

Accepted Manuscript

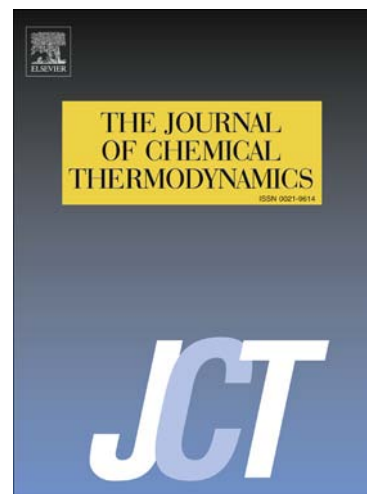
Stability of the $D8_m$ - Ti_5Sn_2Ga compound. Experimental determinations and first principle calculations

Iuliia Fartushna, Marina Bulanova, Catherine Colinet, Jean-Claude Tedenac

PII: S0021-9614(14)00114-1
DOI: <http://dx.doi.org/10.1016/j.jct.2014.04.008>
Reference: YJCHT 3909

To appear in: *J. Chem. Thermodynamics*

Received Date: 25 June 2013
Revised Date: 4 April 2014
Accepted Date: 11 April 2014



Please cite this article as: I. Fartushna, M. Bulanova, C. Colinet, J-C. Tedenac, Stability of the $D8_m$ - Ti_5Sn_2Ga compound. Experimental determinations and first principle calculations, *J. Chem. Thermodynamics* (2014), doi: <http://dx.doi.org/10.1016/j.jct.2014.04.008>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

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

Iuliia Fartushna^a; Marina Bulanova^a; Catherine Colinet^b; Jean-Claude Tedenac^{c*}

^a Frantsevich Institute for Problems of Materials Science of NASU, 3 Krzhynzhansky Str.,
03680 Kiev, Ukraine

^b Science et Ingénierie des Matériaux et Procédés, UMR 5266, CNRS – INP Grenoble - UJF,
BP 75, 38402 Saint Martin d'Hères Cedex

^c I.C.G., UMR-CNRS 5253, Université Montpellier II, Place E. Bataillon, 34095 Montpellier
Cedex 5, France

*** Corresponding author: Jean Claude Tedenac**

Tel.: +33467143342

Fax.: +33467144290

tedenac@univ-montp2.fr

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: $D8_m$ -(Ti_5Sn_2Ga), phase stability, *ab-initio*, ternary system

Download English Version:

<https://daneshyari.com/en/article/215385>

Download Persian Version:

<https://daneshyari.com/article/215385>

[Daneshyari.com](https://daneshyari.com)