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APPLICATION OF COMPUTER METHODS FOR CALCULATION OF  
MULTICOMPONENT PHASE D. (U) MANLABS INC CAMBRIDGE MASS  
L KAUFMAN 23 OCT 84 AFOSR-TR-84-0972 F49620-84-C-0078

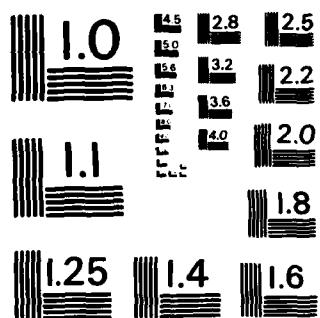
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October 22, 1984

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Major Joseph Heger  
Air Force Office of Scientific Research (AFSC)  
Bolling Air Force Base, D.C. 20332

Subject: ~~Technical~~ Report on Contract  
F49620-84-C-0078

Dear Joe,

Enclosed are six copies of our annual report covering August and September 1984. Provisional results for the Ni-Cr-Si, Ni-Al-Si, NiO<sub>2</sub>-SiO<sub>2</sub> and Cr<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> are enclosed. I expect to be in Washington on 19, 20 November 1984 and would like to see you if you are available.

Best Regards,



Larry Kaufman

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*Technical*  
~~Report~~ Report

on

CONTRACT F49620-84-C-0078

APPLICATION OF COMPUTER METHODS FOR CALCULATION  
OF MULTICOMPONENT PHASE DIAGRAMS OF HIGH TEMPERATURE  
STRUCTURAL CERAMICS

1 August 1984 to 30 September 1984

Air Force of Scientific Research (AFSC)

Bolling Air Force Base, D.C. 20332

23 October 1984

by

Larry Kaufman

ManLabs, Inc.

21 Erie Street

Cambridge, Massachusetts 02139



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| REPORT DOCUMENTATION PAGE                                                                                                                                                                                                                                                                                                                                       |                                           | READ INSTRUCTIONS<br>BEFORE COMPLETING FORM                                               |
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| 18. SUPPLEMENTARY NOTES                                                                                                                                                                                                                                                                                                                                         |                                           |                                                                                           |
| 19. KEY WORDS (Continue on reverse side if necessary and identify by block number)                                                                                                                                                                                                                                                                              |                                           |                                                                                           |
| 20. ABSTRACT (Continue on reverse side if necessary and identify by block number)<br>Computer Coupled Phase Diagram and Thermochemical Data have been<br>used to calculate the NiO-SiO <sub>2</sub> and Cr <sub>2</sub> O <sub>3</sub> -SiO <sub>2</sub> Phase Diagrams and isothermal<br>sections in the Ni-Si-Al and Ni-Cr-Si systems between 700K and 1500K. |                                           |                                                                                           |

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## I PROGRESS DURING THE CURRENT YEAR

The methods developed under the previous Contract F49620-80-C-0020 and described in the final report on that contract dated 30 November 1983 entitled "Computer Based Methods for Thermodynamics Analysis of Materials Processing" by Larry Kaufman are to be employed to carry out the following tasks during the first year of the current program:

1. A combined thermochemical and phase diagram analysis will be performed for the  $\text{GeO}_2$  -  $\text{HfO}_2$ ,  $\text{GeO}_2$  -  $\text{TiO}_2$ ,  $\text{GeO}_2$  -  $\text{Al}_2\text{O}_3$ ,  $\text{GeO}_2$  -  $\text{MgO}$ ,  $\text{GeO}_2$  -  $\text{SiO}_2$ ,  $\text{GeO}_2$  -  $\text{CaO}$ ,  $\text{SiO}_2$  -  $\text{NiO}$  and  $\text{SiO}_2$  -  $\text{Cr}_2\text{O}_3$  quasi-binary systems in order to define the lattice stability, solution and compound phase parameters and expand the current data base.
2. Isothermal sections in the  $\text{GeO}_2$  -  $\text{MgO}$  -  $\text{SiO}_2$ ,  $\text{GeO}_2$  -  $\text{MgO}$  -  $\text{TiO}_2$ ,  $\text{GeO}_2$  -  $\text{CaO}$  -  $\text{MgO}$  systems will be calculated between 700K and 2700K and isothermal sections in the Ni - Cr - Si and Ni - Al - Si systems will be calculated between 700 and 1500K. The calculated phase diagrams will be compared with available experimental phase diagrams to test the data base.

