Isothermal section of the Mg-Mn-Nd System at 450°C: *Experimental Investigation and Thermodynamic Modeling*

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Abstract

The isothermal section of the Mg-Mn-Nd ternary diagram at 450°C was constructed by means of experimental investigation and thermodynamic modeling. Key samples designed to cover the whole system compositions were annealed and analyzed. ICP, XRD, DSC, and SEM/EPMA experiments were applied to reveal the phase equilibria of the annealed samples. Moreover, diffusion couples were designed to present the phase relationships in the system. The composition profile of the diffusion layers was measured using EPMA line scan. Mn-Nd and Mg-Nd binaries were reinvestigated experimentally to overcome the shortcomings that pointed out in the literature. Besides, the system was optimized using CALPHAD methodology in the FactSage software package. The initial ternary model was extrapolated from the databases of its boundary binary systems. Modified quasi-chemical model was used to describe the liquid phases, sublattice model for the intermediate binary and ternary solid solubilities, and BW for terminal solid solubilities. First principle calculations were applied to calculate the heat of formation of the system compounds. The thermodynamic model agrees well with the experimental results.

Introduction

Mg-based alloys are being promising engineering materials for the automotive and aerospace industries, since, they combine the light weight and high specific strength characteristics. In recent development of Mg-based alloys, Mn and Nd are added to increase the mechanical performance at elevated temperatures by forming high stability phases.

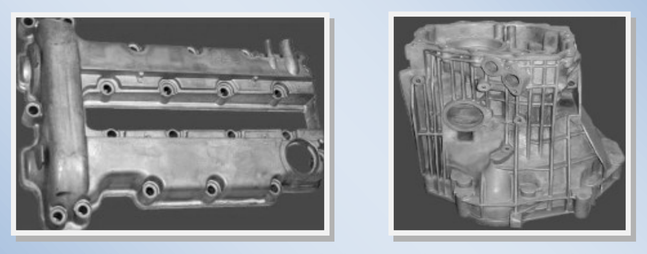


Figure 1: Cam cover and transmission housing made of AZ91D [1]

As part of the MagNET project, attempts are being made to develop a comprehensive database for the Mg-{Mn, Zn}-{Ce, Nd} systems using both thermodynamic modeling and experimental investigations.

Motivation

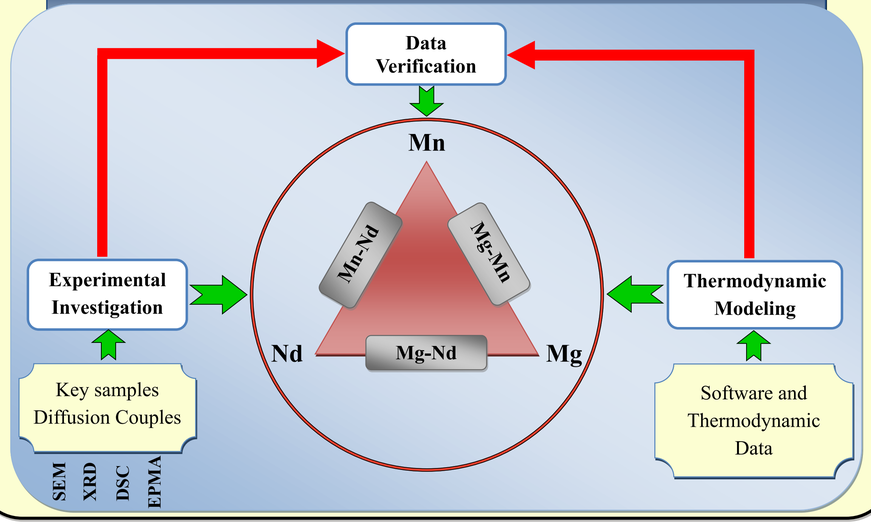
Limited experimental data on the Mg-Mn-Nd ternary diagram was found in the literature. The only covered part was the solubility ranges of Mn and Nd in Mg at 570°, 600°, and 630°C [2].

Many discrepancies regarding the constituent binary systems were reported. Among these discrepancies, three different versions of Mn-Nd phase diagrams were established, and the most recent one was partially covered from 10-85 at.%Mn. Besides, the terminal solid solubility of Nd in Mg of the Mg-Nd system was not revealed. As well as, the intermediate solubilities of MgNd and Mg_3Nd were not resolved.

