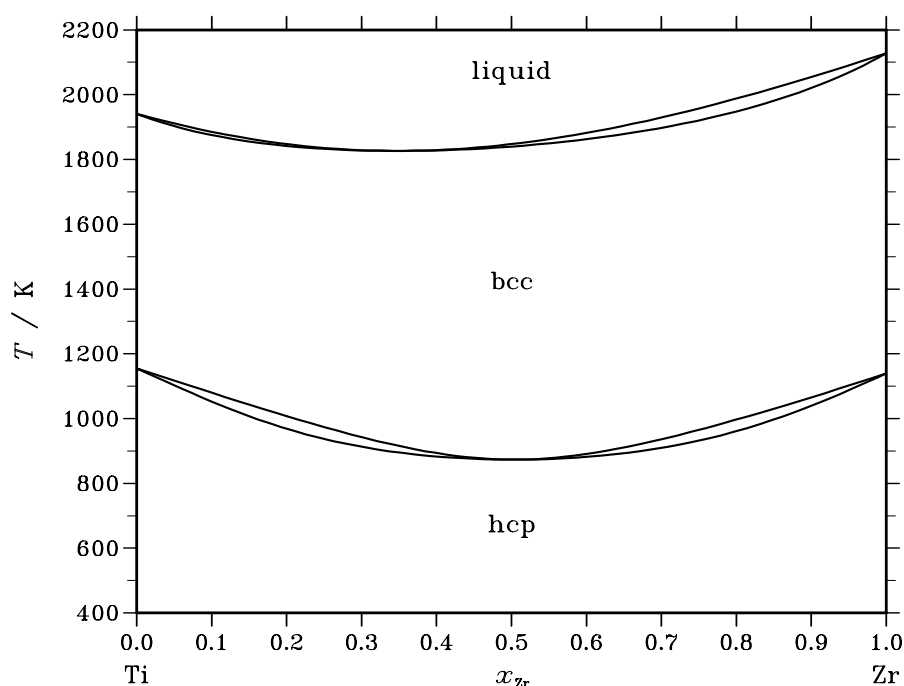


**Ti – Zr** (Titanium – Zirconium)**Fig. 1.** Calculated phase diagram for the system Ti-Zr.

Titanium and zirconium are important additions to many alloys, such as superalloys and refractory alloys. The Ti-Zr system is fairly simple with only three condensed stable phases, liquid, bcc and hcp, each of which shows complete solubility over the entire composition range. Both of the two two-phase equilibria, liquid+bcc and bcc+hcp, show congruent minima. Several thermodynamic descriptions for this system have been developed. The most recent description of [94Har] reproduces the experimental data very well and the small magnitude of the excess parameter reflects the near ideal behaviour of the system.

**Table I.** Phases, structures and models.

| Phase  | Strukturbericht | Prototype | Pearson symbol | Space group                    | SGTE name | Model                |
|--------|-----------------|-----------|----------------|--------------------------------|-----------|----------------------|
| liquid |                 |           |                |                                | LIQUID    | (Ti,Zr) <sub>1</sub> |
| bcc    | A2              | W         | <i>cI2</i>     | <i>Im<math>\bar{3}m</math></i> | BCC_A2    | (Ti,Zr) <sub>1</sub> |
| hcp    | A3              | Mg        | <i>hP2</i>     | <i>P6<sub>3</sub>/mmc</i>      | HCP_A3    | (Ti,Zr) <sub>1</sub> |

**Table II.** Invariant reactions.

| Reaction                        | Type      | <i>T</i> / K | Compositions / <i>x</i> <sub>Zr</sub> |       | $\Delta_r H$ / (J/mol) |
|---------------------------------|-----------|--------------|---------------------------------------|-------|------------------------|
| liquid $\rightleftharpoons$ bcc | congruent | 1826.4       | 0.348                                 | 0.348 | −15901                 |
| bcc $\rightleftharpoons$ hcp    | congruent | 873.5        | 0.503                                 | 0.503 | −3133                  |

