Abstract submitted to the
NATO ADVANCED RESEARCH WORKSHOP
New materials for thermoelectric applications: theory and experiment
September 19 - 25, 2011 Hvar, Croatia

The Ternary Systems Ba-Au-Ge and Ba-Au-Si: Phase Equilibria, Crystal Structures and Physical Properties

I. Zeiringer[1], A. Grytsiv[1], P. Rogl[1], E. Bauer[2], H. Effenberger[3]

[1] *Institute of Physical Chemistry, University of Vienna, Waehringerstrasse 42, A-1090 Wien, Austria*

[2] *Institute of Solid State Physics, TU Vienna, Wiedner Hauptstrasse 8-10, A-1040 Wien, Austria*

[3] *Institute of Mineralogy and Crystallography, University of Vienna, Althanstr. 14, A-1090 Wien, Austria*

Submitted : 08-09-2011

Keywords : Clathrate, Ternary system, Physical property

Formation and homogeneity ranges of the ternary clathrates of type-I, $Ba_8T_xGe_{46-x-y}\square_y$ and $Ba_8T_xSi_{46-x}$ (T = Au and $\square$ is a vacancy; space group Pm-3n) at 800°C and phase relations concerning this region have been investigated. For both ternary systems, Ba-Au-Ge und Ba-Au-Si, partial isothermal sections have been derived at 800°C for the region of 0 to 33 at.% Ba. For characterization of the clathrates and other ternary compounds existing at 800°C, X-ray powder diffraction, electron probe microanalysis (EPMA) and X-ray single crystal diffraction were used. Thermoelectric properties (thermopower, electrical resistivity and thermal conductivity) have been measured for clathrate compositions $Ba_8Au_{5.1}Si_{40.9}$ and $Ba_8Au_6Ge_{40}$ between 4.2 and 900 K from which a thermoelectric figure of merit has been evaluated. These studies evidenced the closeness of the systems to a metal to isolator transition. The phase equlilibria at 800°C are characterized by several new ternary phases in the investigated region up to 33 at.% barium. The homogeneity ranges have been established for $Ba(Au_{1-x}Si_x)_2$ and $Ba(Au_{1-x}Ge_x)_2$ (AlB_2-type) and also for $BaAu_{2+x}Si_{2-x}$ and $BaAu_{1+x}Ge_{3-x}$ ($BaNiSn_3$-type, $Ce(Ni,Sb)_4$-type). The crystal structures of the other novel phases in the gold-rich part have also been determined from single crystal X-ray data: $BaAu_3Si$ and $BaAu_3Ge$ (own type, tP a=0.6459(2), c=0.5487(2) nm), $BaAu_{5+x}Si_{2-x}$ (x = 0, own structure type, space group Pnma, a=0.8981(2), b=0.7106(2) and c=1.0363(2) nm) and $BaAu_{5+x}Ge_{2-x}$, the latter revealing with increasing gold content a closely related derivative structure type (x = 0.3).