During the first two months of the program the  $\text{SiO}_2$  -  $\text{Cr}_2\text{O}_3$  and  $\text{SiO}_2$  -  $\text{NiO}$  quasi binary system have been analysed and ternary sections in the Ni-Cr-Al and Ni-Al-Si systems have been calculated. Figures 1-12 show the present (provisional) results of this work.

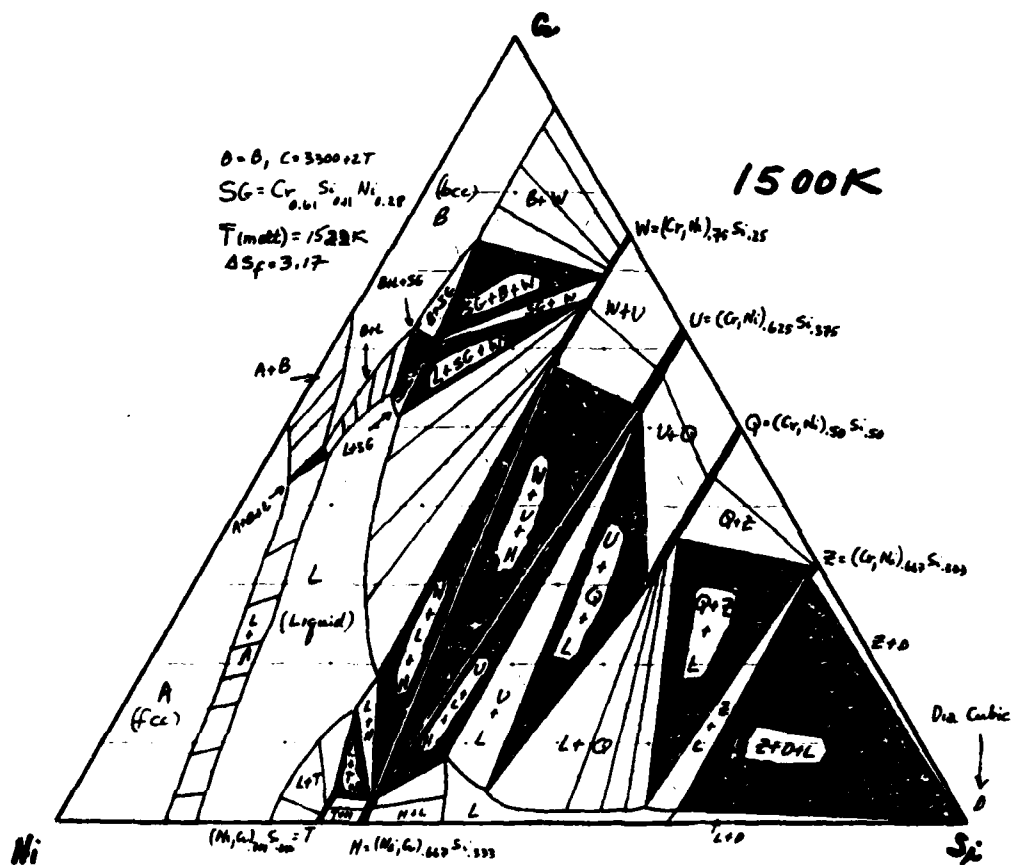


Figure 1 Calculated Isothermal Section in the Cr-Si-Ni System at 1500K





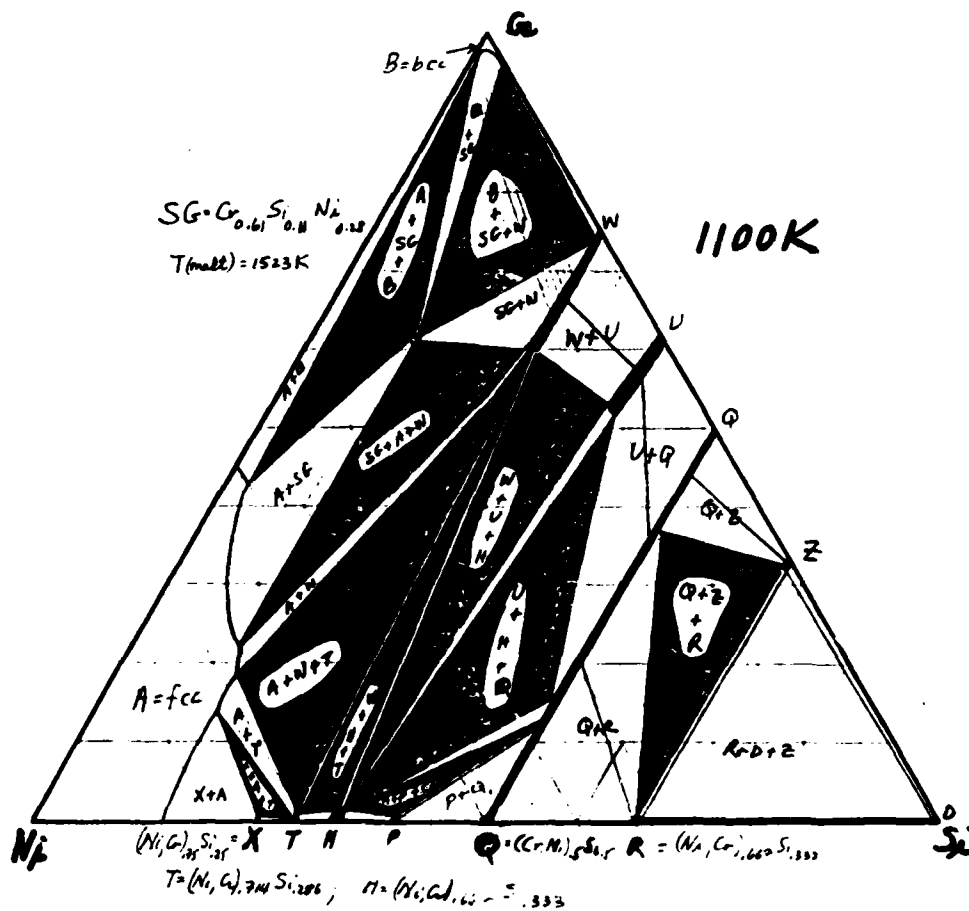