**Table IIIa.** Integral quantities for the liquid phase at 2200 K.

| $x_{\text{Zr}}$ | $\Delta G_{\text{m}}$<br>[J/mol] | $\Delta H_{\text{m}}$<br>[J/mol] | $\Delta S_{\text{m}}$<br>[J/(mol·K)] | $G_{\text{m}}^{\text{E}}$<br>[J/mol] | $S_{\text{m}}^{\text{E}}$<br>[J/(mol·K)] | $\Delta C_P$<br>[J/(mol·K)] |
|-----------------|----------------------------------|----------------------------------|--------------------------------------|--------------------------------------|--|-----------------------------|
| 0.000           | 0                                | 0                                | 0.000                                | 0                                    | 0.000                                    | 0.000                       |
| 0.100           | −6034                            | −87                              | 2.703                                | −87                                  | 0.000                                    | 0.000                       |
| 0.200           | −9308                            | −155                             | 4.161                                | −155                                 | 0.000                                    | 0.000                       |
| 0.300           | −11377                           | −203                             | 5.079                                | −203                                 | 0.000                                    | 0.000                       |
| 0.400           | −12543                           | −232                             | 5.596                                | −232                                 | 0.000                                    | 0.000                       |
| 0.500           | −12921                           | −242                             | 5.763                                | −242                                 | 0.000                                    | 0.000                       |
| 0.600           | −12543                           | −232                             | 5.596                                | −232                                 | 0.000                                    | 0.000                       |
| 0.700           | −11377                           | −203                             | 5.079                                | −203                                 | 0.000                                    | 0.000                       |
| 0.800           | −9308                            | −155                             | 4.161                                | −155                                 | 0.000                                    | 0.000                       |
| 0.900           | −6034                            | −87                              | 2.703                                | −87                                  | 0.000                                    | 0.000                       |
| 1.000           | 0                                | 0                                | 0.000                                | 0                                    | 0.000                                    | 0.000                       |

Reference states: Ti(liquid), Zr(liquid)

**Table IIIb.** Partial quantities for Ti in the liquid phase at 2200 K.

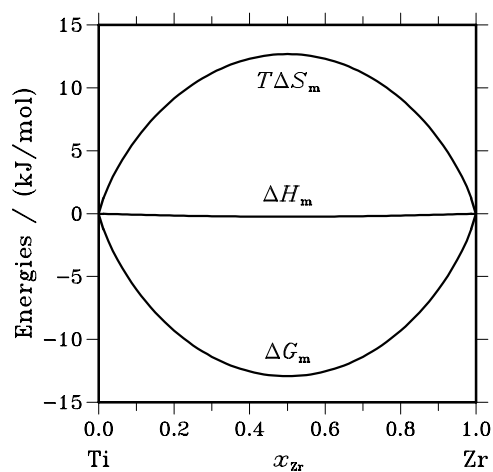
| $x_{\text{Ti}}$ | $\Delta G_{\text{Ti}}$<br>[J/mol] | $\Delta H_{\text{Ti}}$<br>[J/mol] | $\Delta S_{\text{Ti}}$<br>[J/(mol·K)] | $G_{\text{Ti}}^{\text{E}}$<br>[J/mol] | $S_{\text{Ti}}^{\text{E}}$<br>[J/(mol·K)] | $a_{\text{Ti}}$ | $\gamma_{\text{Ti}}$ |
|-----------------|-----------------------------------|-----------------------------------|---------------------------------------|---------------------------------------|---|-----------------|----------------------|
| 1.000           | 0                                 | 0                                 | 0.000                                 | 0                                     | 0.000                                     | 1.000           | 1.000                |
| 0.900           | −1937                             | −10                               | 0.876                                 | −10                                   | 0.000                                     | 0.900           | 0.999                |
| 0.800           | −4120                             | −39                               | 1.855                                 | −39                                   | 0.000                                     | 0.798           | 0.998                |
| 0.700           | −6611                             | −87                               | 2.966                                 | −87                                   | 0.000                                     | 0.697           | 0.995                |
| 0.600           | −9499                             | −155                              | 4.247                                 | −155                                  | 0.000                                     | 0.595           | 0.992                |
| 0.500           | −12921                            | −242                              | 5.763                                 | −242                                  | 0.000                                     | 0.493           | 0.987                |
| 0.400           | −17109                            | −348                              | 7.619                                 | −348                                  | 0.000                                     | 0.392           | 0.981                |
| 0.300           | −22497                            | −474                              | 10.010                                | −474                                  | 0.000                                     | 0.292           | 0.974                |
| 0.200           | −30059                            | −620                              | 13.382                                | −620                                  | 0.000                                     | 0.193           | 0.967                |
| 0.100           | −42903                            | −784                              | 19.145                                | −784                                  | 0.000                                     | 0.096           | 0.958                |
| 0.000           | −∞                                | −968                              | ∞                                     | −968                                  | 0.000                                     | 0.000           | 0.948                |

