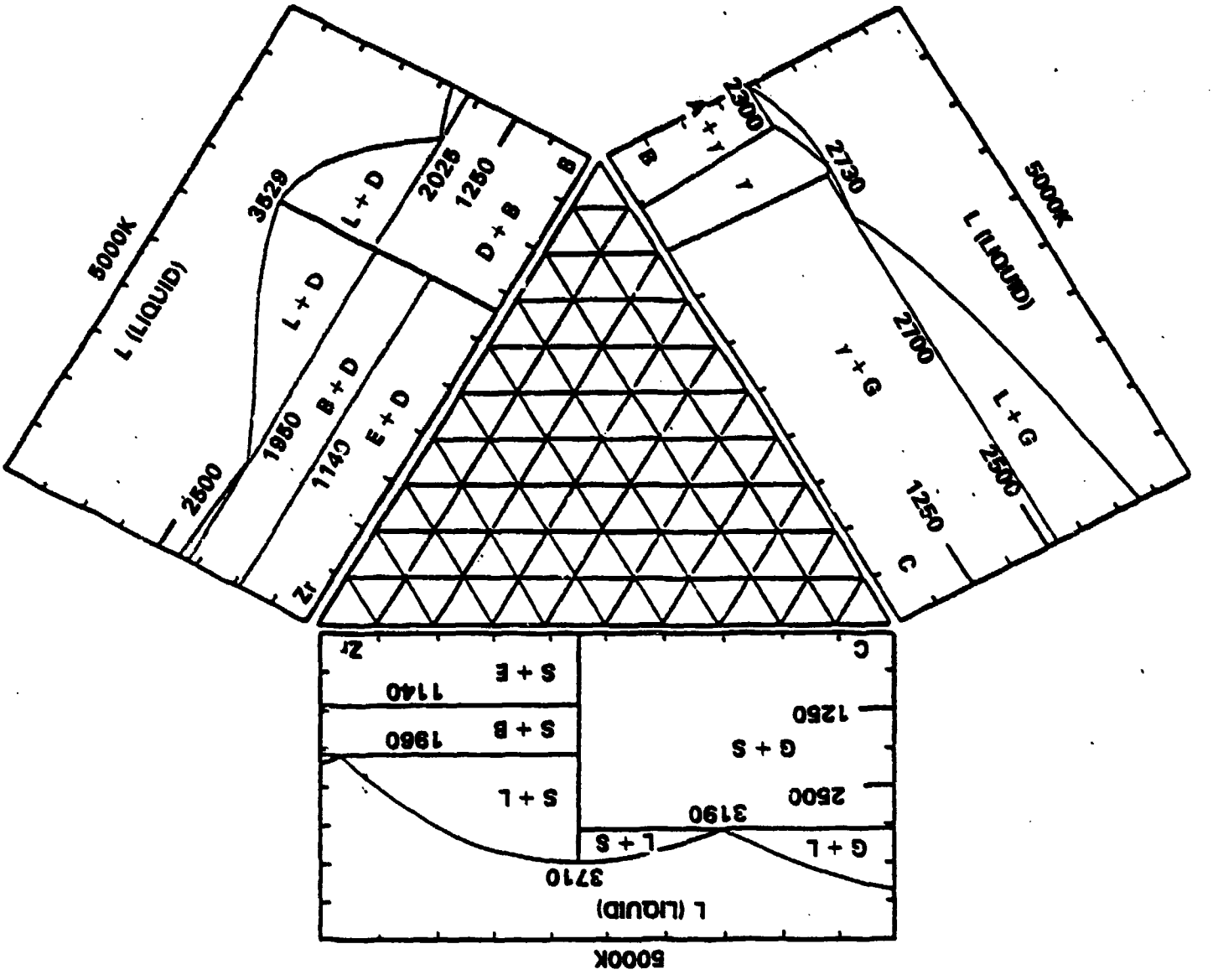

FIGURE 7. CALCULATED ISOTHERMAL SECTIONS IN THE B-C-Zr SYSTEM

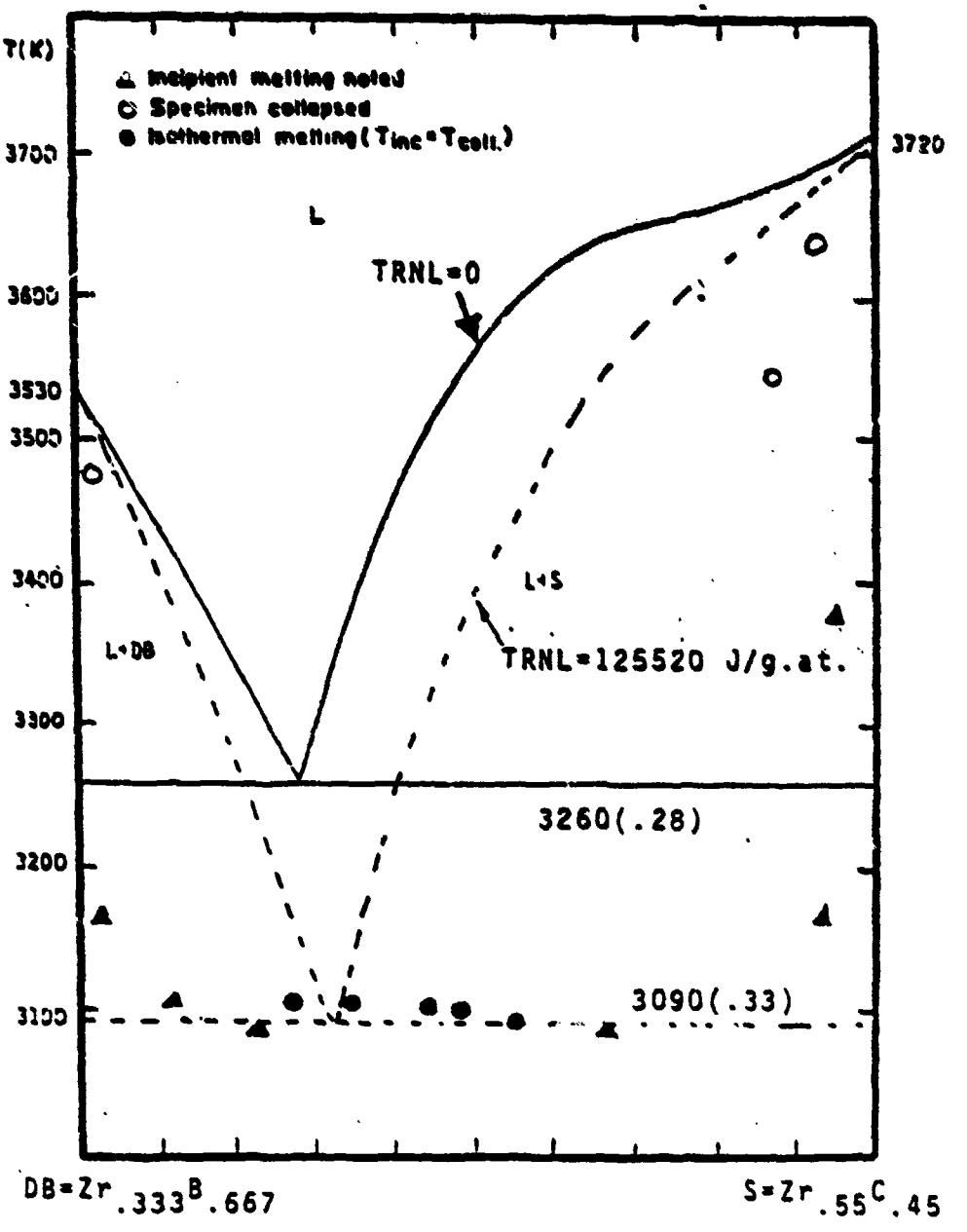

FIGURE 8. CALCULATED QUASI-BINARY JOIN BETWEEN ZrB_2 AND ZrC WITH TWO DIFFERENT TERNARY LIQUID INTERACTION PARAMETERS COMPARED WITH EXPERIMENTAL RESULTS

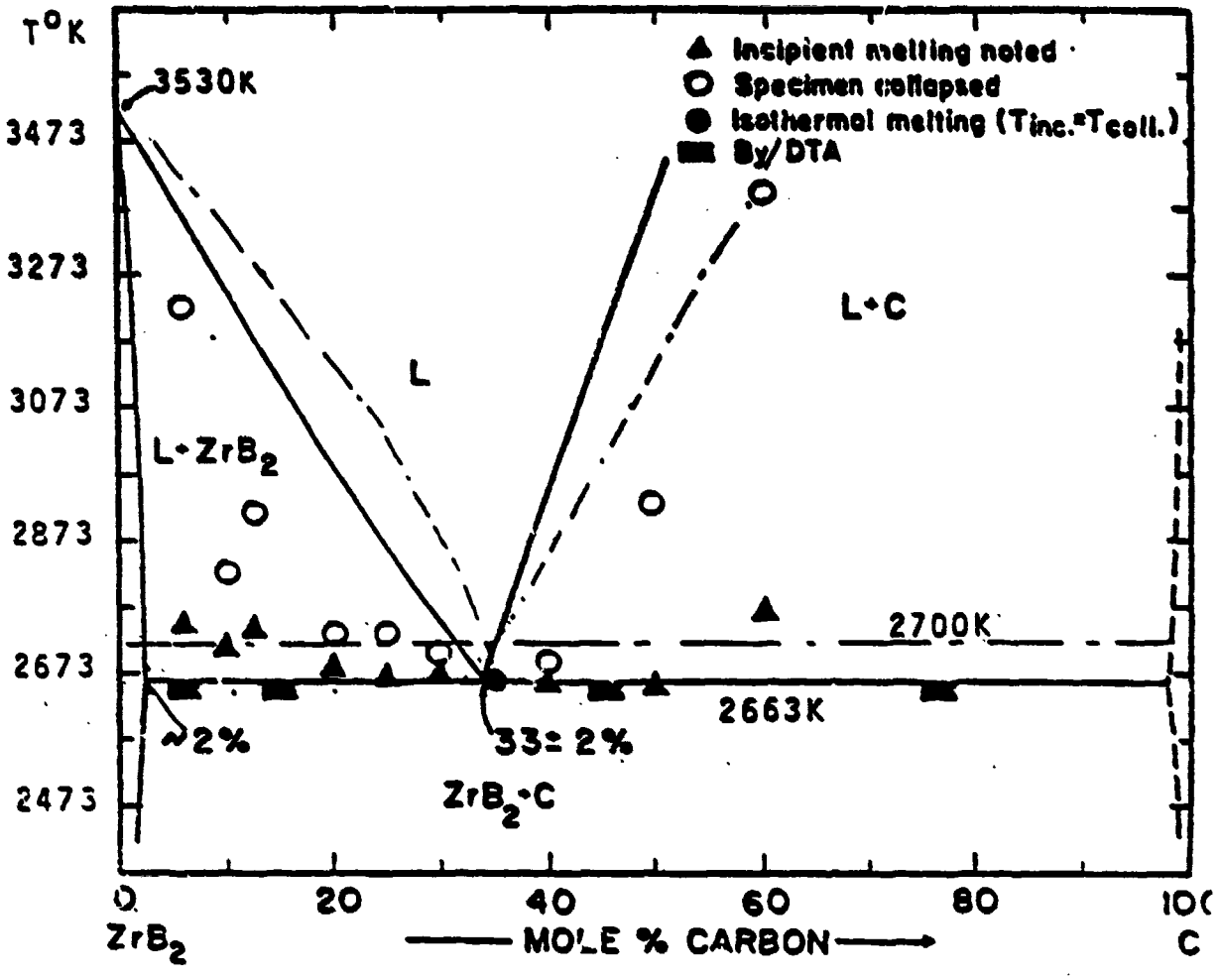

FIGURE 9. CALCULATED AND OBSERVED QUASI-BINARY JOIN BETWEEN ZrB_2 AND C (THE CALCULATED BOUNDARIES ARE SHOWN BY THE DASH-DOTTED CURVES AND LINES WITH TRNL = -125,520 JOULES/g.at)

