Contribution ID: **32** Type: 口头报告

钇及钇基合金氢化过程中的相转变机制及热力学性质的第一性原理研究

摘要

氢化钇（YHx）因其优异的中子慢化能力和热稳定性，在高温反应堆中具有广阔的应用前景。然而，金属氢化物固有的脆性，以及金属吸氢过程中因氢致相变引发的开裂，使得无裂纹氢化钇的制备面临挑战。微合金化是缓解氢致开裂的有效手段。本研究采用第一性原理计算方法，系统研究了钇基合金中的氢扩散行为、氢致相变及压力-组分-温度（PCT）曲线。结果表明，微合金化提高了氢在钇基合金中的扩散系数，而低浓度掺杂不会阻碍 YHx 沿 {0001}HCP/{111}FCC 路径发生的相结构转变；同时，本研究基于纯计算方法准确描述了钇及钇基合金的 PCT 曲线。

关键词

氢化钇；第一性原理计算；扩散；相变；PCT

Abstract

Yttrium hydride (YHx) exhibits excellent neutron moderating capability and thermal stability, giving it broad application prospects in high-temperature reactors. However, the inherent brittleness of metal hydrides, along with cracking induced by hydrogen-induced phase transformation during the hydrogen absorption process, poses challenges to the fabrication of crack-free yttrium hydride. Microalloying is an effective approach to mitigate hydrogen-induced cracking. In this study, first-principles calculations were employed to systematically investigate hydrogen diffusion behavior, hydrogen-induced phase transformation, and pressure–composition–temperature (PCT) curves in yttrium-based alloys. The results show that microalloying increases the diffusion coefficient of hydrogen in the yttrium-based alloy, while low-concentration doping does not hinder the phase transformation of YHx along the {0001}HCP/{111}FCC path. Moreover, this study accurately describes the PCT curves of yttrium and yttrium-based alloys using a purely computational approach.

Keywords

Yttrium hydride; first-principles calculations; diffusion; phase transformation; PCT

Author: 楠, 周 (四川大学物理学院)

Co-authors: Dr 展泽, 施 (四川大学物理学院); Mr 翔, 李 (四川大学物理学院); Prof. 逊祥, 胡 (四川大学物理学院); Dr 苛衣, 赵 (四川大学物理学院); Dr 国庆, 闫 (有色金属研究总院); Dr 贵洋, 黄 (四川大学物理学院); Mr 模超, 龚 (江西理工大学稀土学院)

Presenter: 楠, 周 (四川大学物理学院)

Session Classification: 核能科学与工程

Track Classification: 口头报告: 核能科学与工程