Reference state: Ti(liquid)

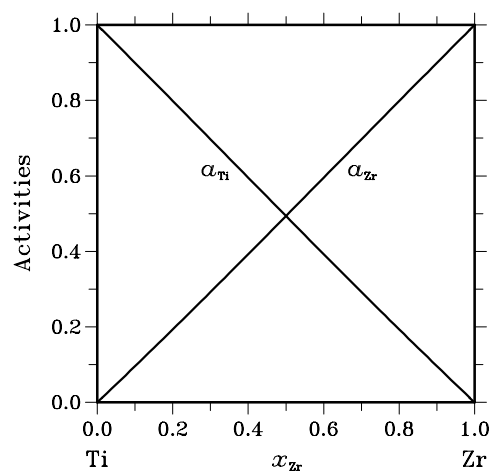
**Table IIIc.** Partial quantities for Zr in the liquid phase at 2200 K.

| $x_{\text{Zr}}$ | $\Delta G_{\text{Zr}}$<br>[J/mol] | $\Delta H_{\text{Zr}}$<br>[J/mol] | $\Delta S_{\text{Zr}}$<br>[J/(mol·K)] | $G_{\text{Zr}}^{\text{E}}$<br>[J/mol] | $S_{\text{Zr}}^{\text{E}}$<br>[J/(mol·K)] | $a_{\text{Zr}}$ | $\gamma_{\text{Zr}}$ |
|-----------------|-----------------------------------|-----------------------------------|---------------------------------------|---------------------------------------|---|-----------------|----------------------|
| 0.000           | −∞                                | −968                              | ∞                                     | −968                                  | 0.000                                     | 0.000           | 0.948                |
| 0.100           | −42903                            | −784                              | 19.145                                | −784                                  | 0.000                                     | 0.096           | 0.958                |
| 0.200           | −30059                            | −620                              | 13.382                                | −620                                  | 0.000                                     | 0.193           | 0.967                |
| 0.300           | −22497                            | −474                              | 10.010                                | −474                                  | 0.000                                     | 0.292           | 0.974                |
| 0.400           | −17109                            | −348                              | 7.619                                 | −348                                  | 0.000                                     | 0.392           | 0.981                |
| 0.500           | −12921                            | −242                              | 5.763                                 | −242                                  | 0.000                                     | 0.493           | 0.987                |
| 0.600           | −9499                             | −155                              | 4.247                                 | −155                                  | 0.000                                     | 0.595           | 0.992                |
| 0.700           | −6611                             | −87                               | 2.966                                 | −87                                   | 0.000                                     | 0.697           | 0.995                |
| 0.800           | −4120                             | −39                               | 1.855                                 | −39                                   | 0.000                                     | 0.798           | 0.998                |
| 0.900           | −1937                             | −10                               | 0.876                                 | −10                                   | 0.000                                     | 0.900           | 0.999                |
| 1.000           | 0                                 | 0                                 | 0.000                                 | 0                                     | 0.000                                     | 1.000           | 1.000                |

Reference state: Zr(liquid)



