HEAT OF FUSION OF REFRACTORY HCP METALS FROM FIRST-PRINCIPLE SIMULATIONS AND TROUTON′S RULE

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There is a well-known empirical systematic relation for the enthalpy of vaporization and boiling temperature proposed by F.T. Trouton and known as Trouton's rule. A similar relation is often used for the estimation of enthalpy of fusion of refractory metals in case of lack of accurate consistent experimental data. The closely packed metals with hcp and fcc lattice are generally considered to have a similar entropy of fusion [1, 2]. According to this suggestion an analysis of entropy of fusion of such refractory fcc metals as rhodium, platinum and iridium leads to estimations of enthalpy of fusion for refractory HCP metals rhenium and osmium of around 60.4 and 57.9 kJ/mol correspondingly. These thermal properties are currently provided by some handbooks, including the well-known CRC Handbook of Chemistry and Physics [3]. However, some experiments for rhenium based on the rapid pulse heating technique do not confirm the existing estimation and provide significantly lower values of heat of fusion of about 30 kJ/mol [4]. In this work we present direct calculations of heat of fusion of refractory hcp metals using first-principle method of quantum molecular dynamics. Our calculations do not confirm high values of heat of fusion of hcp refractory metals, predicted by the linear extrapolation of thermal data for refractory fcc metals, however are in good agreement with measurements by the pulse-heating method.

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