Po62

Structural, Electronic, Elastic and Thermodynamic Properties of ReAuSn

Halima HAMADA*, Kadda AMARA, Friha KHALFAOUI; Fatiha SAADAUI, Samira HAMADA

Laboratoire physico-chimique Université Dr Moulay Tahar de Saida, Saida, Algerie

*Corresponding author

INTRODUCTION

Among Intermetallic phases, the compounds containing rare-earth atoms from numerous Class, well studied for many years in both fundamental and applied research. all known phases are binary or ternary compounds, with some general features [1]. The equiatomic intermetallic ReTX, where (Re) rare- earth element, T=transition metal and X= element of the 3 rd, 4th or 5th main group [2]. In this work, The electronic, structurasl properties of the Intermetallic ReAuSn (Re=Sc,Lu) have been calculated using the full potential l linearized Augmented plane wave (FP-LAPW) method within GGA and LDA approximation.

EXPERIMENTAL/THEORETICAL STUDY

Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method was used for the first-principles calculations within the density functional theory DFT [3-4]. using WIEN2K code [5]. We have investigated the structural, electronic, elastic and thermal properties of ReAuSn (Re=Sc,Lu). and the exchange-correlation energy was calculated using the approximation (GGA) (PBE) LDA and GGAPBsol for the calculation of structural properties. so that the electronic elastic thermal properties compute with GGA. In this calculation we have used 2000 K-point in the first Brillouin zone for the structural properties and 4000K-point for the electronic elastic properties. which marks the separation of valence and core states was chosen as –6 Ry.

RESULTS AND DISCUSSION

Table 1. The calculated values of the lattice parameter (A°), bulk modulus (GPa), and its pressure derivative of ReAuSn

compond		a (A°)	B	B’	Expt
ScAuSn	PBE	6.5187	90.0866	4.9687	6.4194
	PBEsol	6.4271	100.6010	5.0794	
	LDA	6.3672	111.1603	5.0124	
LuAuSn	PBE	6.6639	83.6716	4.8745	6.5652
	PBEsol	6.5618	95.7994	5.1533	
	LDA	6.4976	106.3989	5.0478	

DOI: 10.21467/abstracts.122 ISBN: 978-81-954993-3-5

Table 2:Calculated elastic constants C_{11}, C_{12}, and C_{44} (GPa); bulk modulus B (GPa); shear modulus G (GPa); Young's modulus E(GPa); Poisson's ratio v; for ReAuSn(Re=Sc,Lu):

Paramètres	ScAuSn	LuAuSn
C11	132.8858	129.5031
C12	69.3442	63.6711
C44	73.1487	66.5420
B(Gp)	90.524	85.615
G(Gpa)	52.345	50.164
E(Gpa)	131.658	125.902
v	0.257	0.254

