

论文题目 Pt、Re、Ta、W 在 Ni₃Al 稳定性的影响研究

成任务、B 为完成任务、C 为完成任务不好

摘 要

镍基高温合金是目前使用最多的、温度最高的一类高温合金，是发展先进航空发动机、航海汽轮机等的首选材料。通过加入不同的合金元素进行合金化，是提高镍基高温合金性能的重要方法。为了更加了解不同合金元素对镍基高温合金的影响，本文以 Ni_3Al 基合金为研究目标，通过研究 Pt 元素对 Re、Ta、W 在 Ni_3Al 相中择优占位的影响，来分析合金元素对 Ni_3Al 在性能上的影响。此文章通过应用基于密度泛函理论的第一性原理的计算方法。通过研究 Re、Ta、W 等不同合金元素在 Ni_3Al 基合金的超晶胞结构中的占位情况，通过态密度、电荷密度差、电荷布居数等电子结构分析原子间的成键情况，通过体系能量的变化来分析合金的强度及稳定性，从而得到不同元素占同一位置的情况。通过以上的计算及分析，为日后 Ni_3Al 基合金的发展提供理论经验,为 Ni_3Al 基合金的发展打下一定的基础。

关键词：镍基高温合金；第一性原理方法； Ni_3Al ；择优占位

Abstract

Nickel-based superalloys are the most used superalloys at present and the highest temperature, and are the preferred materials for the development of advanced aero-engines and marine steam turbines. Alloying by adding different alloying elements is an important method to improve the properties of nickel-based superalloy. to better understand the effect of different alloy elements on nickel-based superalloys, In this paper, Ni₃Al-based alloy was taken as the research target, and the influence of Pt element on the selective occupying of Re, Ta and W in Ni₃Al phase was studied to analyze the influence of alloy element on the performance of Ni₃Al. In this paper, a first-principles calculation method based on density functional theory is applied. By studying the occupation of different alloy elements in Ni₃Al supercell structure, the bonding between atoms is analyzed by electronic structures such as density of states, charge density difference, charge population, etc. the strength and stability of the alloy are analyzed by the change of system energy, so that the situation of different elements in the same position is obtained. Through the above calculation and analysis, it provides theoretical experience for the development of Ni₃Al base alloys in the future, and lays a certain foundation for the development of Ni₃Al base alloys.

Keywords: Nickel-based superalloy; First principle method; Ni₃Al; preferred occupancy

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