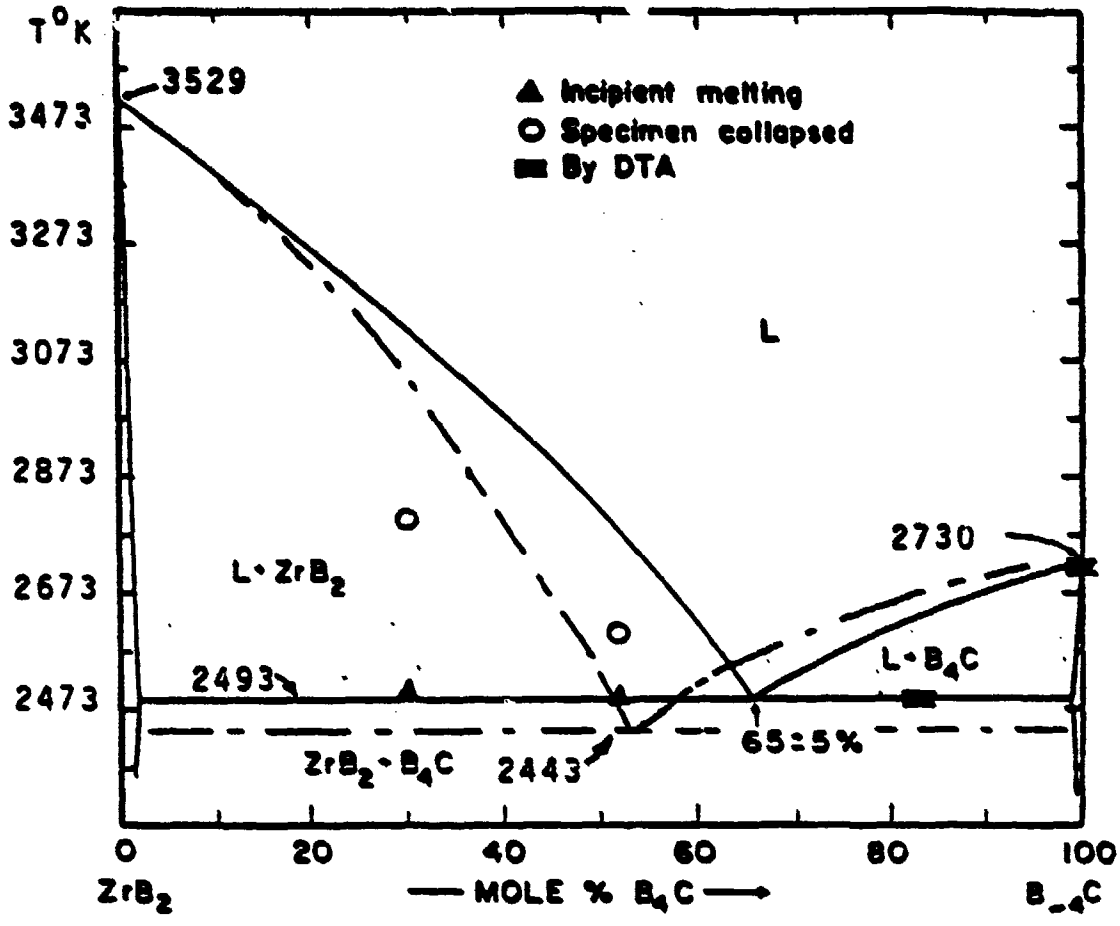

FIGURE 10. CALCULATED AND OBSERVED QUASI-BINARY JOIN BETWEEN ZrB_2 AND B_4C (THE CALCULATED BOUNDARIES ARE SHOWN BY DASH-DOTTED CURVES AND LINES WITH TRNL = −125,520 JOULES/g.at)

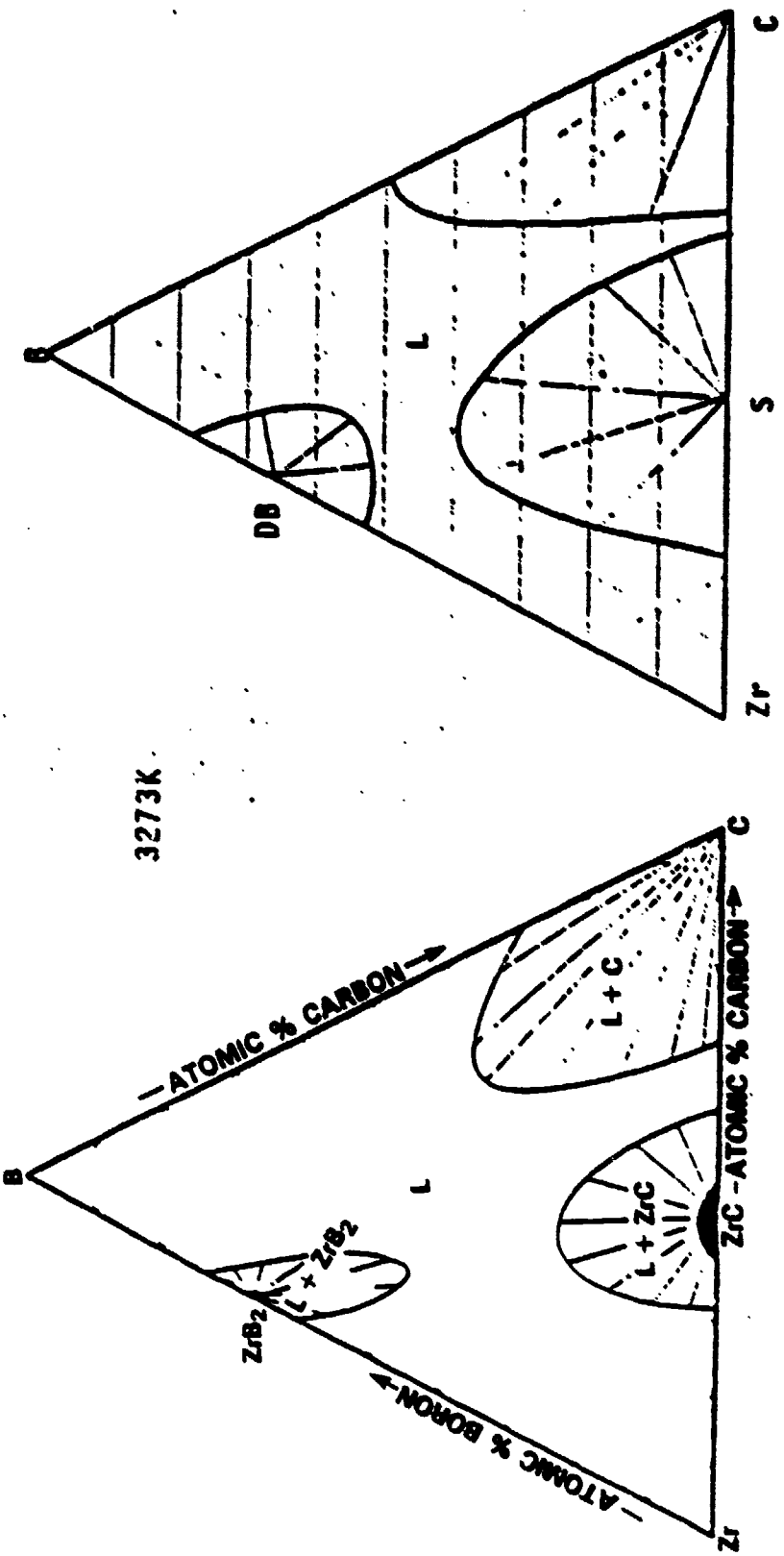

FIGURE 11. CALCULATED ISOTHERMAL B-C-Zr SECTION AT 3273K (SECTION PROPOSED BY RUDY[6] ON THE LEFT)

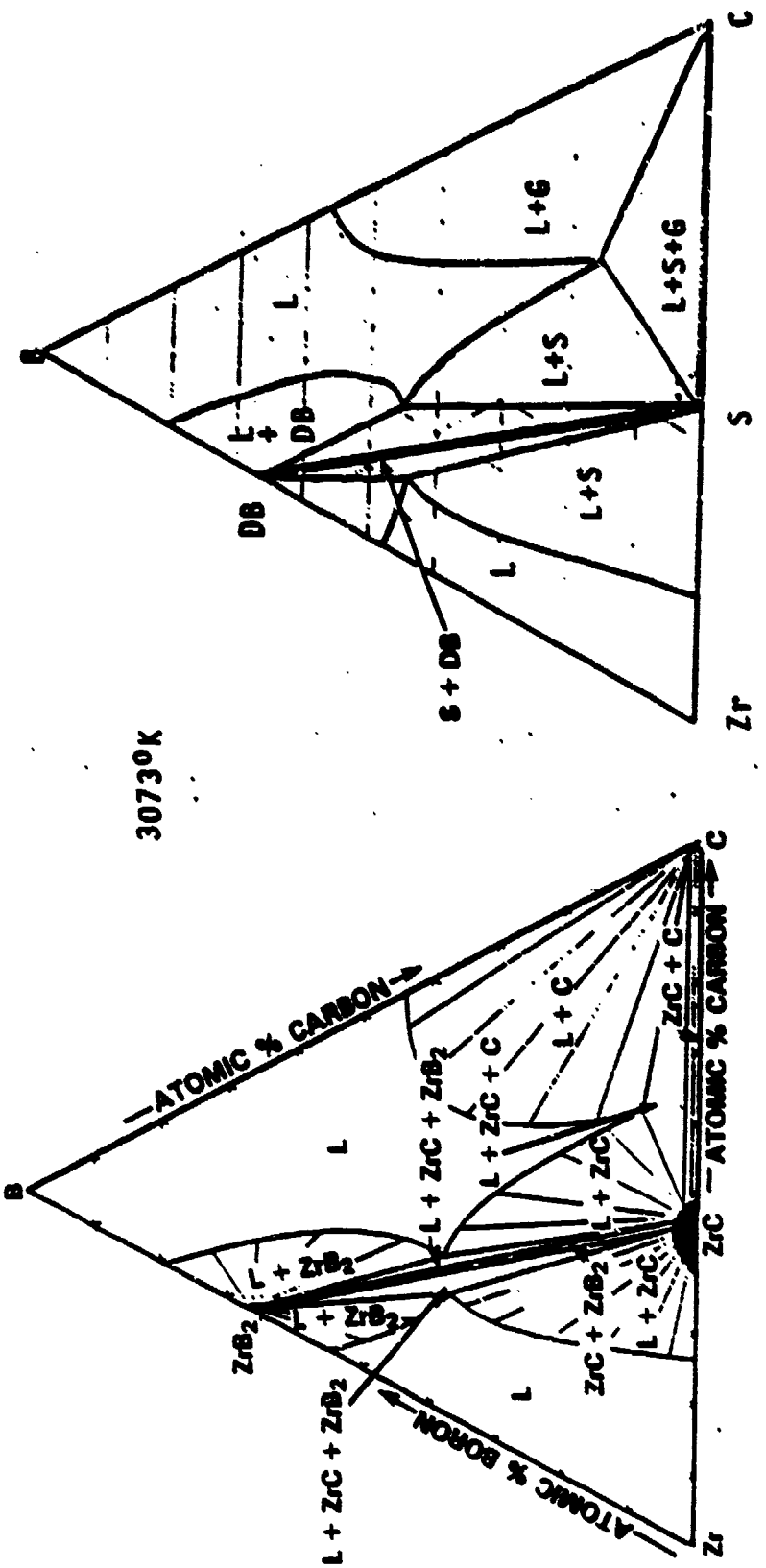

FIGURE 12. CALCULATED ISOTHERMAL B-C-Zr SECTION AT 3073K (SECTION PROPOSED BY RUDY[4] ON THE LEFT)