**Fig. 2.** Integral quantities of the liquid phase at  $T=2200$  K.



**Fig. 3.** Activities in the liquid phase at  $T=2200$  K.

**Table IVa.** Integral quantities for the stable phases at 1500 K.

| Phase | $x_{Zr}$ | $\Delta G_m$<br>[J/mol] | $\Delta H_m$<br>[J/mol] | $\Delta S_m$<br>[J/(mol·K)] | $G_m^E$<br>[J/mol] | $S_m^E$<br>[J/(mol·K)] | $\Delta C_P$<br>[J/(mol·K)] |
|-------|----------|-------------------------|-------------------------|-----------------------------|--------------------|------------------------|-----------------------------|
| bcc   | 0.000    | 0                       | 0                       | 0.000                       | 0                  | 0.000                  | 0.000                       |
|       | 0.100    | -3704                   | -391                    | 2.209                       | 350                | -0.494                 | 0.000                       |
|       | 0.200    | -5619                   | -695                    | 3.282                       | 622                | -0.878                 | 0.000                       |
|       | 0.300    | -6802                   | -913                    | 3.926                       | 816                | -1.153                 | 0.000                       |
|       | 0.400    | -7461                   | -1043                   | 4.278                       | 933                | -1.317                 | 0.000                       |
|       | 0.500    | -7673                   | -1087                   | 4.391                       | 972                | -1.372                 | 0.000                       |
|       | 0.600    | -7461                   | -1043                   | 4.278                       | 933                | -1.317                 | 0.000                       |
|       | 0.700    | -6802                   | -913                    | 3.926                       | 816                | -1.153                 | 0.000                       |
|       | 0.800    | -5619                   | -695                    | 3.282                       | 622                | -0.878                 | 0.000                       |
|       | 0.900    | -3704                   | -391                    | 2.209                       | 350                | -0.494                 | 0.000                       |
|       | 1.000    | 0                       | 0                       | 0.000                       | 0                  | 0.000                  | 0.000                       |

Reference states: Ti(bcc), Zr(bcc)

**Table IVb.** Partial quantities for Ti in the stable phases at 1500 K.

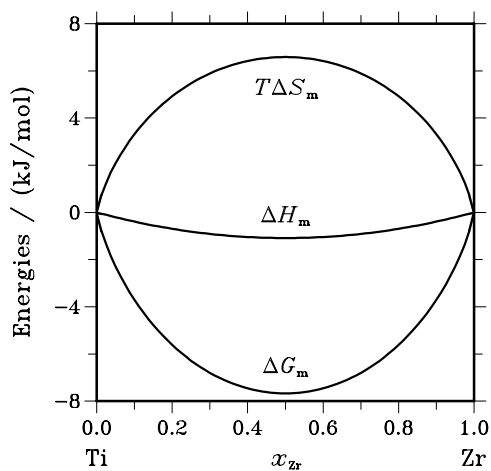
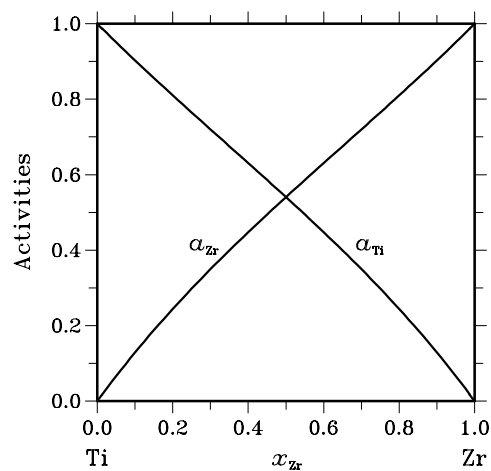
| Phase | $x_{Ti}$ | $\Delta G_{Ti}$<br>[J/mol] | $\Delta H_{Ti}$<br>[J/mol] | $\Delta S_{Ti}$<br>[J/(mol·K)] | $G_{Ti}^E$<br>[J/mol] | $S_{Ti}^E$<br>[J/(mol·K)] | $a_{Ti}$ | $\gamma_{Ti}$ |
|-------|----------|----------------------------|----------------------------|--------------------------------|-----------------------|---------------------------|----------|---------------|
| bcc   | 1.000    | 0                          | 0                          | 0.000                          | 0                     | 0.000                     | 1.000    | 1.000         |
|       | 0.900    | -1275                      | -43                        | 0.821                          | 39                    | -0.055                    | 0.903    | 1.003         |
|       | 0.800    | -2628                      | -174                       | 1.636                          | 156                   | -0.220                    | 0.810    | 1.013         |
|       | 0.700    | -4098                      | -391                       | 2.472                          | 350                   | -0.494                    | 0.720    | 1.028         |
|       | 0.600    | -5749                      | -695                       | 3.369                          | 622                   | -0.878                    | 0.631    | 1.051         |
|       | 0.500    | -7673                      | -1087                      | 4.391                          | 972                   | -1.372                    | 0.541    | 1.081         |
|       | 0.400    | -10028                     | -1565                      | 5.642                          | 1400                  | -1.976                    | 0.448    | 1.119         |
|       | 0.300    | -13111                     | -2130                      | 7.321                          | 1905                  | -2.690                    | 0.350    | 1.165         |
|       | 0.200    | -17585                     | -2781                      | 9.869                          | 2488                  | -3.513                    | 0.244    | 1.221         |
|       | 0.100    | -25568                     | -3520                      | 14.699                         | 3149                  | -4.446                    | 0.129    | 1.287         |
|       | 0.000    | $-\infty$                  | -4346                      | $\infty$                       | 3888                  | -5.489                    | 0.000    | 1.366         |

