



Contribution ID: 248

Type: Poster Presentation

Modelling the thermodynamic properties of TiCl_3 medium

The reduction of titanium tetrachloride (TiCl_4) with magnesium (Mg) results in the production of intermediates such as titanium trichloride (TiCl_3) and titanium dichloride (TiCl_2). Experimental work has been done to develop a continuous reduction process using TiCl_3 and TiCl_2 . However, more investigations still need to be done to understand these mediums and their interactions. In this study, we will be looking at two TiCl_3 polymorphs as a potential medium for titanium production. We employ the DL_POLY code to understand the effect of temperature on the TiCl_3 mediums with R-3 and P3112 space groups. It was noted from the Gibbs free energy that reactions in the R-3 medium are not favourable at 50 K – 2000 K. The results of this study give us more insight into the TiCl_3 medium as a potential medium for evaluating titanium.

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