An Innovative Complex Quantum Advanced Material Regular Full Heussler : Au2LaB .

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Abstract

Heusler ‘s alloys , are investigated in a deep new varied , so exclusive study prediction based on Ab Initio first principle.In order to use them in so many advanced technology matter , we must identify their nature and determine after their several physic chemical characteristic proprieties like : structural , elastic, mechanic, acoustic, thermodynamic , magnetic, electronic ,dielectric, optical , nuclear . There is a new state matter definition : half metallic. Heussler s’ materials as nanostructures develop peculiar effects on their surfaces sits , so that a new types induced quasi particles appear created when interacting , as : Exciton , Phonon , Magnon , Plasmon , photons ,Polaron , ….Generally Heusler ‘s materials develop interesting applications in : spintronics , electronic advanced devices , optoelectronics , super conductivity , mechatronics , atomic mirrors and magnetic lenses , electrodynamics engines, energy efficiency, nanotechnologies , Radar wave guide antenna , optical fiber ,then so multiples academic scientific and industrial fields.

KeyWords :Solid State Physics , Heussler ‘s Materials , Quantum well, Transport Phenomena , Condensed Matter ,Thermo Dynamic functions ,DFT(LDA,GGA),Spin Polarization ,Spin-Orbit coupling ,Nanostructures.

Introduction

Let remind quoted different five types of Heussler’s materials , well identified in scientific literature , like :

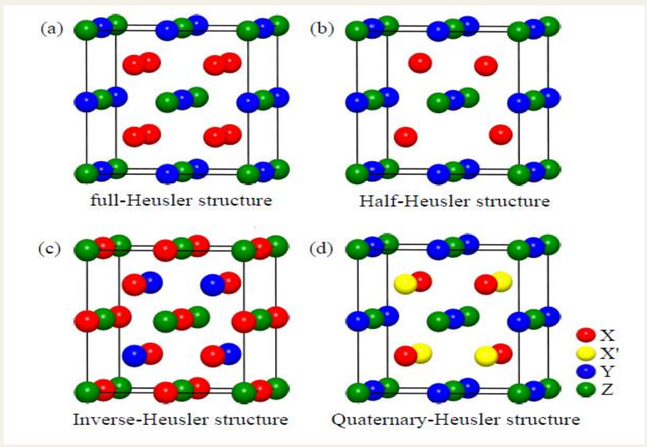


Fig . 1. Heussler ‘s material four types

The fiveth Heussler ‘s material type is : Tetragonal Distorted Heusler . Spherical radial Schrödinger‘s equation, allows for a potential interaction of quantum well with structural parameter and conditions work assumed, to determine solutions: Eigen modes. Schrödinger‘s linear stationary equation is resolved using DFT (Functional Density Theory) of State Energy ρ(E) with complementary tools : LDA , LSDA , (LSDA +L.S),GGA , (GGA+ S) , (GGA+ S+ L.S), for a crystal of two C.F.C parcels. Calculus are based on GGA tools, taking in account :spin(S) and spin–orbit coupling (L.S). A focused study is operated about X_2YZ Regular Full Heusler justified when: Z(Y) < Z(X) . Our investigation assume that atoms‘s Wyckoff geometric positions below, chemical concentrations influences more intensively the wondered researched properties :

4c : X(1)=Au (0.25 , 0.25 , 0.25) ; 4c : X(2) =Au (0.25 , 0.25, 0.25) ;

4b: Y= La (0.5, 05 , 0.5) ; 4a: Z=B (0. 0 , 0.0 , 0.0).

Table .1.Chemical data components of (Au2La B) alloy.

C : Component Concentration (%)	Z :Atomic Number	M : Molar Mass (g / mol)	Electro Negativity Index	Oxidation Numbers
B : 1.988735	5	10,811	2.0	3+
Au : 72.5582	79	196,96657	2.4	3+
La : 25.55231	57	138,9055	1.1	3+

Table .2.Electronic configuration components of (Au2LaB) alloy.

Component	Electronic configuration	Fusion Temperature (°C)	Boiling Temperature (° C)	Density ($g \cdot /cm^{-3}$)
B	$1s^2\ 2s^2\ \mathbf{2p^1}$	2 300	2550	2,46
Au	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^6\ \mathbf{6s^1}\ 4f^{14}\ \mathbf{5d^{10}}$	1064 .4	2940	19.32
La	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^6\ 6s^2\ \mathbf{5d^1}$	920	3454	6,16

Table .3.Electronic configuration components of (Au2LaB) alloy.

Alloy	Molar Mass (g / mol)	Equivalent Mass – Energy (Gev)	Density ($Kg \cdot /m^{-3}$)
(Au2LaB)	543.61228	50.96106909	44087.73004

Sustainable development encourage investigations research efforts to discover and produce new components indifferent fields : medicine, telecommunications , industries , astronomy, aviation ,….to offer a modern comfort life and strong continuous economy , actually and for future generations.