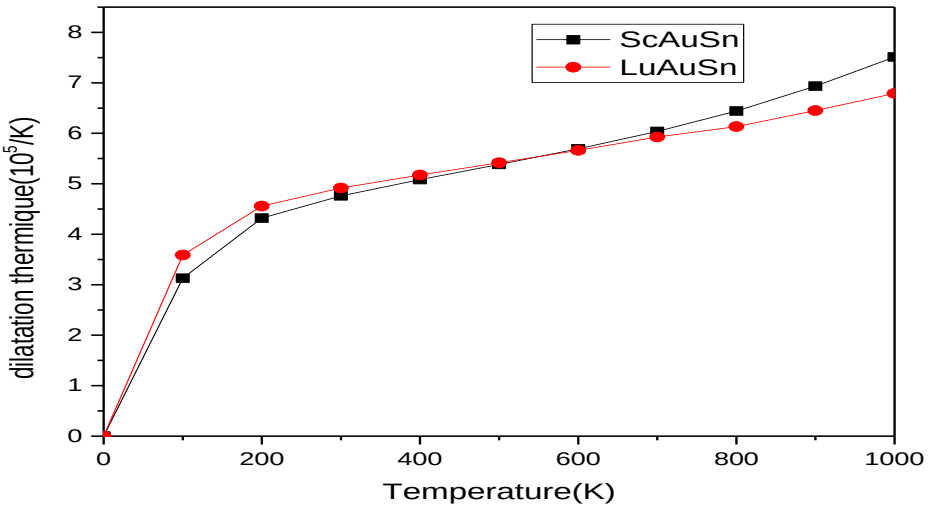

Fig1.Variation of the dilatation thermic en fonction de la temperatura at P=0

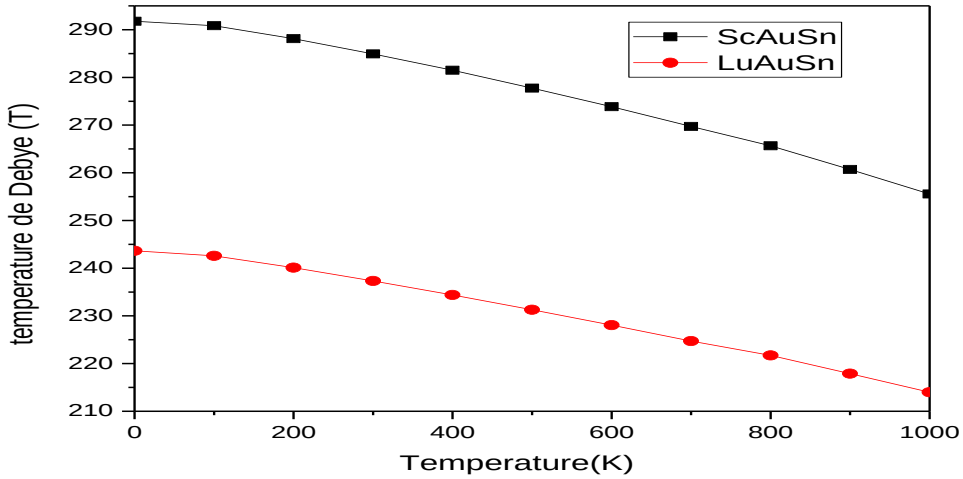

Fig 2 Variation of the Debye temperature as a function temperature at P=0 .

ISBN: 978-81-954993-3-5
DOI: 10.21467/abstracts.122
Series: AIJR Abstracts

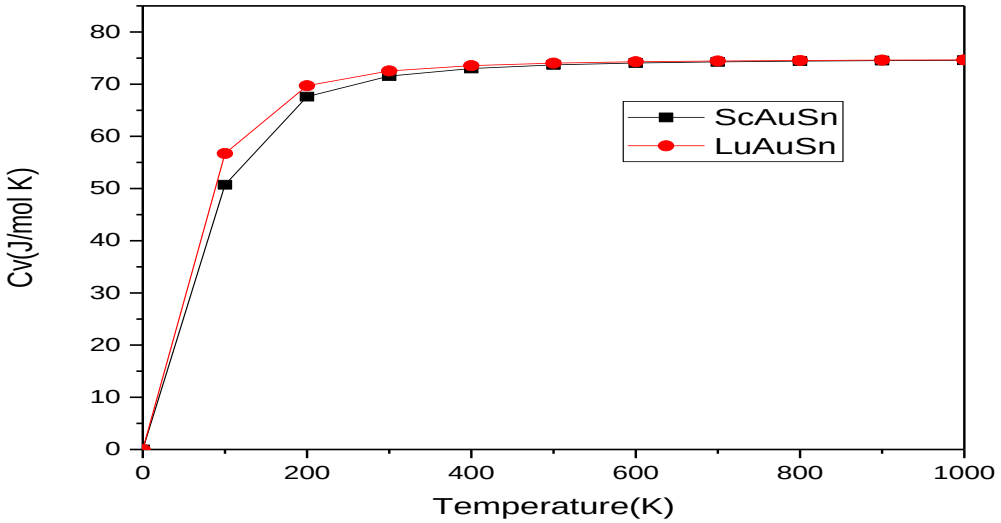

Fig 2 Variation of the CV as a function temperature at P=0

CONCLUSION

The structural, mechanical, electronic and thermal properties of ReAuSn (Re=Sc,Lu) ternaries are investigated using the FPLAPW method with PBE-GGA exchange correlation. The results reveal that ReAuSn (Re=Sc,Lu) is stable for (NM) configuration structure. According to the elastic properties results, we found that our material ReAuSn (Re=Sc,Lu) is mechanically stable. For the electronic properties, we have observed that have indirect gap**.**

ACKNOWLEDGMENTS

The authors acknowledge the Algerian Ministry of Higher Education and Scientific Research (MESRS)

REFERENCES

1. Sudhindra Rayaprol, C .peter Sebastian, Rainer PÖttgen, J of solid state chemistry 1979 (2006) 2014-2046.
2. P.Hohenberg and W.Kohn.phys .Rev.136(1964)B864 W.Kohn and L.JSham. phys .Rev 140(1965)A1133.
3. P. Hohenberg, W. Kohn, Density functional theory (DFT), Phys. Rev, 136 (1964) B864
4. W. Kohn, L.J. Sham, Self-consistent equations including exchange and correlation effects, Physical review, 140 (1965) A1133.
5. D. Kvasnicka, J. Luitz, wien2k, An augmented plane wave+ local orbitals program for calculating crystal properties, (2001).

ISBN: 978-81-954993-3-5
DOI: 10.21467/abstracts.122
Series: AIJR Abstracts