Figure 3 Calculated Isothermal Section in the Cr-Si-Ni System at 1100K

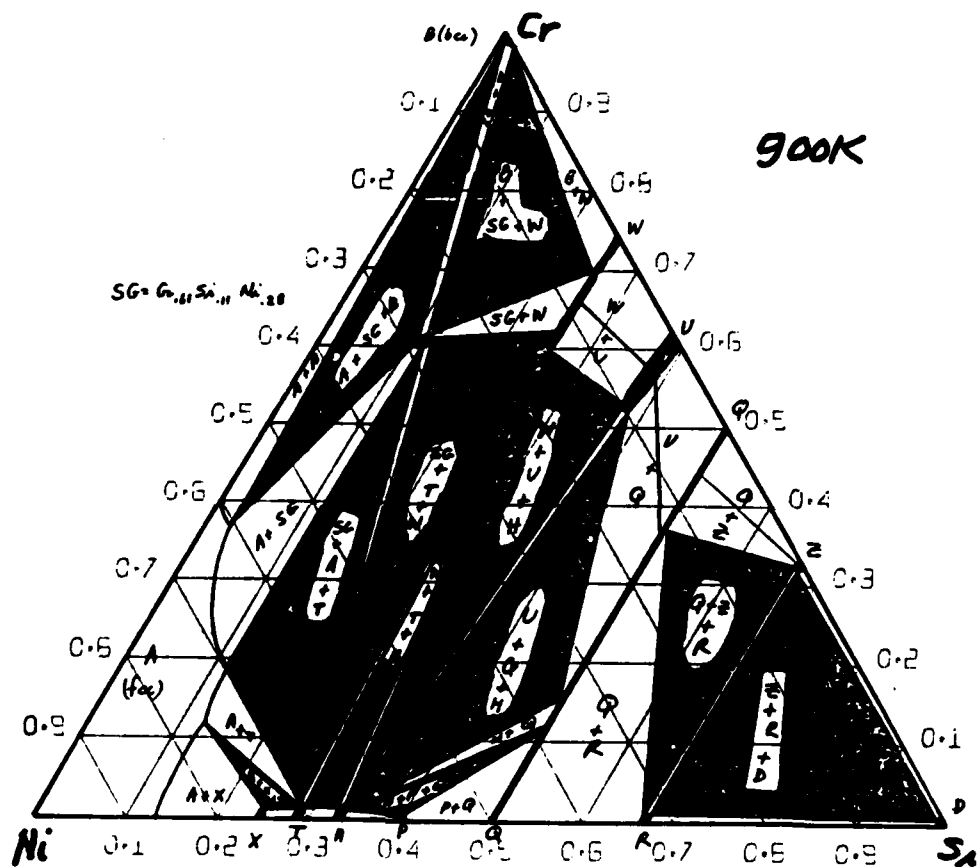


Figure 4 Calculated Isothermal Section in the Cr-Si-Ni System at 900K

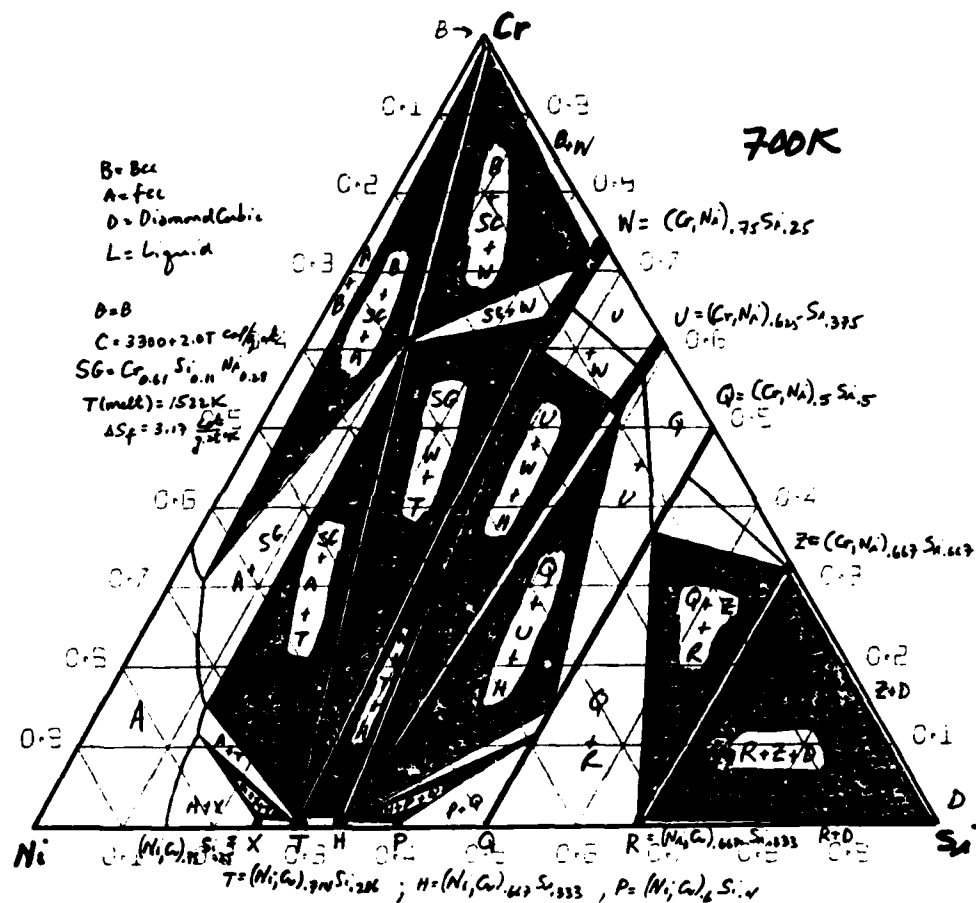


