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## Letter

# Thermodynamic assessment of the $YO_{1.5}$–MgO system

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The $YO_{1.5}$–MgO phase diagram has been measured by several authors [1–4]. The most detailed and accurate one was by Tresvyatsky *et al.* [4]. The phase diagram calculated recently by Kaufman [5] is shown in Fig. 1. The figure shows that Kaufman's assessment does not satisfactorily describe the experimental solid solubilities [4] of either MgO in $YO_{1.5}$ and/or $YO_{1.5}$ in MgO. Furthermore, new experimental data on the transformation temperatures and enthalpies [6–9] should slightly modify the lattice stabilities

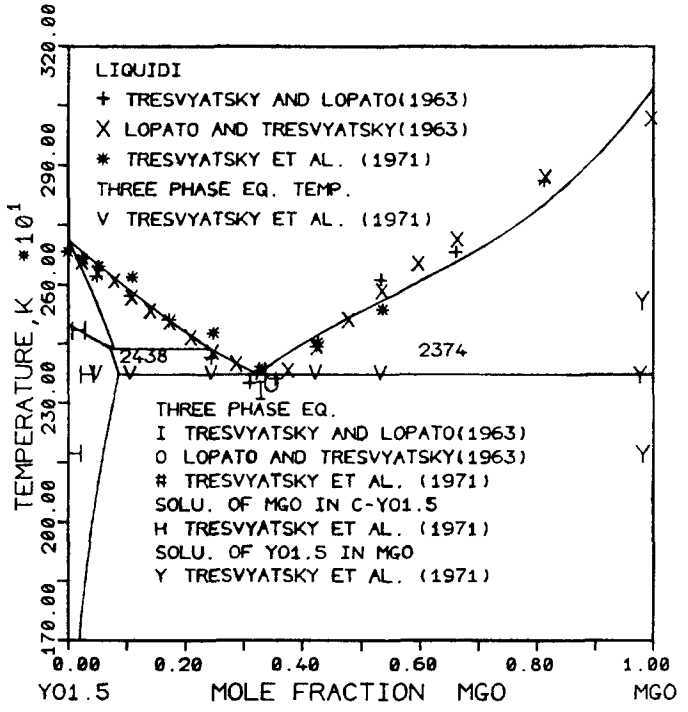


Fig. 1. Calculated $YO_{1.5}$–MgO phase diagram using parameters evaluated by Kaufman [5].

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of Kaufman [5]. Therefore a recalculation of the $YO_{1.5}$–MgO system is of interest.

For convenience the hexagonal and cubic forms of $YO_{1.5}$ are denoted h-$YO_{1.5}$ and c-$YO_{1.5}$ respectively. The solid solutions based on h-$YO_{1.5}$, c-$YO_{1.5}$ and MgO are designated Hss, Yss and MgO.ss respectively.

The phase diagram data used in the optimization are the solid solubilities and $YO_{1.5}$ liquidus [4], the MgO liquidus [3] together with one liquidus temperature at 43 mol.% MgO [4] and the eutectic reaction data [4]. The compound $3MgO–Y_2O_3$ [1] was not included in the optimization because the later authors [3, 4, 10, 11] could not confirm its existence.

Table 1 summarizes the lattice stabilities employed in the current work. The metastable stabilities are from Kaufman's work [5]. However, his data for the stable forms are slightly modified to reflect the currently accepted transition temperatures and enthalpies for MgO [6] and $YO_{1.5}$ [7–9].

The Gibbs free energy of the individual phase $v$ is given by

$$G_m^v(x,T) = \sum_{i=1}^{2} x_i {}^{\circ}G_i^v(T) + RT\sum_{i=1}^{2} x_i \ln x_i + x_1 x_2 \sum_{i=0}^{n} {}^{i}L(x_1 - x_2)^i \qquad (1)$$

where the first term corresponds to a mechanical mixture of the pure oxides, the second term corresponds to an ideal solution and the last term is the excess Gibbs energy function.

