

学校编码: 10384

密级\_\_\_\_\_

学号: 19120051403049

# 厦 门 大 学

## 博 士 学 位 论 文

### 部分铁基合金系相图的热力学数据库的建立及其在非晶态合金设计中的应用

#### Development of Thermodynamic Database of some Fe-based Alloy Systems and Its Application in the Design of Amorphous Alloys

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论文提交日期: 2 0 0 9 年 8 月

论文答辩日期: 2 0 0 9 年 9 月

2009年8月

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## 摘要

由于铁基非晶态合金具有高饱和磁感应强度、高导磁和低损耗等优异磁学性能，而成为非晶态合金研究领域的一个热点。目前，大部分非晶态合金材料的制备研究主要采用“炒菜法”，但这会浪费大量的人力、物力，并且研发效率低、研发周期长。相图计算在材料的研究设计方面具有重要的指导作用，并且成为研究比较活跃的领域之一。铁基合金热力学数据库的建立将为铁基非晶态合金的设计和开发提供有效的指导作用。

在本研究中主要针对部分铁基合金（Fe-B-C-Mo-Cr-W-RE-Ag）体系进行展开研究，利用相图计算的方法，对 Fe-B-C-Mo-Cr-W-RE-Ag 体系中的部分二元系进行热力学优化，初步建立 Fe-B-C-Mo-Cr-W-RE-Ag 系合金相图的热力学数据库，并探讨相图计算在铁基非晶态合金材料设计中的应用。本研究的主要内容如下：

(1) 系统地收集和整理现有的相图实验数据和热力学信息，采用合理的热力学模型，利用CALPHAD（相图计算）方法，对Ag-X (X: Gd, Ho, Nd, Sc, Sm, Tb, Y, Er), B-X (X: Er, Sc, Tm), Er-X (X: Sc, Y), Sc-X (X: Th, Y), Mo-X (X: Sc, Y), Cr-X (X: Er, Sc, Y, Gd, Dy, Ho), W-X (X: Er, Sc, Y, Nd, Gd, Dy, Tb, Ho, Lu, Tm) 各二元系相图进行热力学优化，计算结果与实验结果取得了很好的一致性，初步建立Fe-B-C-Mo-Cr-W-RE-Ag系合金相图的热力学数据库。

(2) 利用初步建立的 Fe-B-C-Mo-Cr-W-RE-Ag 系合金相图的热力学数据库，运用 CALPHAD 方法，计算了 Fe-B-Er 三元系、Fe-B-Sc 三元系、Fe-Cr-Mo-C-B 五元系、Fe-Cr-Mo-C-B-W 六元系和 Fe-Cr-Mo-C-B-Gd 六元系的液相面，确定低熔点共晶反应的成分和温度，实现对非晶态合金成分的设计。在此基础上，利用急冷设备在不同冷速条件下制备合金薄带，并对合金薄带进行 X-ray 衍射分析，确定合金薄带的结构类型。

(3) 在 Fe-B-X (X: Co, Ni, Mn, Al, Mo, W) 三元系富铁侧选取不同的合金成分，利用急冷设备制备合金薄带，并对合金薄带进行 X-ray 衍射分析，进而确定富铁侧非晶形成的成分范围，为 Fe-B 基非晶合金的制备提供了理论依据。

本研究优化获得的热力学参数, 将作为铁基合金相图热力学数据库的部分内容, 同时为铁基非晶态合金的设计提供重要的理论依据。

**关键词:** CALPHAD 非晶态合金 热力学 铁基合金

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## Abstract

Fe-based amorphous alloys are being paid much attention due to its excellent magnetic properties and considered to be a hotspot in the field of amorphous alloys. At present, most of amorphous alloys are usually obtained by the method of “try and error”, which squanders manpower and material resources. CALPHAD (CALCulation of Phase Diagrams) method, which is a powerful tool to cut down on cost and time during development of materials, plays an important role in materials design. Development of Fe-based thermodynamic database will provide an effective guideline for design and preparation of Fe-based amorphous alloys.

In the present work, most of binary systems in the Fe-B-C-Mo-Cr-W-RE-Ag multicomponent systems were thermodynamically assessed by using CALPHAD method, and thermodynamic database of Fe-B-C-Mo-Cr-W-RE-Ag systems was basically developed. The details of the results are described as follows:

(1) The phase diagrams of the Ag-X (X: Gd, Ho, Nd, Sc, Sm, Tb, Y, Er), B-X (X: Er, Sc, Tm), Er-X (X: Sc, Y), Sc-X (X: Th, Y), Mo-X (X: Sc, Y), Cr-X (X: Er, Sc, Y, Gd, Dy, Ho), W-X (X: Er, Sc, Y, Nd, Gd, Dy, Tb, Ho, Lu, Tm) binary systems have been thermodynamically optimized based on the available experimental data. A set of self-consistent and reasonable thermodynamic parameters was obtained for each binary system, which describes the Gibbs energies of the solution phases and the intermediate phases. And thermodynamic database of Fe-B-C-Mo-Cr-W-RE-Ag systems was primarily developed.

(2) Liquidus projection of the Fe-B-Er, Fe-B-Sc, Fe-Cr-Mo-C-B, Fe-Cr-Mo-C-B-W and Fe-Cr-Mo-C-B-Gd systems are calculated by CALPHAD methods. The compositions of eutectic reactions in the Fe-rich part of the multicomponent system were optimized and the thin ribbon alloys were made by liquid quench technique. X-ray technique was carried out to determine the crystal structure of these alloy samples.

(3) Many compositions in the Fe-rich part in Fe-B-X (X: Co, Ni, Mn, Mo, W,

Al) ternary systems were optimized and the thin ribbon alloys were made by liquid quench technique. X-ray technique was carried out to determine the crystal structure of these alloy samples. Glass formation region in the Fe-rich part in Fe-B-X (X: Co, Ni, Mn, Mo, W, Al) ternary system was determined, which can provide theoretical guidance on preparation for Fe-B base amorphous alloys.

The obtained results in this work can be applied to establish the thermodynamic database of Fe-based alloys system. In addition, the results in this work can provide important theoretical guidance on designing Fe-based amorphous alloys.

**Keywords:** CALPHAD; Amorphous alloys; Thermodynamics; Fe-based alloys



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