Figure 5 Calculated Isothermal Section in the Cr-Si-Ni System at 700K

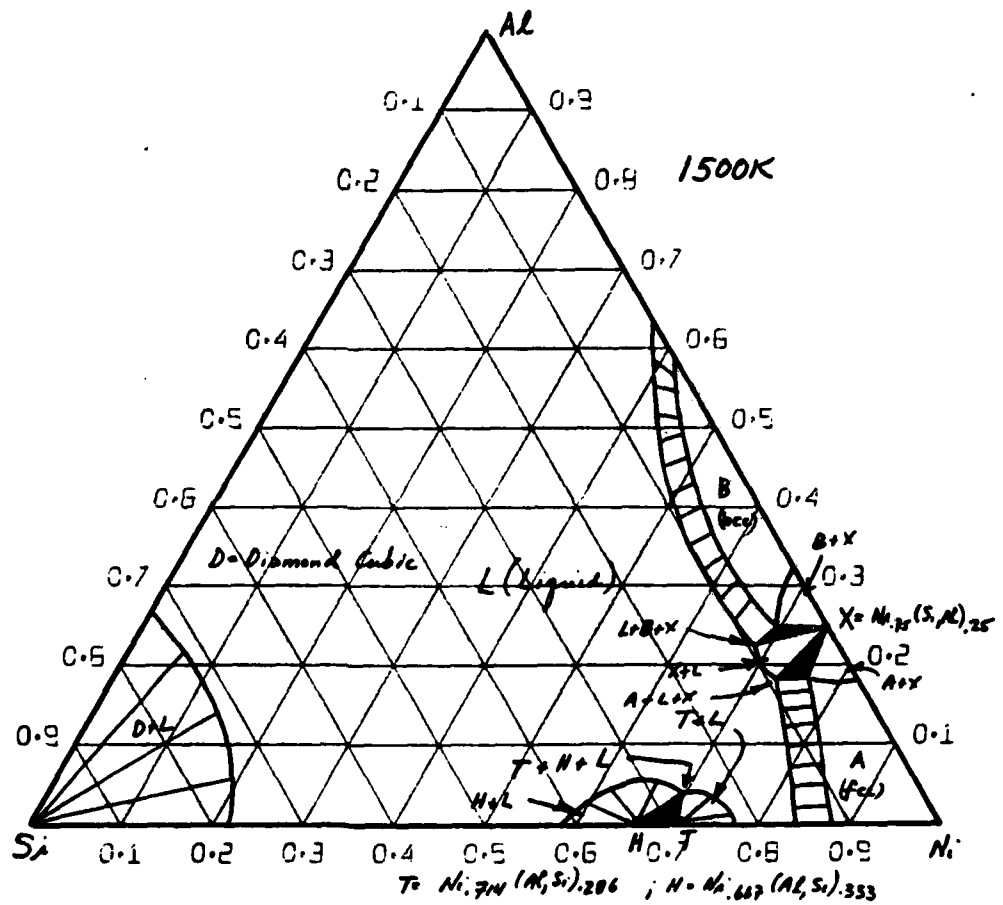


Figure 6 Calculated Isothermal Section in the Al-Ni-Si System at 1500K

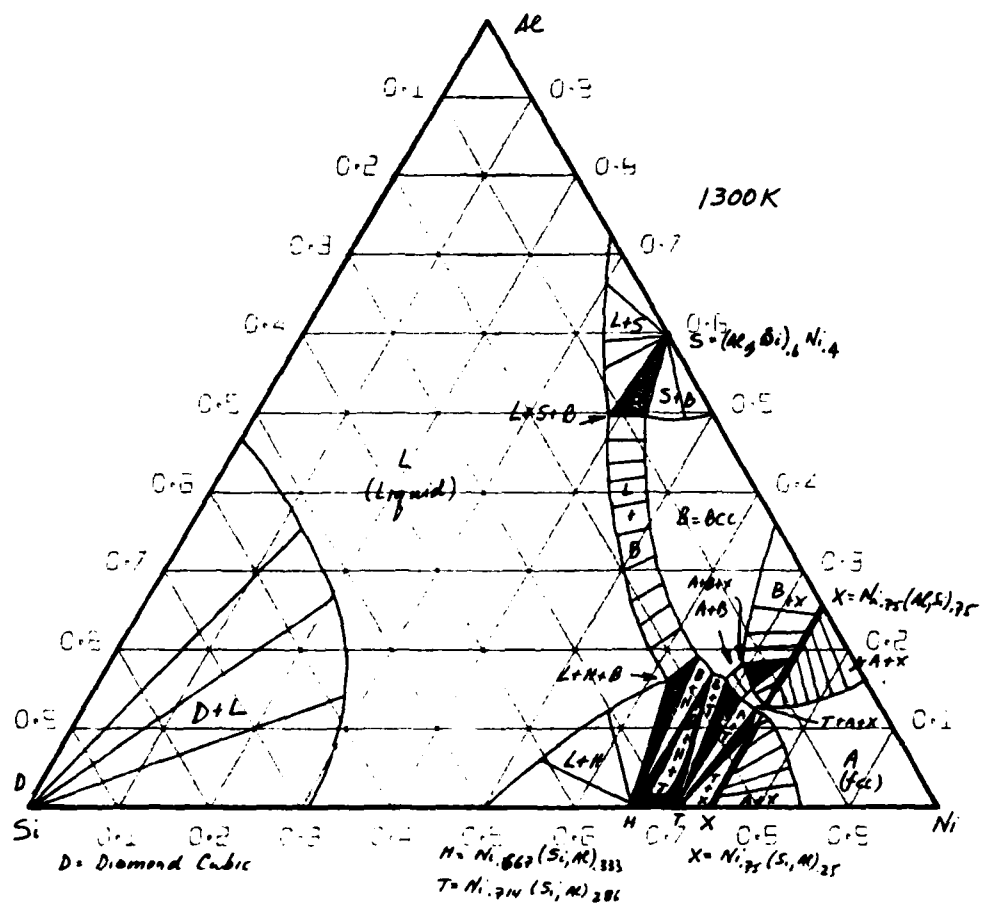