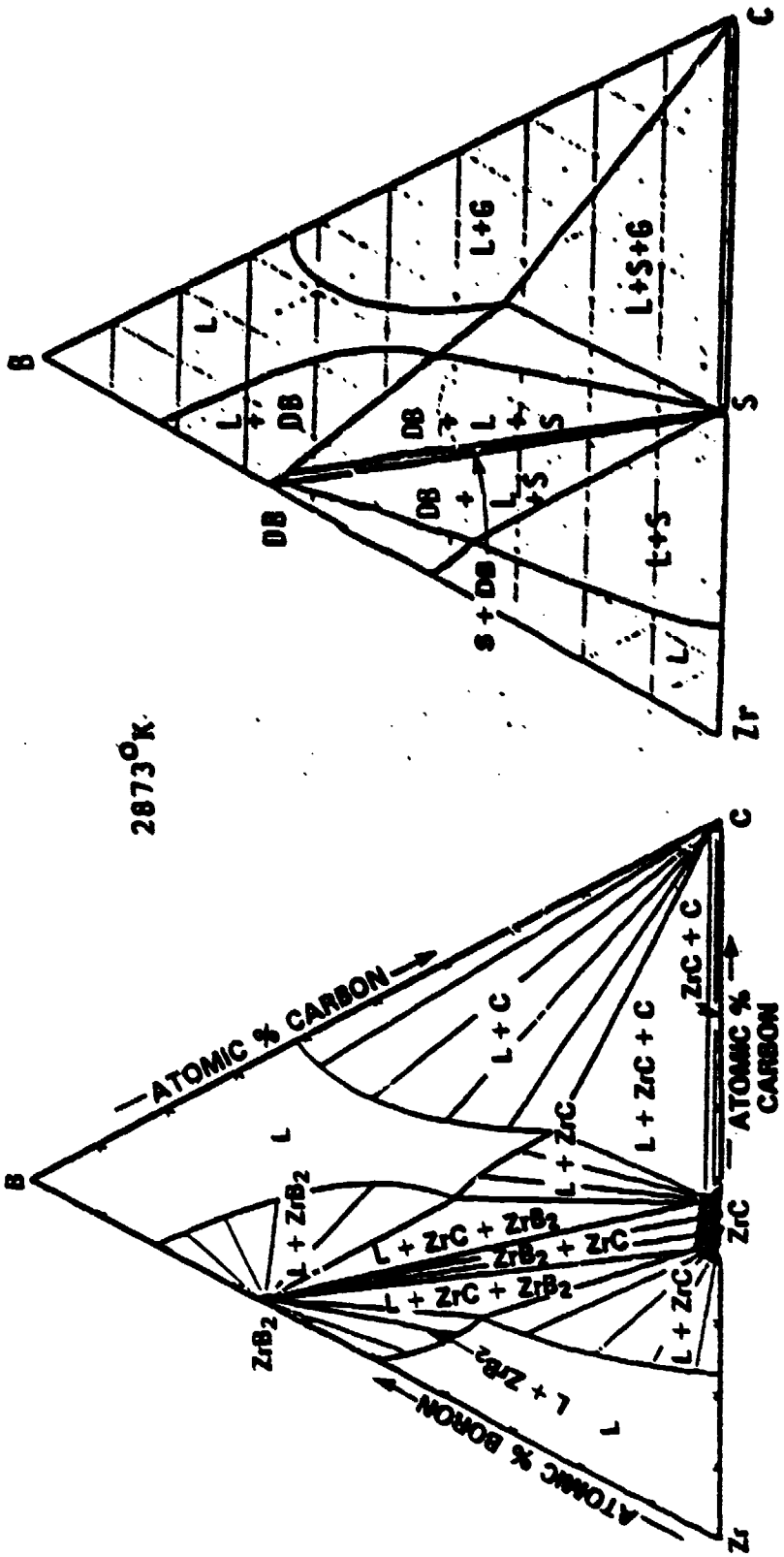

FIGURE 13. CALCULATED ISOTHERMAL B-C-Zr SECTION AT 2873K (SECTION PROPOSED BY RUDY[6] ON THE LEFT)

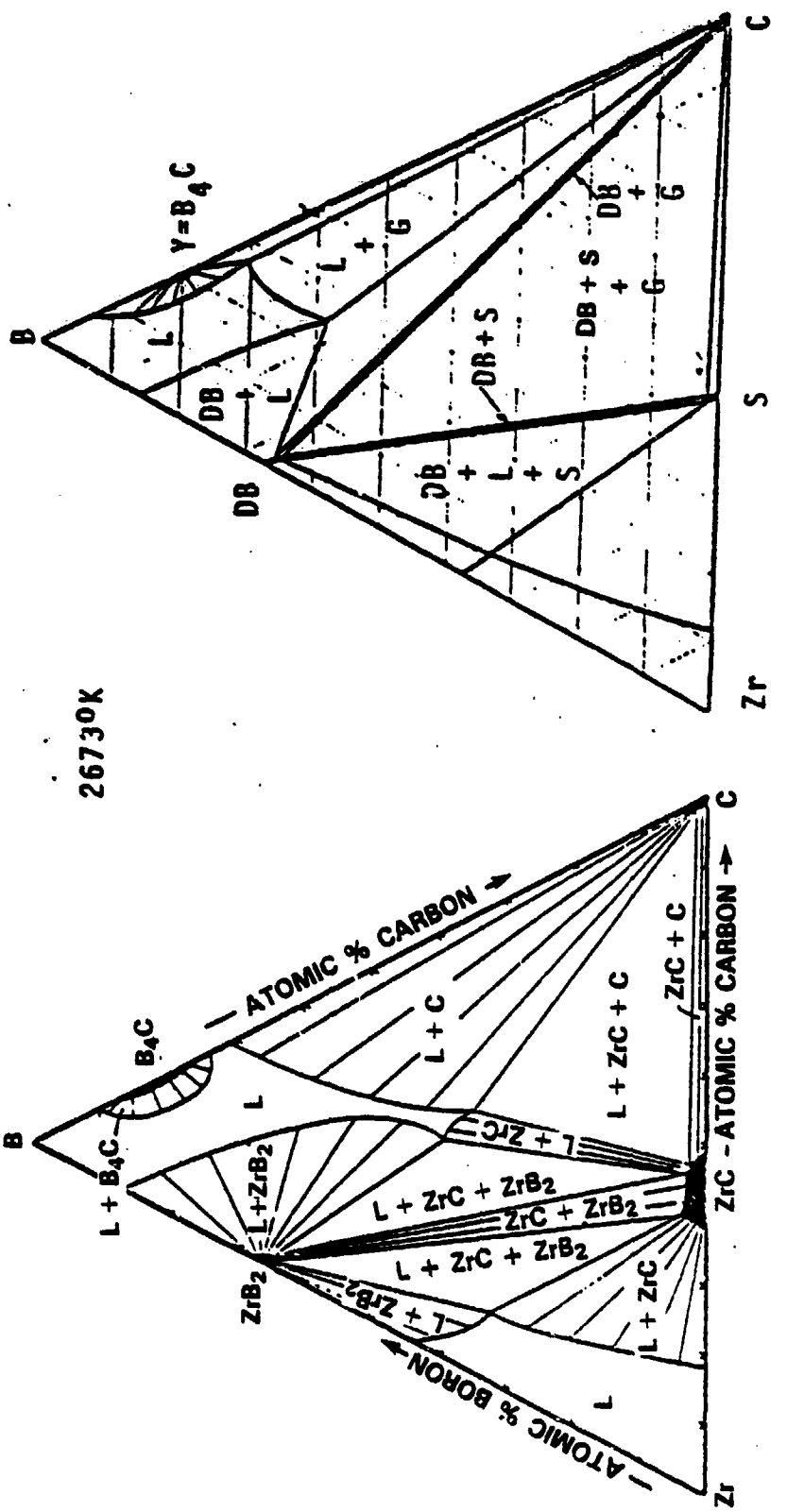

FIGURE 14. CALCULATED ISOTHERMAL B-C-Zr SECTION AT 2673K (SECTION PROPOSED BY RUDY[6] ON THE LEFT)

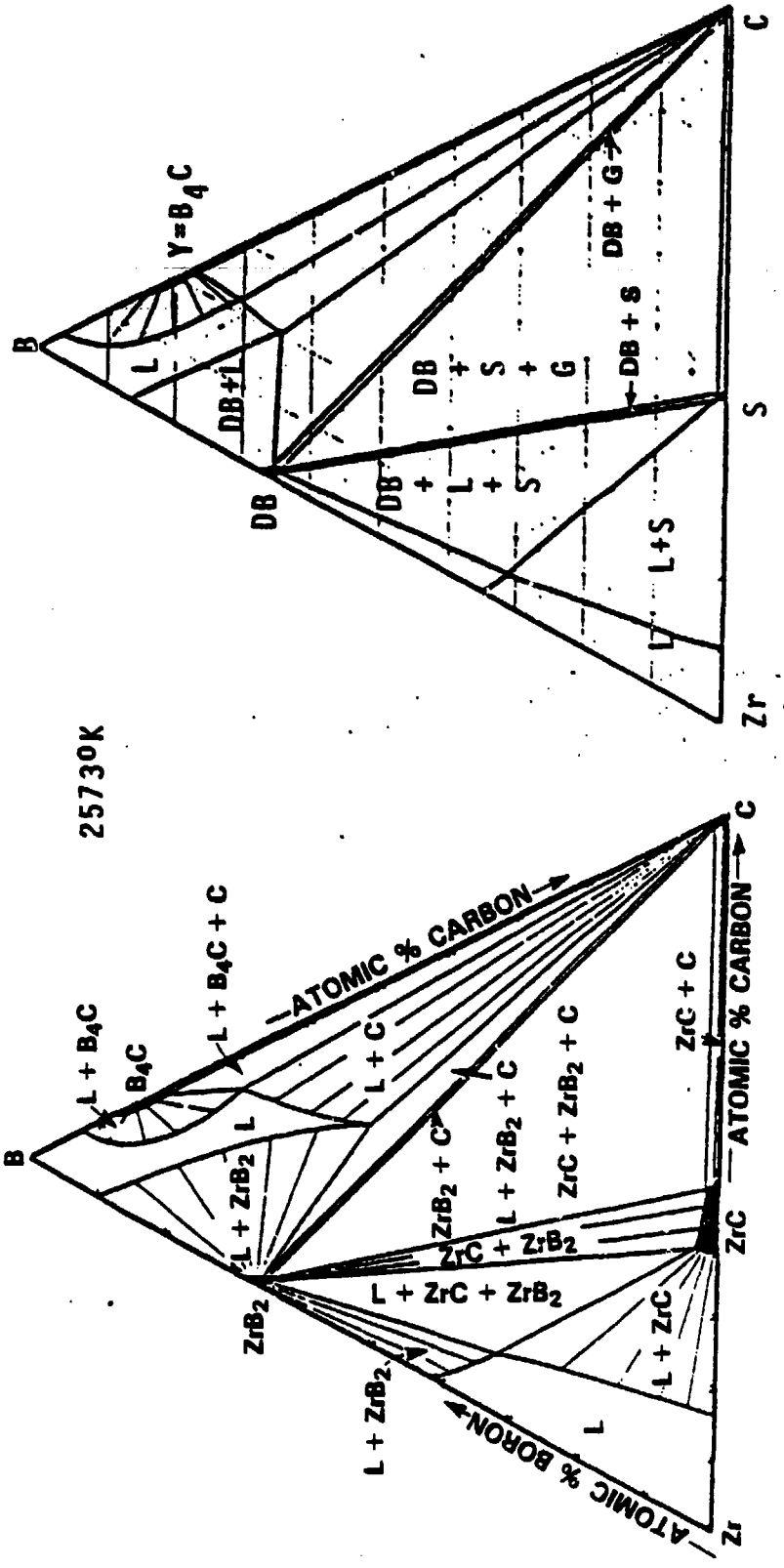

FIGURE 15. CALCULATED ISOTHERMAL B-C-Zr SECTION AT 2573K (SECTION PROPOSED BY RUDY[6] ON THE LEFT)