Objectives

In this work, an experimental investigation coupled with thermodynamic modeling were performed to provide better understanding on the phase relationships of Mg-Mn-Nd ternary system. Diffusion couples techniques were designed to measure the diffusion coefficients of the system binary and ternary compounds.

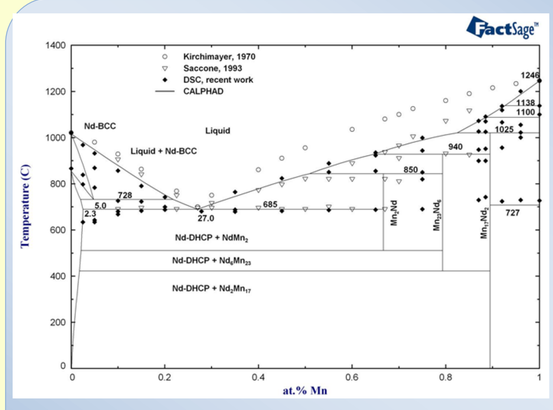
Methodology



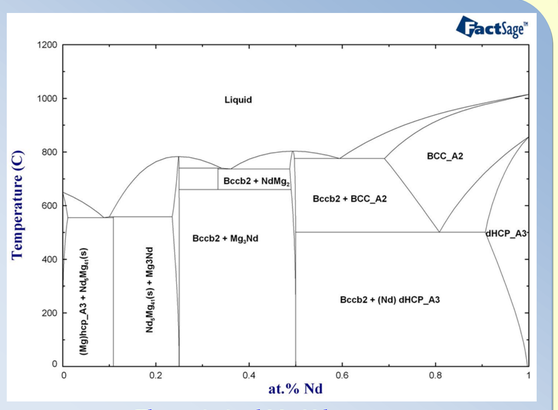
Experimental Procedure and Thermodynamic Modeling

- The alloys were prepared initially from pure metals (99.98% Mg, 99.90% Mn, and 99.95%Nd).
- The samples were prepared in an electrical arc-melting furnace with water-cooled copper crucible under argon.
- ICP was used to check the chemical composition.
- XRD was used to identify the phases, and to find the relative amount of each phase.
- EPMA to identify the phases composition.
- DSC for the phase transformation temperatures.
- The Mn-Nd system was reoptimized according to the new experimental findings.
- First principle calculations were used to compute the heat of formation of the system compounds.
- The ternary model was extrapolated from the models of its constituent binary systems.
- QCM was used to describe the liquid phase, sublattice model for the intermediate solid solubilities of the binary and ternary compounds, and BW for the terminal solid solutions.

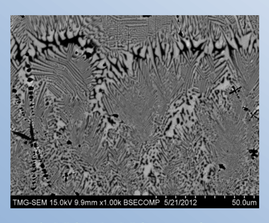
Investigated binaries



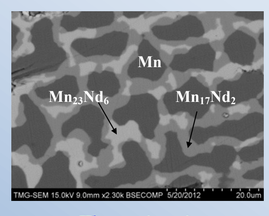
The complete Mn-Nd phase diagram consructed based on experimental investigation and thermodynamic modeling



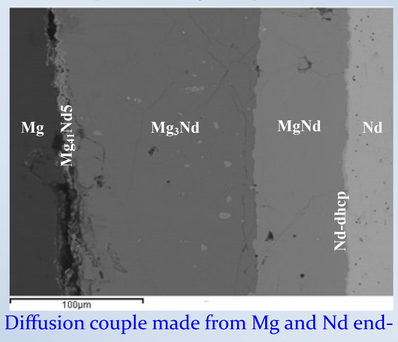
The optimized Mg-Nd system



A-Nd-Mn_2Nd eutectic at 27at.% Mn.

