Phase Equilibria in the Transition Metal-Ga-Sb Systems

S. E. Mohney and Wayne Liu
Department of Materials Science and Engineering
109 Steidle Building
The Pennsylvania State University
University Park, PA 16802
mohney@ems.psu.edu

Electrical contacts to the 6.1 Å family of semiconductors will be required for many new devices currently under development. As part of a program to develop contacts to these semiconductors, we have performed thermodynamic calculations to estimate ternary phase diagrams for the transition metal-Ga-Sb systems. Similar phase diagrams have been a valuable tool in the development of contacts to other III-V semiconductors. The diagrams have been used to identify candidates for shallow and/or thermally stable contacts as well as for designing alloyed contacts with engineered electrical performance. Unfortunately, such information is lacking for the majority of the metal-III-Sb systems. For the Metal-Ga-Sb systems, experimental studies of the phase equilibria have been reported only for Ni, Pd, Pt, and Au.

We will present the results of our estimates of the phase equilibria in the transition metal-Ga-Sb systems where no diagrams were previously available, describing the necessary approximations we have made in the calculations. We then categorize the phase diagrams according to the dominant features in their tie-line configurations to highlight trends in the contact metallurgy across the periodic table. For comparison, we have also applied the same method for estimating phase diagrams to the Ni-, Pd-, Pt-, and Au-Ga-Sb systems. Excellent agreement was found between the types of tie-line configurations predicted and reported from experiments, although minor discrepancies in some of the tie-lines were observed in two systems. According to our calculations, W, Re, and Os are the only transition metals anticipated to be in thermodynamic equilibrium with GaSb under the conditions considered in our calculations. We are currently using the phase diagrams we calculated together with information on other metal-III-V systems in our work on contacts to alloy semiconductors that contain GaSb.