Figure 7 Calculated Isothermal Section in the Al-Ni-Si System at 1300K

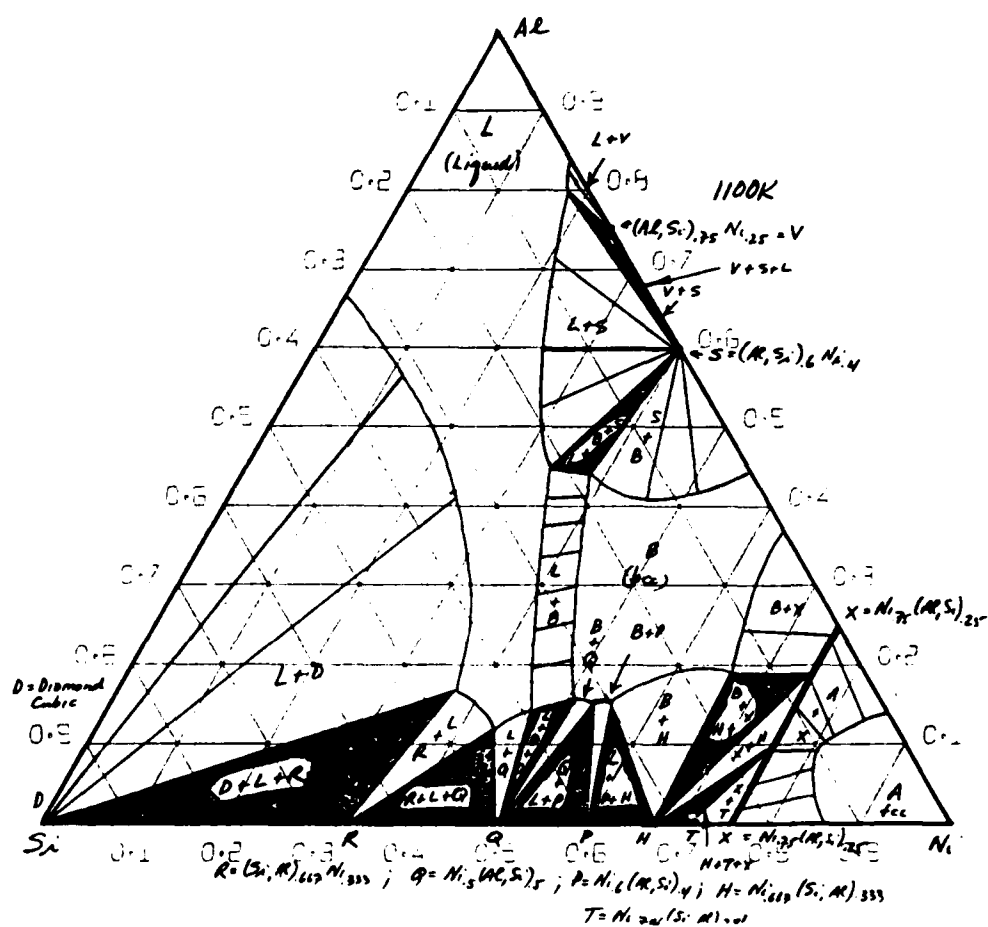


Figure 8 Calculated Isothermal Section in the Al-Ni-Si System at 1100K







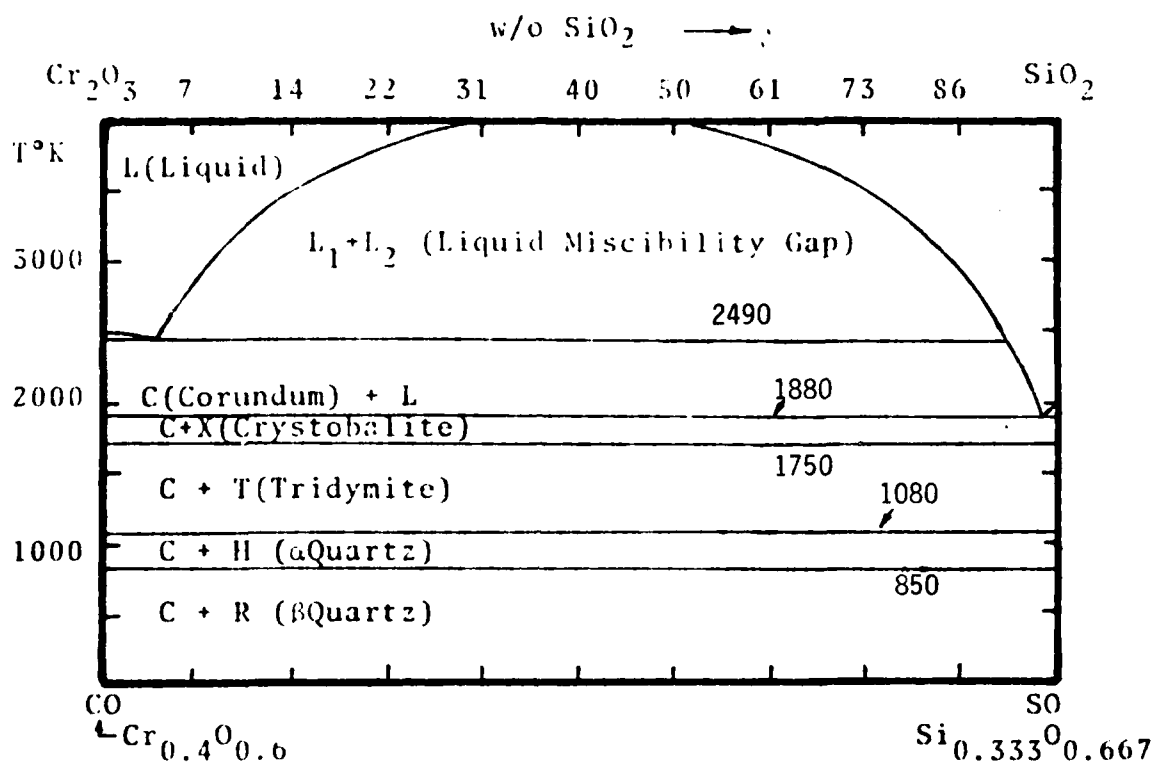