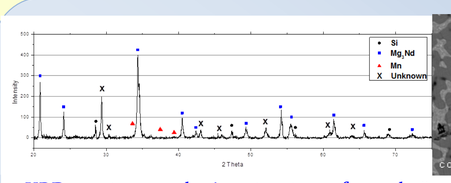


The peritectic microstructure of $Mn_{17}Nd_2$

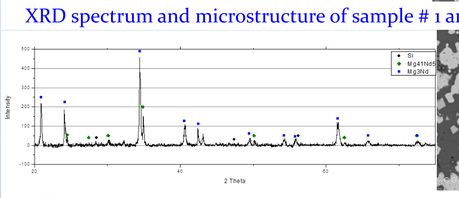


Diffusion couple made from Mg and Nd end-members annealed at 450°C for 17 days

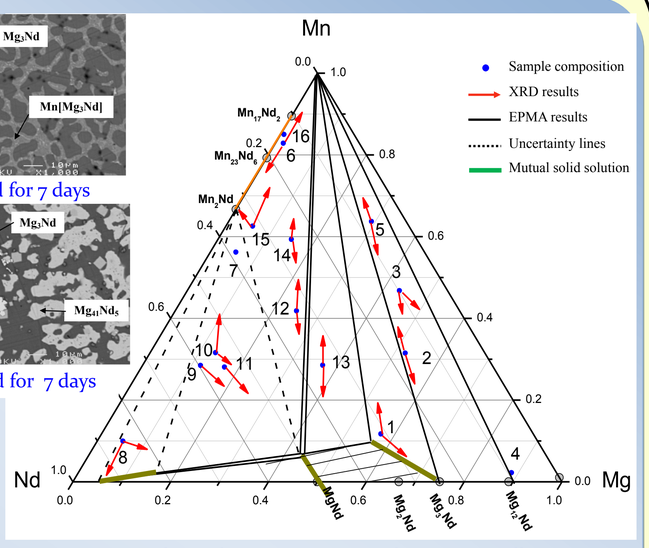
Mg-Mn-Nd isothermal Section at 450°C



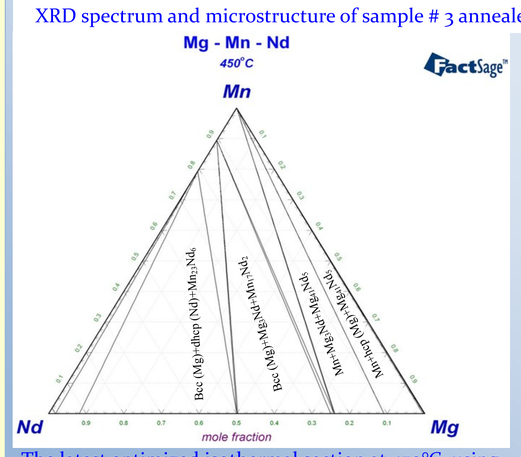
XRD spectrum and microstructure of sample # 1 annealed for 7 days



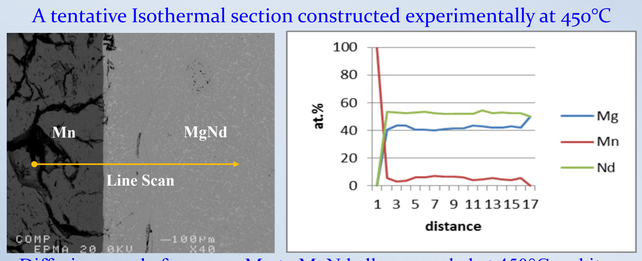
XRD spectrum and microstructure of sample # 3 annealed for 7 days



A tentative Isothermal section constructed experimentally at 450°C



The latest optimized isothermal section at 450°C using FactSage software



Diffusion couple from pure Mn to MgNd alloy annealed at 450°C and its composition profile

Conclusions

- The Mn-Nd phase diagram was completely constructed by experimental investigation and thermodynamic modeled. The heats of formation of the Mn-Nd binary system, computed by the first principle calculations, are in good agreement with the values obtained by CALPHAD.
- Diffusion couple from Mg to Nd end-members was prepared to reveal the phase equilibria in the binary system.
- The isothermal section of Mg-Mn-Nd system at 450°C was constructed experimentally based on XRD, EPMA, and metallography studies.
- The thermodynamic model of the ternary system was not completed, since some regions in the system were not resolved experimentally yet.

Acknowledgments

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NSERC CRSNG

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