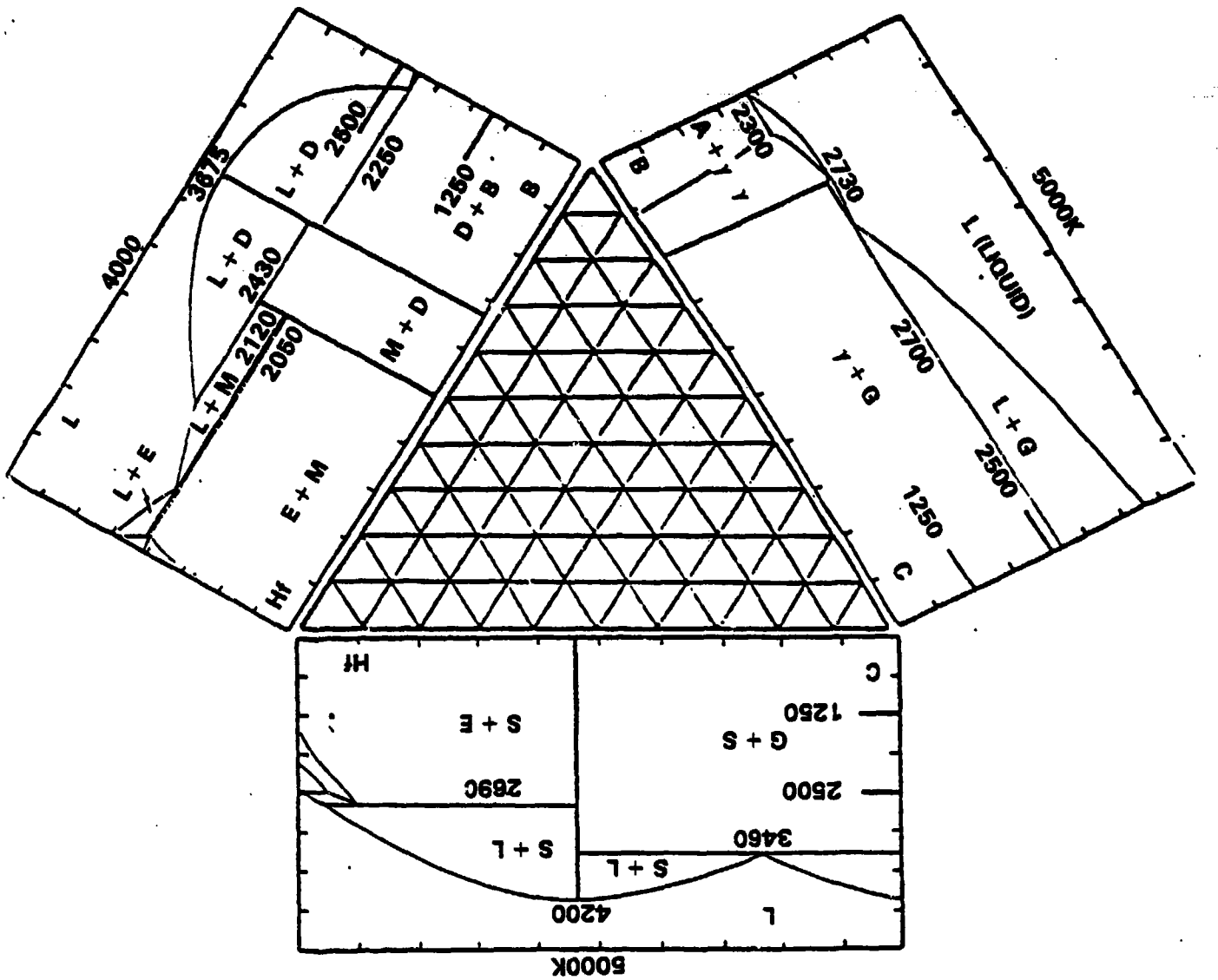

FIGURE 16. CALCULATED ISOTHERMAL SECTIONS IN THE B-C-Hf SYSTEM

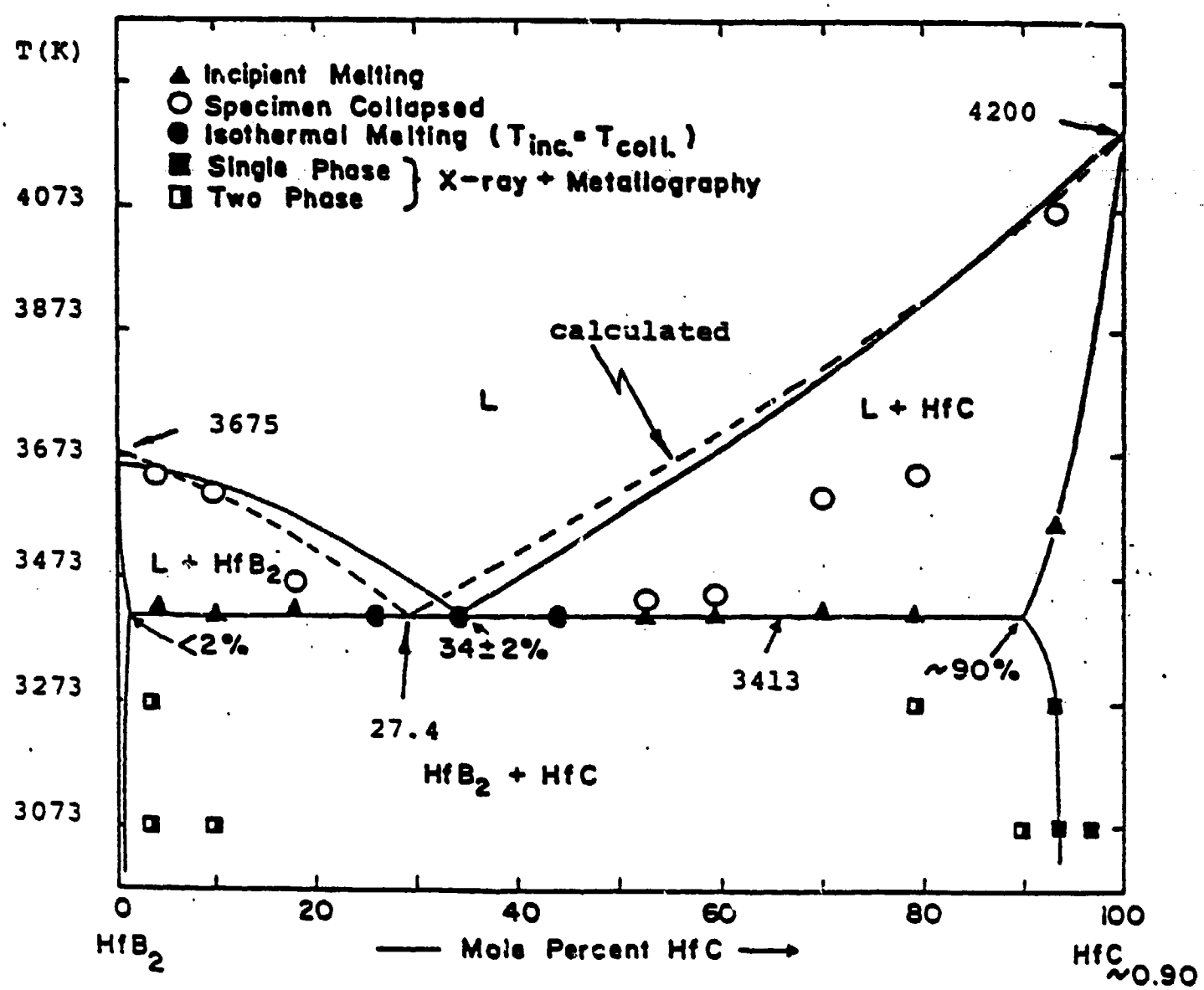

FIGURE 17. COMPARISON OF EXPERIMENTAL[6] HfB_2-HfC QUASI-BINARY JOIN WITH CALCULATED RESULTS (DASHED CURVE) BASED ON TRNL = -12,552 JOULES/g.at

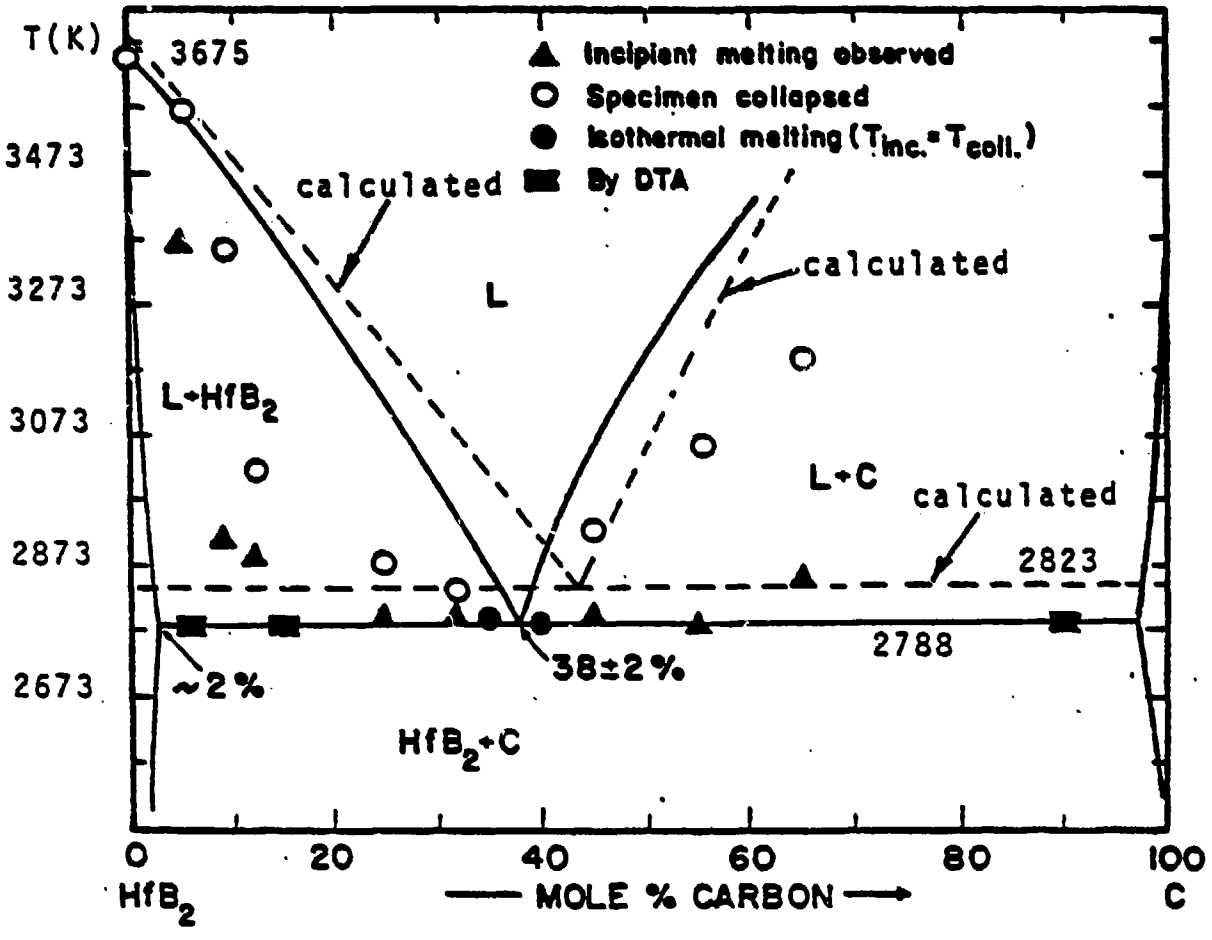

FIGURE 18. COMPARISON OF EXPERIMENTAL[6] HfB_2-C QUASI-BINARY JOIN WITH CALCULATED RESULTS (DASHED CURVES) BASED ON TRNL = -12,552 JOULES/g.at

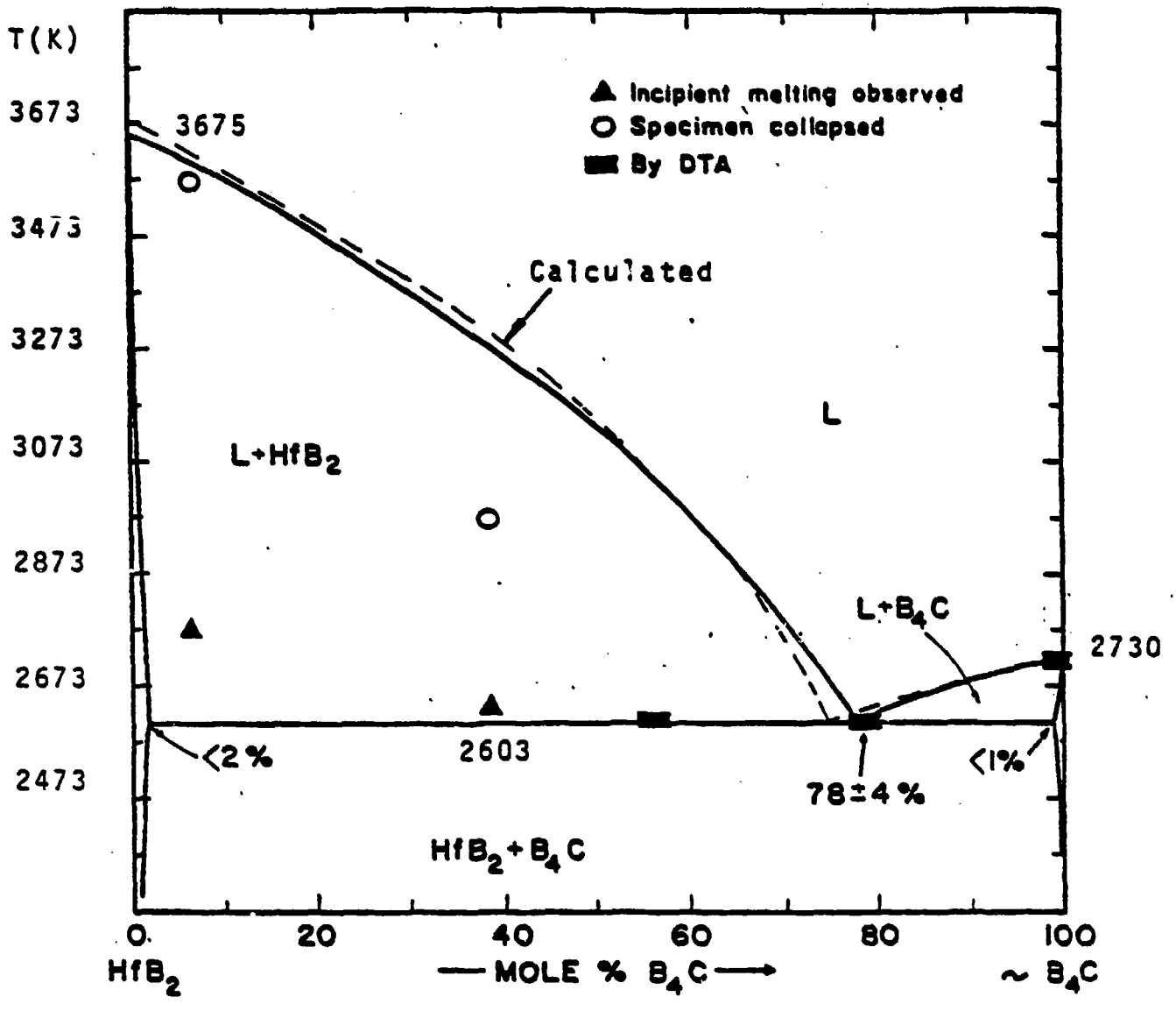

FIGURE 19. COMPARISON OF EXPERIMENTAL[6] HfB_2-B_4C QUASI-BINARY JOIN WITH CALCULATED RESULTS (DASHED CURVES) BASED ON TRNL = -12,552 JOULES/g.at

