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Authors: Zhu Li, Jing Wang, Baotong Li, Shusen Wang, Ali Wajid, Shihua Wang, Xueguang Wang, Xionggang Lu, Chonghe Li, Kun Wang

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## ACCEPTED MANUSCRIPT

### Thermodynamic evaluation of the BaO-CaO-YO<sub>1.5</sub> system

Zhu Li<sup>a</sup>, Jing Wang<sup>a</sup>, Baotong Li<sup>a</sup>, Shusen Wang<sup>a</sup>, Ali Wajid<sup>a</sup>, Shihua Wang<sup>c</sup>, Xueguang Wang<sup>a</sup>, Xionggang Lu<sup>a,b</sup>, Chonghe Li<sup>a,b,\*</sup>, Kun Wang<sup>d,\*</sup>

<sup>a</sup> State Key Laboratory of Advanced Special Steel & Shanghai Key Laboratory of Advanced Ferrometallurgy & School of Materials Science and Engineering, Shanghai University, Shanghai 200072, China

<sup>b</sup> Shanghai Special Casting Engineering Technology Research Center, Shanghai 201605, China

<sup>c</sup> Shanghai University Library, Shanghai University, Shanghai, 200072, China

<sup>d</sup> Department of Chemical and Materials Engineering, University of Alberta, Edmonton, AB T6G
2V4, Canada

\*Corresponding author A: Chonghe Li; E-mail address: chli@staff.shu.edu.cn.

\*Corresponding author B: Kun Wang; E-mail address: akun22951@163.com.

#### **ABSTRACT:**

A series of experiments were performed to study the solid solubility of CaO in BaY<sub>2</sub>O<sub>4</sub>, and the observed results were then adopted to the present thermodynamic evaluation to derive a set of thermodynamic database for the BaO-CaO-YO<sub>1.5</sub> system. The database was constructed by the CALPHAD method where the binary parameters from the BaO-CaO and CaO-YO<sub>1.5</sub> systems were presently optimized, those from the BaO-YO<sub>1.5</sub> system were simulated by our previous assessments, and only limited amount of ternary parameters were introduced. All the model parameters were emanated from the Bragg-Williams approximation where the liquid and terminal solid-solution phases were treated by the one-sublattice model, and two ternary intermediate phases, named BCY (BaCa<sub>2</sub>Y<sub>6</sub>O<sub>12</sub>) and BaY<sub>2</sub>O<sub>4</sub>, were described by the three-sublattice and two-sublattice models, respectively. Good agreement between the experimental data and the calculated results demonstrates that the present thermodynamic database is self-consistent and credible and able to be used to design novel refractory.

**Keywords:** Refractory; Thermodynamic modeling; CALPHAD; BaO-CaO-YO<sub>1.5</sub>; Phase diagram

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