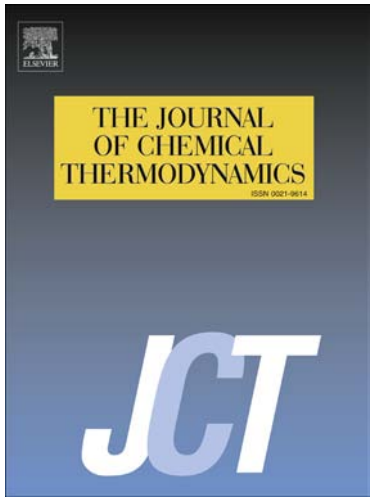

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Stability of the $D8_m$-Ti_5Sn_2Ga compound. Experimental determinations and first principle calculations.

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Abstract.

In this paper we discuss the formation of the ternary compound Ti_5Sn_2Ga (τ) with the $D8_m$ structure. Phase equilibria with participation of the τ-phase were studied experimentally, and partial solidus projection and isothermal section at 1300°C were plotted. At the solidus temperatures the ternary compound is in equilibria with two continuous solid solutions: (1) between Ti_2Sn and Ti_2Ga (named $Ti_2(Sn,Ga)$) and (2) between Ti_5Sn_3 and Ti_5Ga_4 (named $Ti_5(Sn,Ga)_{3-4}$). At 1300°C Ti_2Sn and Ti_2Ga do not form continuous solid solution, and the ternary compound participates in equilibria with $Ti_5(Sn,Ga)_{3-4}$, and Ti_2Sn, Ti_2Ga and Ti_3Sn based phases. The formation energy of the $D8_m$-Ti_5Sn_2Ga compound is calculated by using electronic density-functional theory (DFT) using pseudopotentials constructed by the projector augmented waves (PAW) method in the generalized gradient (GGA) approximation for the exchange and correlation energy. The calculated lattice parameters are in good agreement with the experimental values. According to the experiments and the *ab-initio* calculations, the $D8_m$-Ti_5Sn_2Ga compound is stable and possesses a domain of off-stoichiometry.

Keywords: D8m-(Ti_5Sn_2Ga), phase stability, ab-initio, ternary system