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Thermodynamic Assessment of the In-Ni-Sb System and Predictions for Thermally Stable Contacts to InSb

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Thermodynamic assessment of the In-Ni-Sb ternary system has been performed using the CALPHAD technique. The phases $\zeta(Ni_2In)$ and $\zeta(NiSb)$ with the same B8-type structure in the subbinary systems are modified using the same three-sublattice model: $(Ni,Va)_{1/3}(Ni,Va)_{1/3}(Ni,X)_{1/3}$ (X = In, Sb), in order to give the continuous solid solution phase ζ in the In-Ni-Sb ternary system a better description. This modification is also made to the Gibbs free energy expression of the InSb phase. The parameters of the thermodynamic descriptions of the In-Ni-Sb ternary system are optimized on the basis of the three modified subbinary systems. A set of self-consistent thermodynamic parameters of the In-Ni-Sb system is obtained according to five isothermal sections and three vertical sections. Most of the experimental data can be satisfactorily reproduced by the present parameters. The liquidus projection and the invariant reactions are also presented. By simply considering the standards of melting temperature and thermodynamic stability, part of the ζ-phase is more suitable as a contact material to InSb semiconductor.

Key words: In-Ni-Sb, phase diagram, CALPHAD, thermodynamic assessment, contacts to InSb

INTRODUCTION

There has been considerable interest in the narrow-bandgap semiconductor InSb due to its high electron mobility, which makes it a promising material for many electronic and optoelectronic applications, such as infrared sources, laser diodes, high-efficiency photodetectors, and quantum devices.[1–4] Despite all these applications, ohmic contacts to InSb have not yet been investigated in detail compared with the more traditional material GaAs. Design of contacts with low contact resistance, good thermal stability, and good adhesion is challenging. Since most of the commonly used ohmic contacts to GaAs and other III–V semiconductors contain either Ni or Pd as one of their major components,[5–7] study of the In-Ni-Sb system is helpful for development of new and improved InSb contact materials. Contacts are usually formed by metallization of the semiconductor surface and subsequent heat treatment. They have to be carefully designed to avoid undesirable problems during the annealing step, for example, formation of a liquid phase and intermediate phases due to reactions of metal layers with the semiconductor surface at elevated temperatures. Hence, knowledge of the thermodynamics and phase diagrams of the In-Ni-Sb ternary system is essential to understand the mechanisms of such reactions during metallization and further heat treatment of InSb semiconductor devices.[8–11]

In this work, the In-Ni-Sb ternary system is thermodynamically assessed using the CALPHAD technique on the basis of the available experimental data. A set of self-consistent parameters for calculation of the phase equilibria and the thermochemical properties of the system are provided. According to our calculations, predictions for thermally stable contacts to InSb are also presented.

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