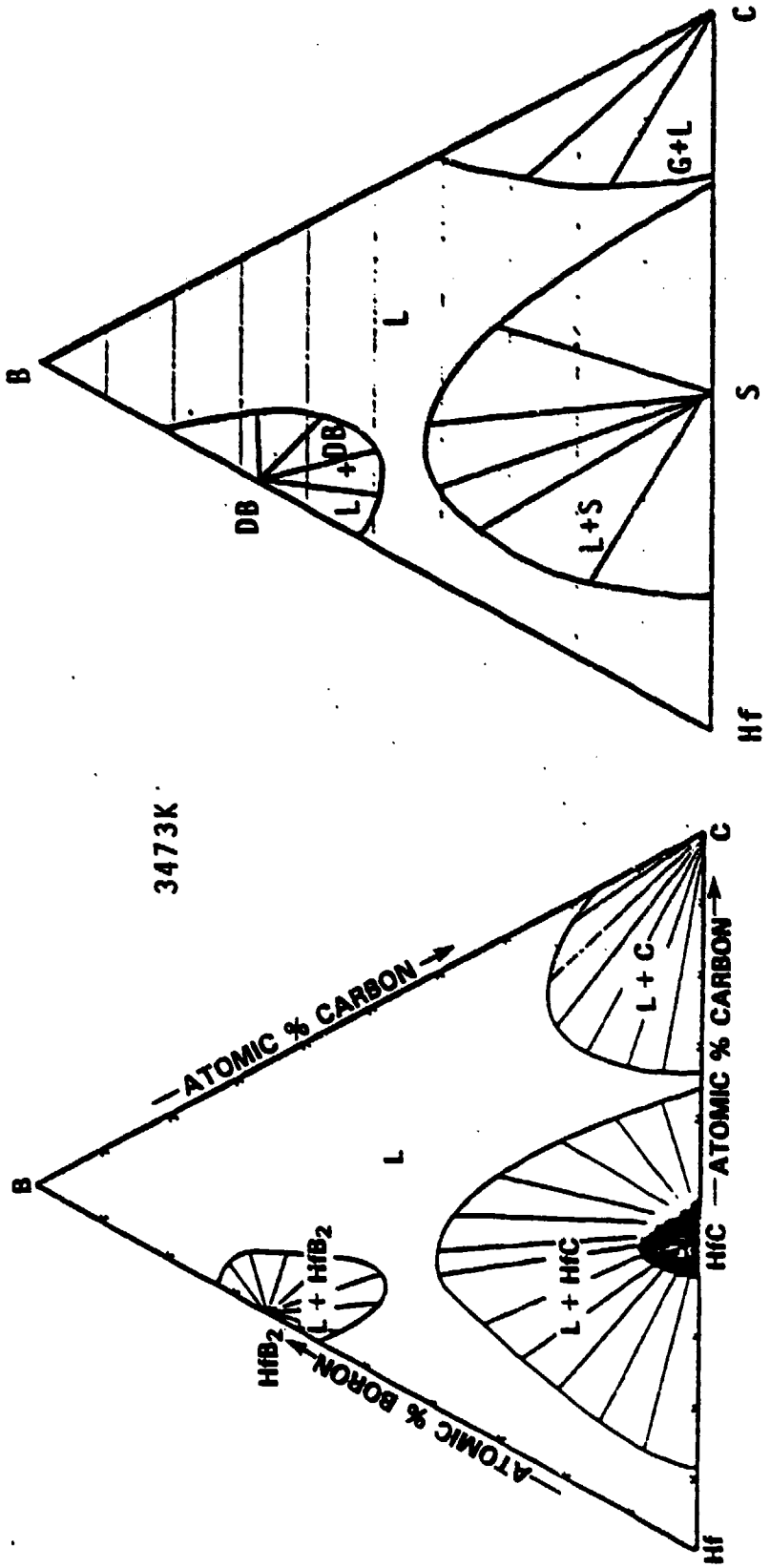

FIGURE 20. CALCULATED B-C-Hf SECTION AT 3473K (SECTION PROPOSED BY RUDY[6] ON THE LEFT)

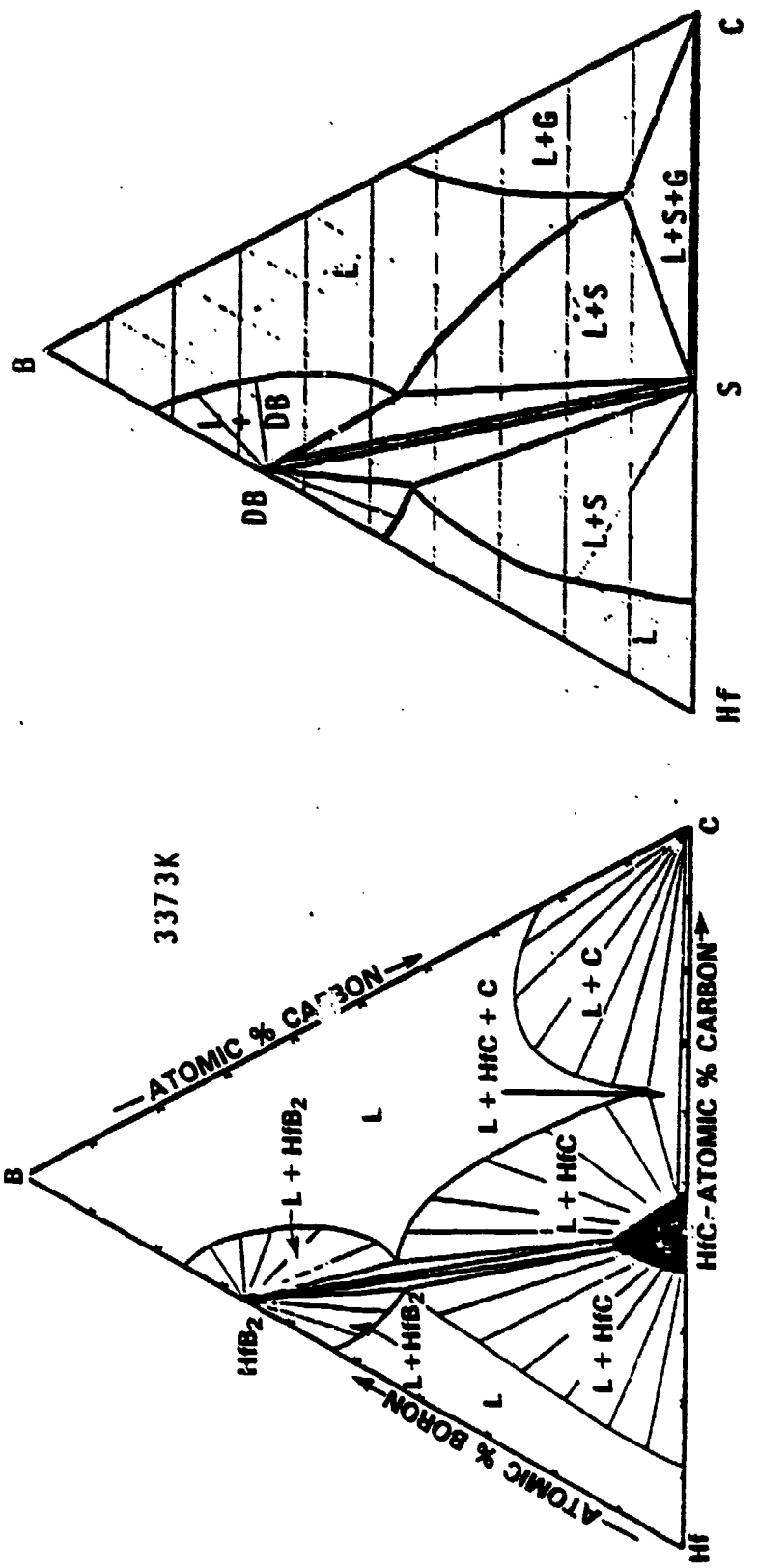

FIGURE 21. CALCULATED B-C-Hf SECTION AT 3373K (SECTION PROPOSED BY RUDY[6] ON THE LEFT)

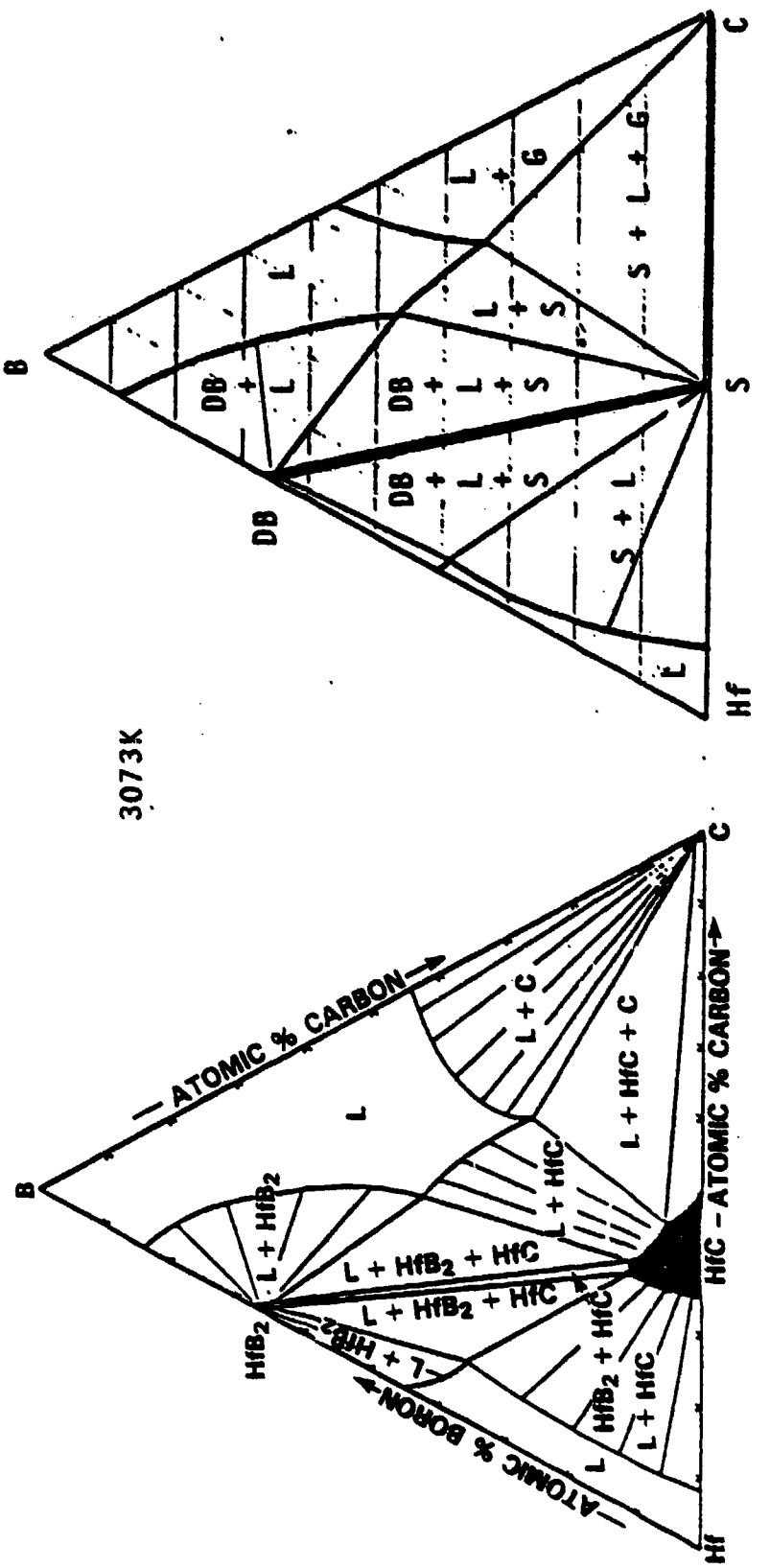

FIGURE 22. CALCULATED B-C-Hf SECTION AT 3073K (SECTION PROPOSED BY RUDY[6] ON THE LEFT)

