

化学

化学气相沉积法制备ZrC涂层的热力学分析

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摘要 ZrC涂层可能在新一代TRISO包覆颗粒上被用作阻挡裂变产物和承受主要载荷的关键层, 是先进高温气冷堆燃料元件研究的一个重要方向。文章利用HSC-CHEMISTRY 4.1软件分析化学气相沉积工艺参数对所制备的ZrC涂层的影响。分析结果表明, 在载气中加入足够的氢气对制备单一ZrC涂层很有必要。ZrCl₄的转化率随着沉积温度的升高而增加, 当温度过高时, 其影响不明显; 较佳的沉积温度范围为1 400~1 600 °C。随着反应物浓度的增加, 获得单一ZrC涂层对应的最低ZrCl₄与CH₄的摩尔分数比增加; 反应物摩尔分数的最佳范围可选为: 甲烷, 1.0%~2.0%; ZrCl₄, 为甲烷的1.5倍。

关键词 [ZrC](#); [化学气相沉积](#); [热力学分析](#)

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Thermodynamic Analysis of Chemical Vapor Deposition Process for ZrC Coating

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Abstract ZrC coating, which may be a key layer to prevent the diffusion of fission products and bear the load in the next-generation TRISO coated particles, is an important research field of the advanced fuel element for high temperature gas-cooled reactor. The influence of chemical vapor deposition process on the phase composition of ZrC coating was studied with HSC-CHEMISTRY 4.1 code. It is found that the addition of enough hydrogen into carrier gas is necessary to obtain pure ZrC coating. Deposition at higher temperature increases with the concentration of ZrC and decreases with the concentration of free carbon in ZrC coatings. Moreover, the conversion rate of ZrCl₄ is increased also. But the influence is not obvious at higher temperature. the optimal deposition temperature is 1 400-1 600 °C. The lowest concentration ratio of ZrCl₄ and CH₄ to obtain pure ZrC increases with the increase of the concentration of reactant. The reactant optimal concentration is 1.0%-2.0% for methane and more than 1.5 times of the concentration of methane for ZrCl₄.

Key words [ZrC](#) _ [chemical](#) [vapor](#) [deposition](#) _ [thermodynamics](#) [analysis](#)

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