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# Predicting thermodynamic stability of crucible oxides in molten titanium alloys

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Titanium and its alloys interstitially dissolve a large amount of impurities, such as oxygen and nitrogen, which degrade the mechanical and physical properties of alloys. The possibilities of eliminating oxygen from titanium and its alloys are important for use in widespread applications. Refractory oxides i.e. oxides based on CaO, $ZrO_2$, $Y_2O_3$ and their spinels, can be used for melting titanium and its alloys. However, the thermodynamic behavior of calcium, zirconium, yttrium on the one side, and oxygen on the other side, in molten Ti and Ti-Al alloys have not been made clear. For that reason, the thermodynamic analysis in crucible oxide-titanium-aluminum system in accordance to determine the crucible oxide stability in molten titanium-aluminum alloys is very interesting for research.

The results of thermodynamic calculations for the most important crucible oxides in molten titanium-aluminum alloys are presented in this paper.

First, the activity-temperature-composition relationships of titanium and aluminium in Ti-Al at temperature range between 1273 K and 2273 K are estimated. Next, thermodynamic calculations of oxides are performed to determine their chemical activity as a function of temperature and composition in liquid Ti-Al. Using the activity of oxygen and the Gibbs free energy of formation of chosen crucible oxides the stability region of these oxides is mapped out as a function of temperature and composition. Finally, the stability of crucible oxides in Ti-Al is estimated using the Gibbs free energy data. All calculations in this paper are done using FactSage thermochemical software and databases.

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