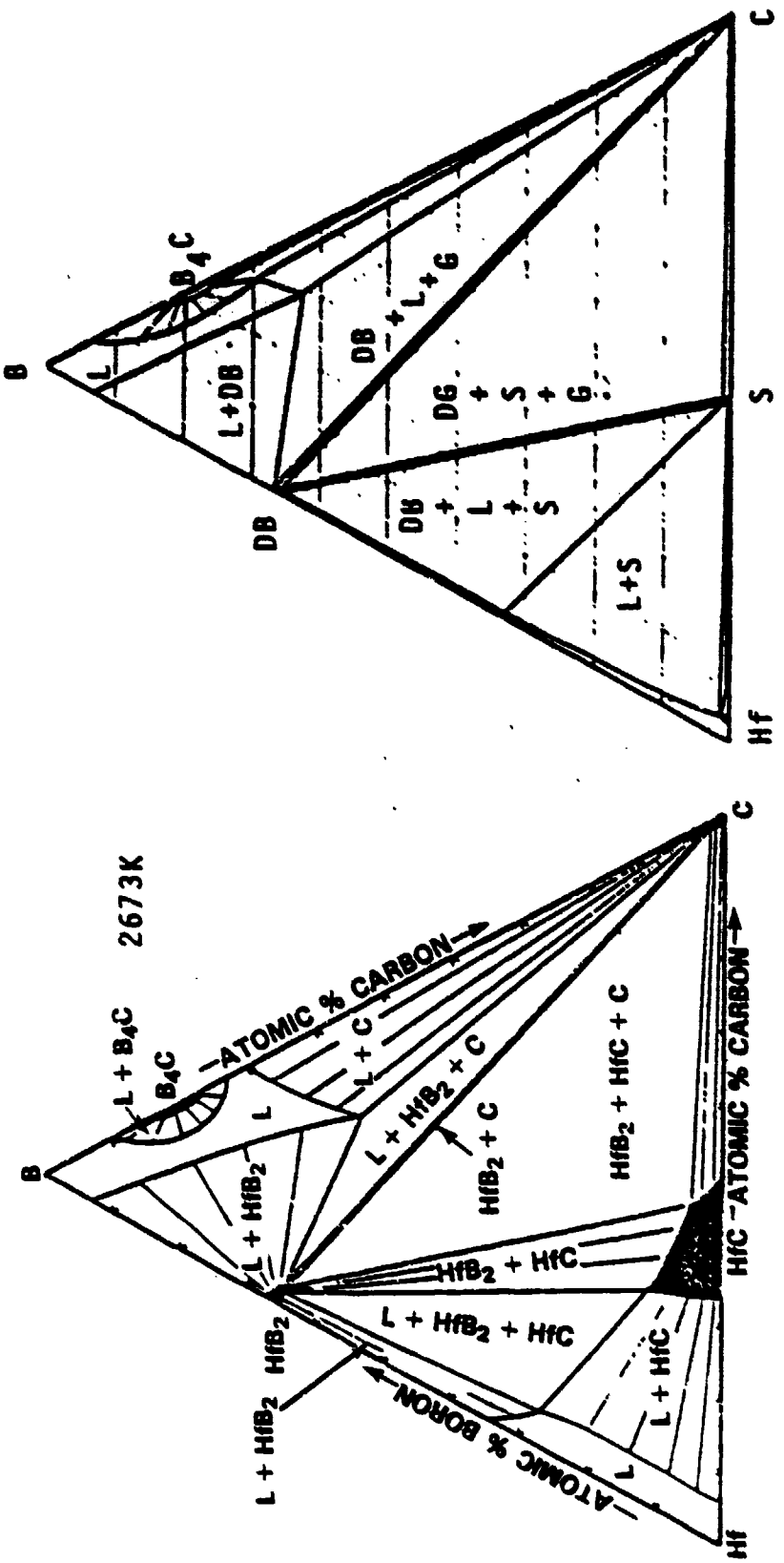

FIGURE 23. CALCULATED B-C-Hf SECTION AT 2673K (SECTION PROPOSED BY RUDY[6] ON THE LEFT)

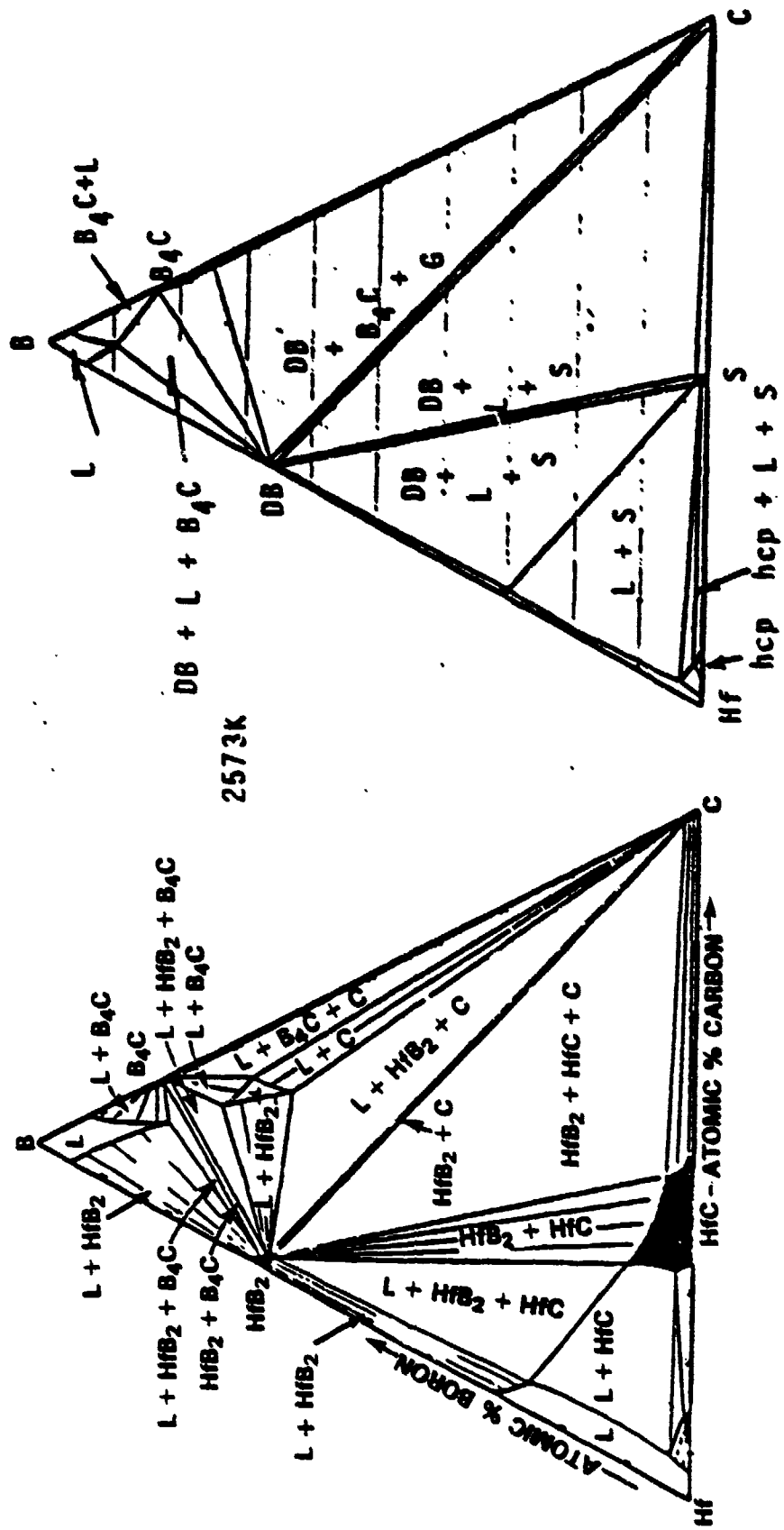

FIGURE 24. CALCULATED B-C-Hf SECTION AT 2673K (SECTION PROPOSED BY RUDY[6] ON THE LEFT)

