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The Mg-Cu-Ni-Y quaternary system: thermodynamic modeling coupled with key experiments

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Mg based alloys provide a promising candidate for bulk metallic glass which has high mechanical strength and good corrosion resistance. Among these alloys, the Mg-Cu-Y system has the largest super-cooled liquid region. Also, the Mg-Ni-Y system has been found to be a potential candidate for the Ni-Metal hydride batteries. These batteries are supposed to replace the existing Ni/Cd rechargeable batteries due to environment concerns. Hence, a sound description of the Mg-Cu-Ni-Y quaternary system is essential. A thorough review and critical evaluation of phase equilibria and thermodynamic data of the phases in the Mg-Cu-Y, Mg-Ni-Y, Mg-Cu-Ni and Cu-Ni-Y and their constituent binary systems have been performed over the entire composition range from room temperature to above the liquidus. These systems are being modeled for the first time using the modified quasichemical model for the liquid phase to account for the presence of the short-range ordering properly. The Gibbs energies of the different phases have been modeled, and the optimal model parameters that reproduce all the experimental data simultaneously within experimental error limits have been obtained. Diffusion couples and key alloys are used to verify the calculated ternary systems. The alloys for diffusion couples and key experiments were prepared from pure metals (Mg-99.8 wt.%, Ni-99.9 wt.%, Cu-99 wt.%, Y wt.99.9%). Some of the samples have also been prepared using arc melting or induction melting furnaces. New ternary phases have been observed and their crystallographic data and homogeneity ranges have been identified using SEM/EPMA and XRD. Also, DSC has been used to determine the melting temperature of the key alloys. The calculated phase diagrams are compared with the current experimental results.

Key words: Diffusion couples, key alloys, XRD, EPMA, SEM, DSC.