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Phase equilibria and thermodynamic evaluation of BaO-TiO_2-$YO_{1.5}$ system

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ABSTRACT：

A series of ceramic samples were prepared and characterized at 1400ºC in the BaO-TiO_2-$YO_{1.5}$ system. The obtained experimental results were adopted to the present thermodynamic evaluation to derive a set of thermodynamic database for the BaO-TiO_2-$YO_{1.5}$ system. The database was constructed by the CALPHAD method where the binary parameters from BaO-TiO_2 and TiO_2-$YO_{1.5}$ systems were re-optimized, those from the BaO-$YO_{1.5}$ system were simulated by our previous assessments. Thermodynamics descriptions of all liquid and terminal solid solution phases were treated by the substitutional solution model, the H-$BaTiO_3$ ($BaTiO_3$, hexagonal structure) and C-$BaTiO_3$ ($BaTiO_3$, cubic structure) were described by the compound energy formalism model, and other binary intermediate phases were treated as the stoichiometric compounds. Finally, some thermodynamic diagrams were calculated and compared with the experimental results. Good agreement between present calculations and