Calculation of Phase Equilibria in the Y203-Yb203-Zr02 System

Rare earth oxide stabilized zirconias have a wide range of applications—from solid electrolytes to thermal barrier coatings. An understanding of phase equilibria is essential for these applications. The Y_2O_3-ZrO_2 system is the most widely used, however stabilized zirconias with other rare earth oxides or combinations of these earth oxides may show improved properties, such as reduced thermal conductivity. There is a good deal of experimental information on the Y_2O_3-ZrO_2 system, but only limited information on the other systems.

In this study we do a Calphad-type thermodynamic assessment of the Y_2O_3-ZrO_2, Yb_2O_3-ZrO_2, and Y_2O_3-Yb_2O_3 psuedo-binary systems. The oxide units are treated as components and lattice stabilities are taken from the SGTE database and estimated where necessary. The solutions are modeled via the standard formalism:

$$G_m(x,T)=\sum_{i=1}^{2} x_i {}^{o}G_i(T)+RT\sum_{i=1}^{2} x_i \ln x_i + {}^{ex}G_m \qquad (1)$$

$${}^{ex}G_m = x_1 x_2 \sum_{j=0}^{n} {}^{j}L(x_1 - x_2)^j \qquad (2)$$

Here $G_m(T)$ is the Gibbs energy of each phase, x_i is the mole fraction, G_i is the Gibbs energy of each component, R is the gas constant, and T is the absolute temperature. The excess Gibbs energy is expressed as a Redlich Kister polynomial with parameters derived from experimental data. Standard computational thermodynamic codes were used*.

The experimental data for each psuedo-binary is reviewed. There is a good deal of excellent phase boundary data for the Y_2O_3-ZrO_2 system, but only limited thermodynamic data. There is only a small amount of phase boundary data for the Yb_2O_3-ZrO_2 system. Ideal solution behavior was assumed for the Y_2O_3-Yb_2O_3 system. The calculated psuedo-binary diagrams show good agreement with the experimental data. All known phase boundaries and invariant points are reproduced. Then the binaries are put together to form isothermal sections for the Y_2O_3-Yb_2O_3-ZrO_2 psuedo-ternary. Additional ternary interaction parameters are added and the basic features of the experimental ternaries are reproduced.

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