The evaluation of the parameters was carried out by the least-squares method [12]. The optimized parameters are shown in Table 2. In the assessment MgO.ss is treated as an ideal solution. Figure 2 shows the presently calculated $YO_{1.5}$–MgO phase diagram along with the experimental data [2–4]. The figure demonstrates that all the solubility data [4] are well reproduced by the present assessment. Thus the solubilities calculated by Kaufman [5] are improved by the present work. The presently calculated $YO_{1.5}$ liquidus agrees well with the liquidus of Tresvyatsky et al. [4] obtained using differential thermal analysis (DTA). The $YO_{1.5}$ liquidus computed by Kaufman [5] is in good agreement with the data [2, 3] obtained by optical pyrometry. In the absence of further data the $YO_{1.5}$ liquidus [4] measured by using DTA would be preferable. For the MgO liquidus the present evaluation also gives rise to better agreement with the experimental data [2–4]. Finally, the currently

TABLE 1

Summary of lattice stability parameters (joules per mole of cation; $T$ in Kelvin)

| | | | |
|---|---|---|---|
| ${}^{\circ}G^{l\text{-}YO_{1.5}}$ | 0.0 | ${}^{\circ}G^{l\text{-}MgO}$ | 0.0 |
| ${}^{\circ}G^{h\text{-}YO_{1.5}}$ | $-56735.0+20.920T$ | ${}^{\circ}G^{p\text{-}MgO}$ | $-77000.0+24.83871T$ |
| ${}^{\circ}G^{c\text{-}YO_{1.5}}$ | $-67419.3+25.105T$ | ${}^{\circ}G^{h\text{-}MgO}$ | $-21756.0+16.73600T$ |
| ${}^{\circ}G^{p\text{-}YO_{1.5}}$ | $31.380T$ | ${}^{\circ}G^{c\text{-}MgO}$ | $-26778.0+20.08400T$ |

l, liquid; p, periclase; h, hexagonal $YO_{1.5}$; c, cubic $YO_{1.5}$.
Values adjusted in the present work are underlined.

TABLE 2

Evaluated interaction parameters for various phases in the $YO_{1.5}$–MgO system (joules per mole of cation; $T$ in Kelvin)

| Phase | Reference state | | $^oL$ |
|---|---|---|---|
| | $YO_{1.5}$ | MgO | |
| Liquid | Liquid | Liquid | 4830.6 |
| Hss | h-$YO_{1.5}$ | h-MgO | 28521.6 |
| Yss | c-$YO_{1.5}$ | c-MgO | 28770.4 |

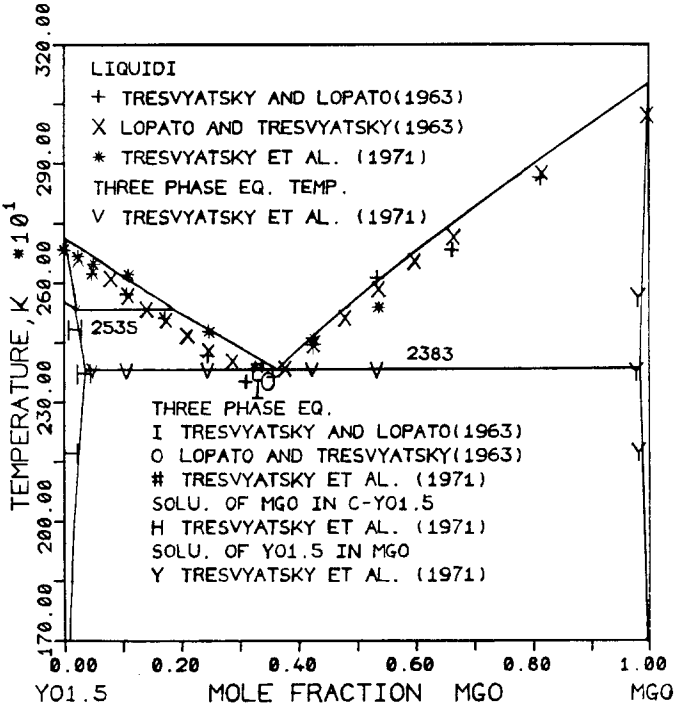


Fig. 2. Comparison of presently calculated phase diagram and experimental data.

calculated invariant equilibria agree with the experimental data [4] better than those of Kaufman [5]. In summary, the presently assessed parameters can describe the $YO_{1.5}$–MgO system better than those evaluated by Kaufman [5].

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