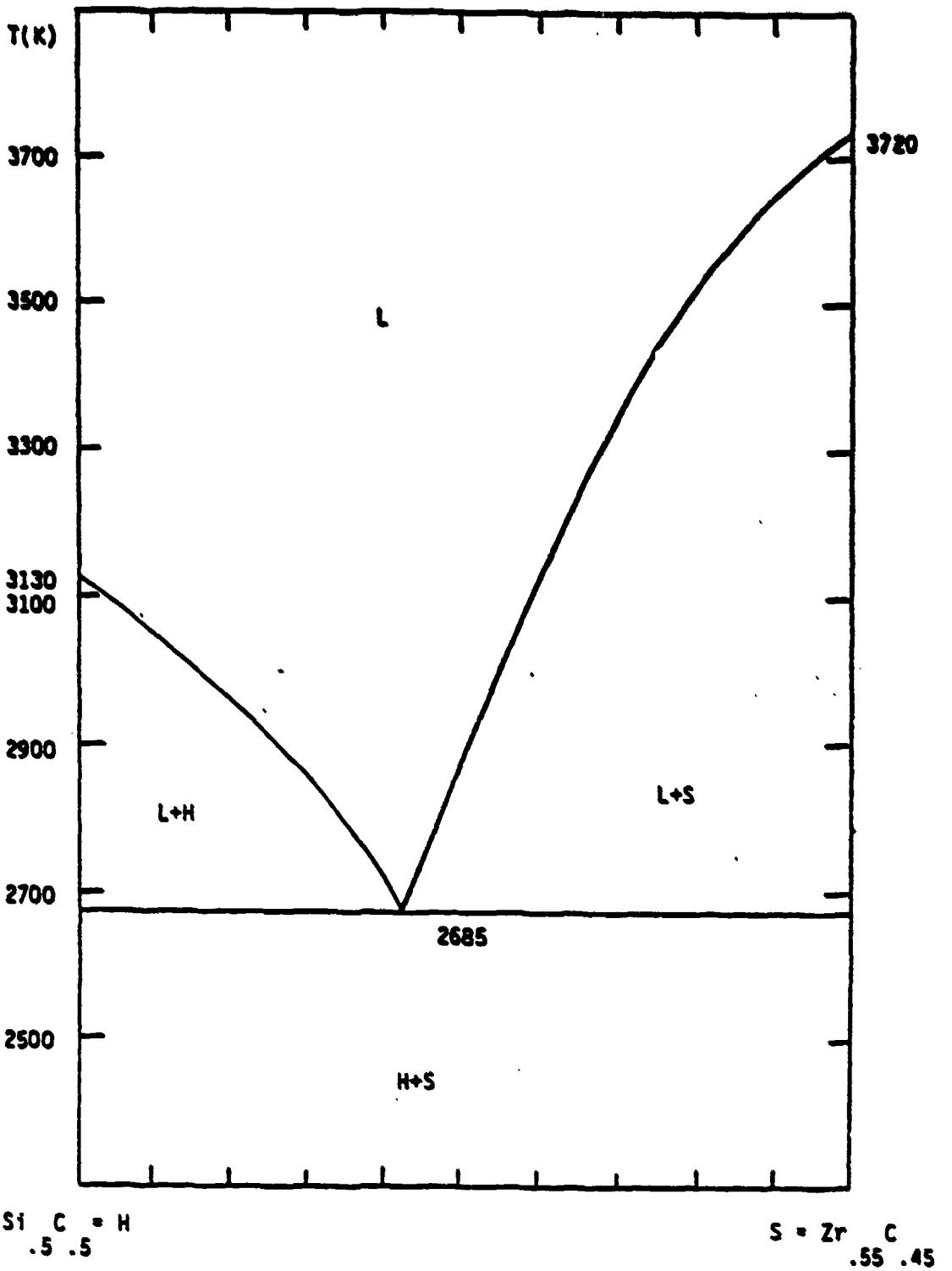

FIGURE 25. CALCULATED QUASI-BINARY JOIN $Si_{.5}C_{.5}$-$Zr_{.55}C_{.45}$

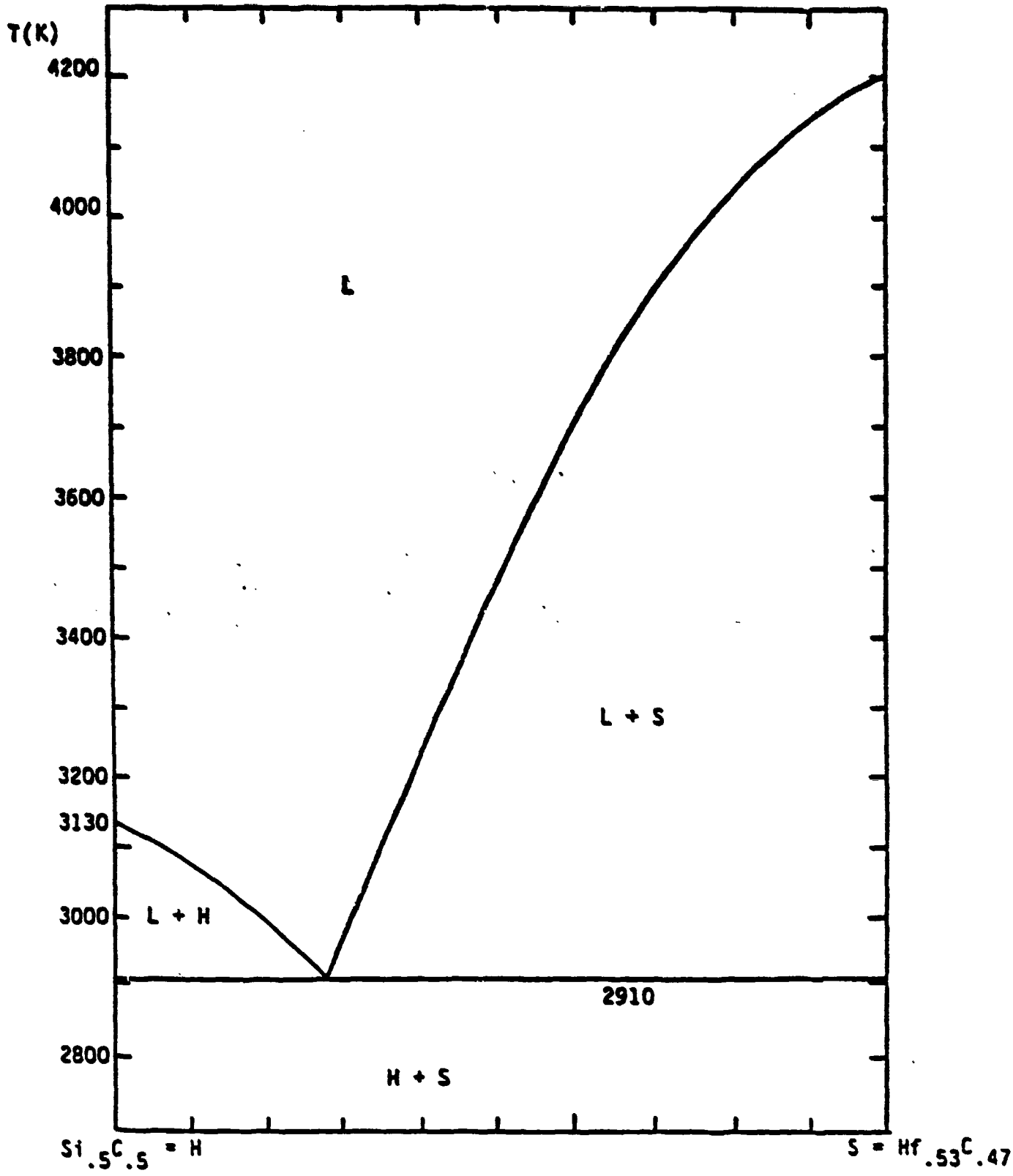

FIGURE 26. CALCULATED QUASI-BINARY JOIN $Si_{.5}C_{.5}$-$Hf_{.53}C_{.47}$

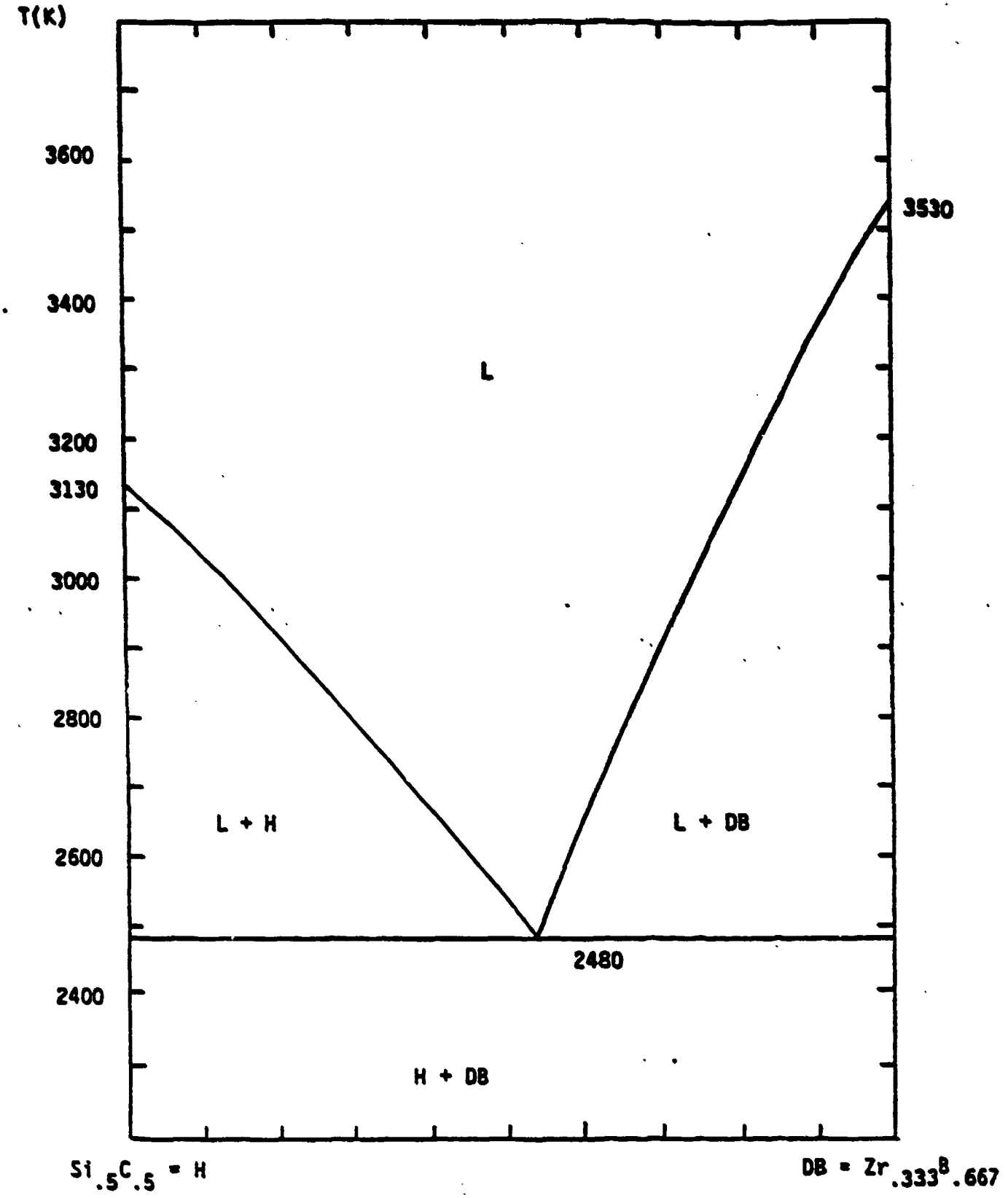

FIGURE 27. CALCULATED QUASI-BINARY JOIN $Si_{.5}C_{.5}$-$Zr_{.333}B_{.667}$

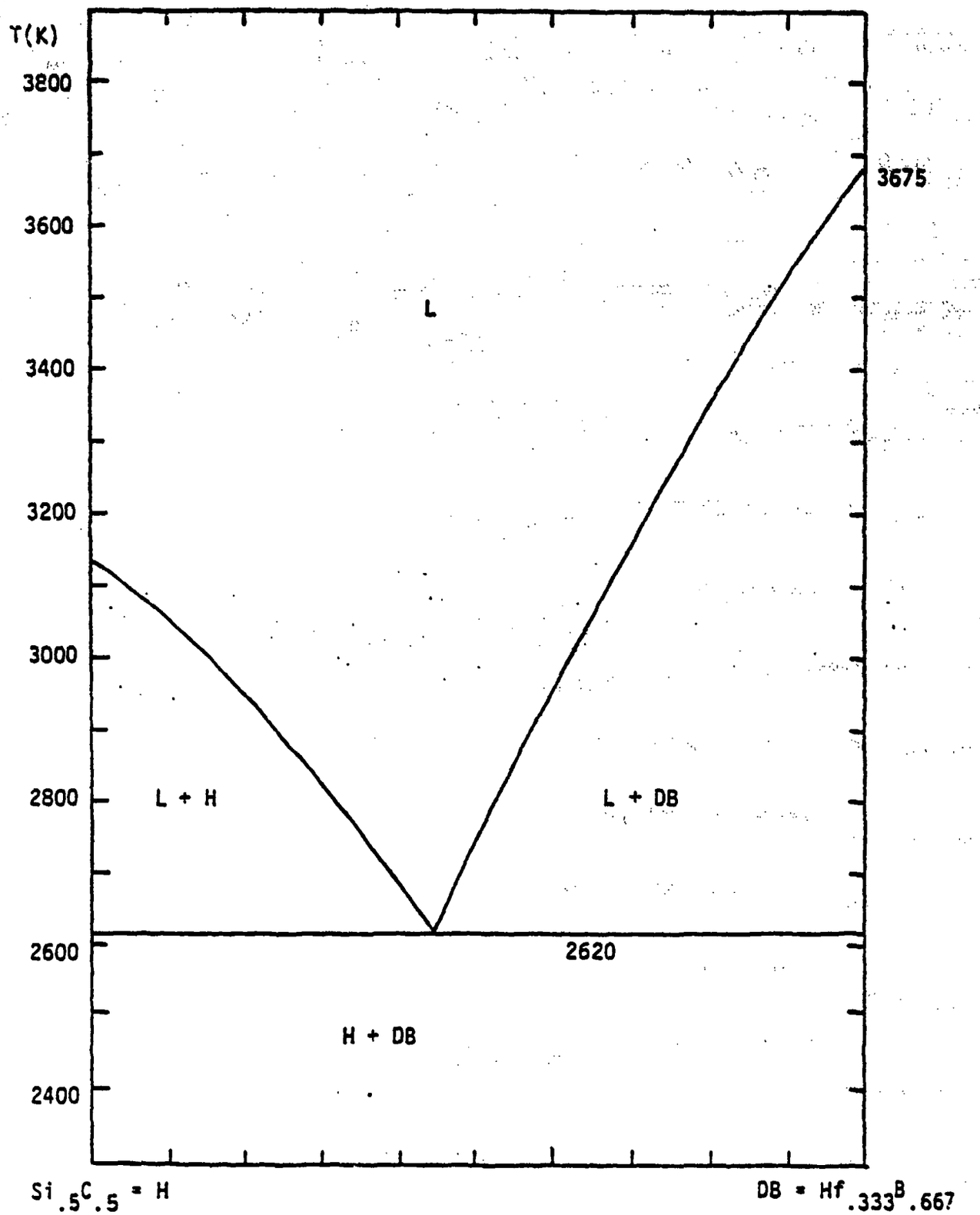

FIGURE 28. CALCULATED QUASI-BINARY JOIN $Si_{.5}C_{.5}$-$Hf_{.333}B_{.667}$

TABLE 1. LATTICE STABILITY VALUES FOR THE ELEMENTS
(Units of J/mol and J/mol K)