Figure 11. Calculated  $\text{Cr}_{0.4}\text{O}_{0.6}$ - $\text{Si}_{0.333}\text{O}_{0.667}$  Phase Diagram

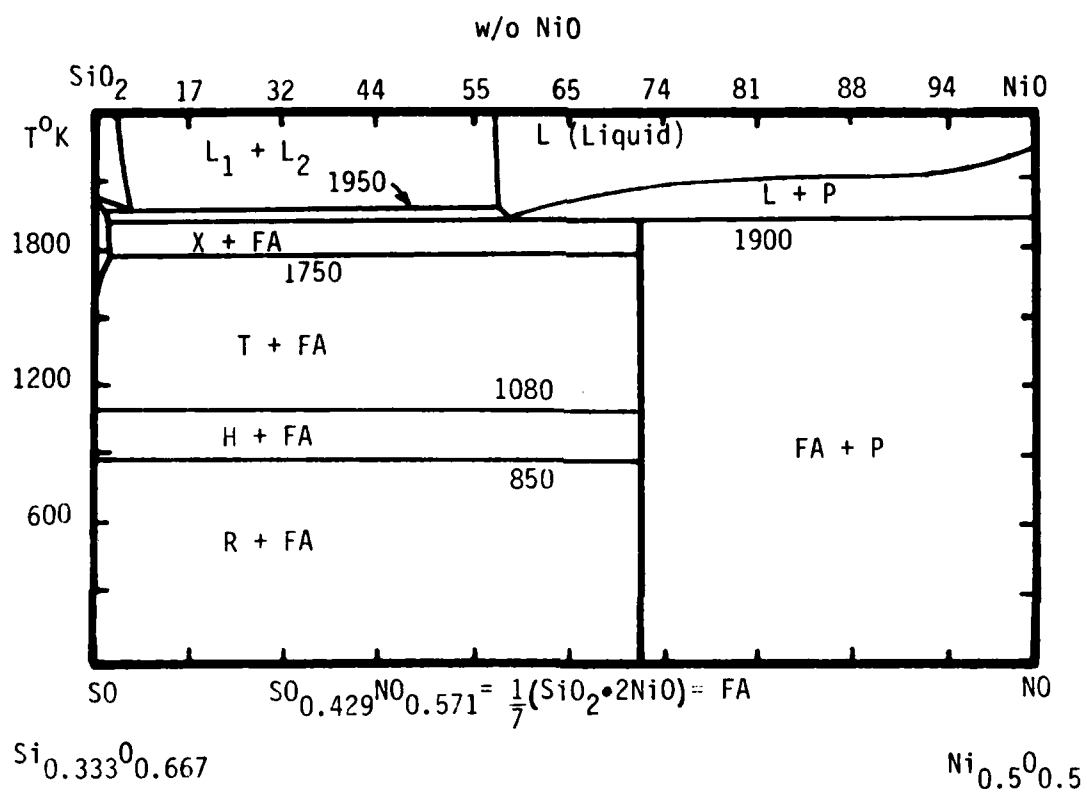


Figure 12 Calculated Si<sub>0.333</sub>O<sub>0.667</sub> - Ni<sub>0.5</sub>O<sub>0.5</sub> Phase Diagram

## II PROGRAM PERSONNEL

Technical activities during the past two months have been carried out by L. Kaufman, D. Birnie, J. Pershan, E.P. Warekois, J. Smith and D. Hay.

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