Reference state: Ti(bcc)

**Table IVc.** Partial quantities for Zr in the stable phases at 1500 K.

| Phase | $x_{\text{Zr}}$ | $\Delta G_{\text{Zr}}$<br>[J/mol] | $\Delta H_{\text{Zr}}$<br>[J/mol] | $\Delta S_{\text{Zr}}$<br>[J/(mol·K)] | $G_{\text{Zr}}^{\text{E}}$<br>[J/mol] | $S_{\text{Zr}}^{\text{E}}$<br>[J/(mol·K)] | $a_{\text{Zr}}$ | $\gamma_{\text{Zr}}$ |
|-------|-----------------|-----------------------------------|-----------------------------------|---------------------------------------|---------------------------------------|---|-----------------|----------------------|
| bcc   | 0.000           | $-\infty$                         | -4346                             | $\infty$                              | 3888                                  | -5.489                                    | 0.000           | 1.366                |
|       | 0.100           | -25568                            | -3520                             | 14.699                                | 3149                                  | -4.446                                    | 0.129           | 1.287                |
|       | 0.200           | -17585                            | -2781                             | 9.869                                 | 2488                                  | -3.513                                    | 0.244           | 1.221                |
|       | 0.300           | -13111                            | -2130                             | 7.321                                 | 1905                                  | -2.690                                    | 0.350           | 1.165                |
|       | 0.400           | -10028                            | -1565                             | 5.642                                 | 1400                                  | -1.976                                    | 0.448           | 1.119                |
|       | 0.500           | -7673                             | -1087                             | 4.391                                 | 972                                   | -1.372                                    | 0.541           | 1.081                |
|       | 0.600           | -5749                             | -695                              | 3.369                                 | 622                                   | -0.878                                    | 0.631           | 1.051                |
|       | 0.700           | -4098                             | -391                              | 2.472                                 | 350                                   | -0.494                                    | 0.720           | 1.028                |
|       | 0.800           | -2627                             | -174                              | 1.636                                 | 156                                   | -0.220                                    | 0.810           | 1.013                |
|       | 0.900           | -1275                             | -43                               | 0.821                                 | 39                                    | -0.055                                    | 0.903           | 1.003                |
|       | 1.000           | 0                                 | 0                                 | 0.000                                 | 0                                     | 0.000                                     | 1.000           | 1.000                |

Reference state: Zr(bcc)

**Fig. 4.** Integral quantities of the stable phases at  $T=1500$  K.**Fig. 5.** Activities in the stable phases at  $T=1500$  K.

## References

[94Har] K.C. Hari Kumar, P. Wollants, L. Delaey: J. Alloys Comp. **206** (1994) 121–127.