(L = Liquid, R = Rhombohedral, fcc = face centered cubic
bcc = body centered cubic, hcp = hexagonal close packed,
D = Diamond cubic, G = Graphite, Y = "B_4C" Structure)

Element			
B	${}^{\circ}G^{L} - {}^{\circ}G^{R}$	= 50208	- 21.84T
	${}^{\circ}G^{L} - {}^{\circ}G^{fcc}$	= 6694	- 9.623T
	${}^{\circ}G^{L} - {}^{\circ}G^{bcc}$	=	- 8.368T
	${}^{\circ}G^{L} - {}^{\circ}G^{hcp}$	=	- 12.134T
	${}^{\circ}G^{L} - {}^{\circ}G^{D}$	=	- 30.00T
	${}^{\circ}G^{L} - {}^{\circ}G^{G}$	=	- 27.20T
	${}^{\circ}G^{L} - {}^{\circ}G^{Y}$	= 44560	- 20.836T
C	${}^{\circ}G^{L} - {}^{\circ}G^{Y}$	= 61923	- 53.974T
	${}^{\circ}G^{L} - {}^{\circ}G^{G}$	=114223	- 27.196T
	${}^{\circ}G^{L} - {}^{\circ}G^{bcc}$	= 32635	- 12.552T
	${}^{\circ}G^{bcc} - {}^{\circ}G^{hcp}$	= 32635	
	${}^{\circ}G^{hcp} - {}^{\circ}G^{fcc}$	=	- 24267
	${}^{\circ}G^{L} - {}^{\circ}G^{R}$	=	- 21.84T
Zr	${}^{\circ}G^{L} - {}^{\circ}G^{G}$	=	- 27.20T
	${}^{\circ}G^{L} - {}^{\circ}G^{bcc}$	= 17782	- 8.368T
	${}^{\circ}G^{L} - {}^{\circ}G^{hcp}$	= 22092	- 12.134T
	${}^{\circ}G^{L} - {}^{\circ}G^{fcc}$	= 18744	- 12.134T
	${}^{\circ}G^{L} - {}^{\circ}G^{Y}$	=	- 25.10T
	${}^{\circ}G^{L} - {}^{\circ}G^{R}$	=	- 21.84T
Hf	${}^{\circ}G^{L} - {}^{\circ}G^{G}$	=	- 27.20T
	${}^{\circ}G^{L} - {}^{\circ}G^{bcc}$	= 20878	- 8.368T
	${}^{\circ}G^{L} - {}^{\circ}G^{hcp}$	= 28535	- 12.134T
	${}^{\circ}G^{L} - {}^{\circ}G^{fcc}$	= 25188	- 12.134T
	${}^{\circ}G^{L} - {}^{\circ}G^{Y}$	=	- 25.10T
	${}^{\circ}G^{L} - {}^{\circ}G^{R}$	=	- 21.84T

TABLE 2. ANALYTICAL DESCRIPTION OF THE CARBON-BORON SYSTEM (Joules/g.at., °K)

Phase	$E_H = H_M - x_C {}^\circ H_C - x_B {}^\circ H_B$	$E_S = S - x_C {}^\circ S_C - x_B {}^\circ S_B + R[x_C \ln x_C + x_B \ln x_B]$	Composition Range	Comments
Liquid	$-x_C x_B 29288$	0	$0<x_B<1$	$2000<T<4200$ °Refers To Liquid
Rhombohedral	$-x_C x_B 83680$	0	$0<x_B<1$	$300<T<2300$ °Refers to Rhombohedral
"B_4C Structure"	$-x_C x_B 351456$	0	$0<x_B<1$	$300<T<2800$ °Refers to "B_4C Structure"
Graphite	0	0	$0<x_B<1$	$300<T<4200$ °Refers to Graphite

TABLE 3. ANALYTICAL DESCRIPTION OF THE ZIRCONIUM-CARBON SYSTEM

Phase	$E_H = H_M - x_{Zr}{}^{\circ}H_{Zr} - x_C{}^{\circ}H_C$	$E_S = S - x_{Zr}{}^{\circ}S_{Zr} - x_C{}^{\circ}S_C + R[x_{Zr}\ln x_{Zr} + x_C \ln x_C]$	Composition Range	Comments
Liquid	$-x_{Zr}x_C 253509$	$- x_{Zr}x_C 20.92$	$0<x_C<1$	$1500<T<4200$ °Refers To Liquid
bcc	$-x_{Zr}x_C 253509$	$- x_{Zr}x_C 20.92$	$0<x_C<1$	$1100<T<2200$ °Refers to bcc
hcp	$-x_{Zr}x_C 253509$	$- x_{Zr}x_C 20.92$	$0<x_C<1$	$300<T<2200$ °Refers to hcp
Graphite	$x_{Zr}x_C 83680$	0	$0<x_C<1$	$300<T<4200$ °Refers to Graphite
Compound	$H=H-x^*_{Zr}{}^{\circ}H^{\theta}_{Zr}-x^*_C{}^{\circ}H^{\theta}_C$	$S=S-x^*_{Zr}{}^{\circ}S^{\theta}_{Zr}-x^*_C{}^{\circ}S^{\theta}_C$	Composition	Comments
$Zr_{0.55}C_{0.45}$	-171996	16.35	$x^*_C=0.45$	θ = fcc

TABLE 4. ANALYTICAL DESCRIPTION OF THE HAFNIUM-CARBON SYSTEM

Phase	$E_H = H_M - x_{Hf}{}^{\circ}H_{Hf} - x_C{}^{\circ}H_C$	$E_S = S - x_{Hf}{}^{\circ}S_{Hf} - x_C{}^{\circ}S_C + R[x_{Hf}\ln x_{Hf} + x_C \ln x_C]$	Composition Range	Comments
Liquid	$-x_{Hf}x_C 104000$	$x_{Hf}x_C 38.49$	$0<x_C<1$	$1500<T<4200$ *Refers To Liquid
bcc	$-x_{Hf}x_C 104000$	$x_{Hf}x_C 38.49$	$0<x_C<1$	$1100<T<2600$ *Refers to bcc
hcp	$-x_{Hf}x_C 195392$	$x_{Hf}x_C 38.49$	$0<x_C<1$	$300<T<2700$ *Refers to hcp
Graphite	$x_{Hf}x_C 83680$	0	$0<x_C<1$	$300<T<4200$ *Refers to Graphite

Compound	$H=H-x^*_{Hf}{}^{\circ}H^{\theta}_{Hf}-x^*_C{}^{\circ}H^{\theta}_C$	$S=S-x^*_{Hf}{}^{\circ}S^{\theta}_{Hf}-x^*_C{}^{\circ}S^{\theta}_C$	Composition	Comments
$Hf_{0.53}C_{0.47}$	-176138	-8.548	$X^*_C=0.47$	θ = fcc

Kohler's equation

$$G^L = (1-x-y)^{\circ}G^L_B + x^{\circ}G^L_C + y^{\circ}G^L_{Hf} + RT[(1-x-y)\ln(1-x-y)+x\ln x+y\ln y]$$
$$+(1-x-y)x(1-y)^{-1}[(1-x-y)LBBCC + xLCCBB] + (1-x-y)y(1-x)^{-1}[(1-x-y)LBBHF+yLHFBB]$$
$$+ xy(x+y)^{-1}[xLCCHF+yLHFCC] + xy(1-x-y)\ \text{TRNL} \quad \text{J./g.at.}$$

$x = x_C$, $y=y_{Hf}$, $(1-x-y) = (1-x-y)_B$

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TABLE 5. ANALYTICAL DESCRIPTION OF THE ZIRCONIUM-BORON SYSTEM (Joules/g.at., °K)

Phase	$^{E}_{H} = H_M - x_{Zr}{}^{\circ}H_{Zr} - x_B{}^{\circ}H_B$	$^{E}_{S} = S - x_{Zr}{}^{\circ}S_{Zr} - x_B{}^{\circ}S_B + R[x_{Zr}\ln x_{Zr} + x_B \ln x_B]$	Composition Range	Comments
Liquid	$-x_{Zr}x_B[x_{Zr}168615 + x_B 63178]$	$- x_{Zr}x_B[x_{Zr}37.66]$	$0<x_B<1$	$1500<T<3800$ °Refers To Liquid
bcc	$-x_{Zr}x_B[x_{Zr}430115 + x_B 314218]$	$- x_{Zr}x_B[x_{Zr}41.84 - x_B 41.84]$	$0<x_B<1$	$1100<T<2100$ °Refers to bcc
hcp	$-x_{Zr}x_B[x_{Zr}430115 + x_B 314218]$	$- x_{Zr}x_B[x_{Zr}41.84 - x_B 41.84]$	$0<x_B<1$	$300<T<2100$ °Refers to hcp
Rhombohedral	$-x_{Zr}x_B 41840$	0	$0<x_B<1$	$300<T<2300$ °Refers to Rhombohedral
Compound	$H = H - x^{\#}_{Zr}{}^{\circ}H^{\theta}_{Zr} - x^{\#}_B{}^{\circ}H^{\theta}_B$	$S = S - x^{\#}_{Zr}{}^{\circ}S^{\theta}_{Zr} - x^{\#}_B{}^{\circ}S^{\theta}_B$	Composition	Comments
$(1/3)ZrB_2$	-142612	-12.473	$x^{\#}_B = 0.667$	θ = hcp

TABLE 6. ANALYTICAL DESCRIPTION OF THE HAFNIUM-BORON SYSTEM (Joules/g.at., °K)

Phase	$E_H = H_M - x_{Hf}{}^{\circ}H_{Hf} - x_B{}^{\circ}H_B$	$E_S = S - x_{Hf}{}^{\circ}S_{Hf} - x_B{}^{\circ}S_B + R[x_{Hf}\ln x_{Hf} + x_B \ln x_B]$	Composition Range	Comments
Liquid	$-x_{Hf}x_B[x_{Hf}9205 + x_B 371434]$	$x_{Hf}x_B[x_{Hf}62.76 - x_B 54.39]$	$0<x_B<1$	$1500<T<3800$ °Refers To Liquid
bcc	$-x_{Hf}x_B[x_{Hf}117152 + x_B 251040]$	0	$0<x_B<1$	$1100<T<2500$ °Refers to bcc
hcp	$-x_{Hf}x_B[x_{Hf}133888 + x_B 267776]$	0	$0<x_B<1$	$300<T<2600$ °Refers to hcp
Rhombohedral	$x_{Hf}x_B 41840$	0	$0<x_B<1$	$300<T<2600$ °Refers to Rhombohedral
Compound	$H=H-x^{\#}_{Hf}{}^{\circ}H^{\theta}_{Hf}-x^{\#}_B{}^{\circ}H^{\theta}_B$	$S=S-x^{\#}_{Hf}{}^{\circ}S^{\theta}_{Hf}-x^{\#}_B{}^{\circ}S^{\theta}_B$	**Composition**	**Comments**
(1/2)HfB	-126030	-14.644	$x^{\#}_B = 0.500$	θ=hcp
(1/3)HfB_2	-146034	-13.163	$x^{\#}_B = 0.667$	θ=hcp

TABLE 7. DESCRIPTION OF THE PARTIAL GIBBS ENERGY OF EACH COMPONENT IN A FIVE COMPONENT SOLUTION ON THE BASIS OF BINARY (i.e., FIIJJ) AND TERNARY (i.e., FIIJJLL) TEMPERATURE AND COMPOSITION DEPENDENT INTERACTION PARAMETERS ACCORDING TO THE KOHLER MODEL (SEE TABLE 4)

$$\bar{G}_i^{\phi} = G_i^{\phi} + RT\ell nX_i$$

$$+ \sum_{\substack{j=1,5 \\ j\neq i}} \frac{X_iX_j}{X_i+X_j}\left[\frac{X_j}{X_i+X_j} + 1-X_i\right] FIIJJ$$

$$+ \sum_{\substack{j=1,5 \\ j\neq i}} X_j\left[\left(\frac{X_j}{X_i+X_j}\right)^2 - \frac{X_iX_j}{X_i+X_j}\right] FJJII$$

$$- \sum_{\substack{j,\ell=1,5 \\ j,\ell\neq i \\ j<\ell}} FJJLL\left[\frac{X_j^2X_\ell}{X_j+X_\ell}\right] + FLLJJ\left[\frac{X_jX_\ell^2}{X_j+X_\ell}\right]$$

$$+ \sum_{\substack{j,\ell=1,5 \\ j,\ell\neq i \\ j<\ell}} X_jX_\ell(1-2X_i) FIIJJLL$$

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