

研究论文

## 欠电势沉积Bi-Te基体系热电材料的平衡热力学分析

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**摘要** 基于普通的能斯特方程, 建立了单原子层平衡电势的热力学模型. 据此, 分析了单原子层覆盖度以及电吸附价与欠电势之间的相互关系, 获得了沉积物与衬底之间干涉特性. 并且分析了Bi-Te基体系欠电势沉积热力学特性. 通过对Bi欠电势沉积在几个不同的金属衬底体系的分析阐明了功函数随覆盖度的变化机制. 研究了铋离子的浓度变化对铋的欠电势及覆盖度的影响关系, 结果表明, 铋在铂上欠电势沉积的体系在整个欠电势范围内具有恒定的电吸附价, 而铋在覆盖了一层碲的铂衬底上欠电势沉积的体系其电吸附价随覆盖度的增加而降低, 从热力学理论角度对铋在碲覆盖的衬底上导致欠电势负移的特性给予了解释.

**关键词** [欠电势沉积](#) [热力学](#) [热电材料](#) [Bi-Te基体系](#)

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## Equilibrium Thermodynamics Analysis of Underpotential Deposition of Bi-Te Substrate System Thermoelectric Material

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**Abstract** Based on the general Nernst equation, thermodynamics model of the submonolayer equilibrium potential was set up. Both the underpotential-coverage and the underpotential-electrosorption valency relationships were analyzed, and the interactional properties between the deposit and substrate were obtained. By mean of the theoretical model, the thermodynamic properties of underpotential deposition of Bi-Te compound were obtained. The mechanism of variation of work function with UPD coverage was elucidated *via* analyzing the system of Bi UPD on several different substrates. The coverage and underpotential of UPD Bi as a function of Bi ion concentration were studied. The results show that the electrosorption valency remains invariant over all underpotential range for Bi UPD in Pt system. However, for Bi UPD in Te-covered Pt system, the electrosorption valency decreases with increasing the Bi coverage. These features will be helpful to explain theoretically the negative shift of Bi UPD on Te-covered substrate.

**Key words** [Underpotential deposition](#) [Thermodynamics](#) [Thermoelectric materials](#) [Bi-Te substrate system](#)

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