Methods

Equilibrium point stable state (E_0 , V_0) fitted data are ta ken in ideal conditions investigations for Heussler ‘s alloy. Seeking through iterations by Mind Lab Mstudio 5.0 code , for : structural , magnetic , electronic , dielectric ,optic , properties. Thermo dynamical functions depending on (T, P) conditions are given by Gibbs code. Elastic and mechanic coefficients obtained when applying a feeble positive variable strain: delta . First step is , begin by lattice parameter , calculated by optimizing total energy E (Ry) according to Murnanghan’s equation non linear fit Implemented in code Origin 5.0 . when external stationary fixed positive feeble mechanical strain (δ) ,is applied on variable compressed lattice parameters ,curve : E= f (δ^^2) assuming orthorhombic tensor for (C11 ,C12) and monoclinic Tensor for (C44) , shows different intervals slopes (positives ,negatives) ,that proof the instability. The elastic coefficients relatives to mechanical strain (δ) are not constants and not always positives .Characteristic mechanic parameters can not be deduced as recommended : Bulk modulus (B) , Shear modulus (G) ,Young modulus (E) , anisotropic elastic parameter (A) , Ratio ductility (B / G) , Debye temperature (θ-D), mean sound velocity , Poisson Ratio (γ) , Poisson ratio function :f (γ),In static ideal conditions , Gibbs code simulation gives parameters related to thermo elasticity like: γ = 0.25 ; f (γ)= 0.859949 ; B0 = 90. 85 (GPa) ; Debye quasi harmonic model temperature : θ-D= 267.30(K°) ; Grussein parameter = 1.802..

$$E\ (V) = \{E_0 + \frac{B_0}{B_0'(B_0'+1)} * [\ v * \left(\frac{v_0}{v}\right)^{B_0'} - v_0\ ] + \frac{B_0}{B_0'}(v - v_0)\}$$

$$B_0 = V.\frac{\partial^2 E(V)}{\partial V^2} \qquad B_0' = \frac{\partial B}{\partial P} \qquad a(p) = a_0[1 + P\ \left(\frac{B'}{B_0}\right)$$

Results

1.Structural parameters :

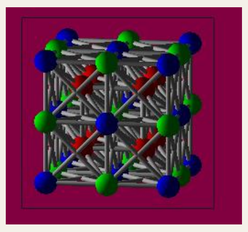


Fig.2.Cristal(Au2LaB).

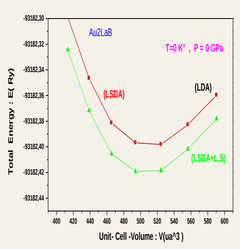


Fig .3.E= f (V)-LDA.

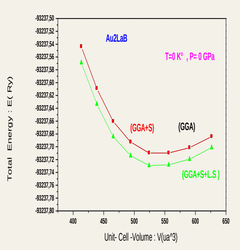


Fig4.E=f (V)-GGA.

Table.4. Equilibrium point parameters at ideal conditions :

Method	a0 (ua)	B0 (GPa)	V0 (ua)^^3	B ’	E 0 (Ry)
LDA	10.071371	116.154	510.782	3.3793	-93182.399
(LDA+S)	10.071326	116.154	510.775	3.3822	-93182.399
(LDA+S+L.S)	10.047085	116.448	507.096	3.8023	-93182.420.
GGA	10.3116121	93.6295	548.213	3.8660	-93237.711.
(GGA+S)	10.3337726	93.6587	545.383	3.7680	-93237.712.
(GGA+S+L.S)	10.3425443	92.0414	542.625	3.8690	-93237.730.

2.Thermodynamic parameters.

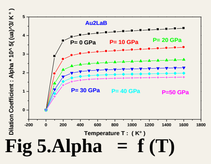


Fig 5.Alpha = f (T)

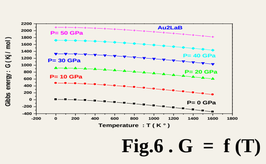


Fig.6 . G = f (T)

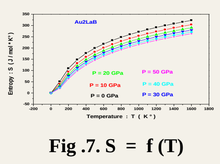


Fig .7. S = f (T)

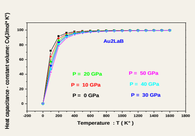


Fig.8 .Cv = f (T)

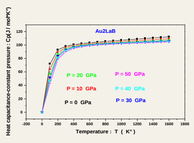


Fig .9.Cp = f (T)

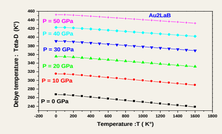


Fig .10.θ-Debye= f (T).

3.Electronic properties.

Au2LaB(GGA+S) : Fermi Energy Ef = 18.898198 (e V) .
Au2LaB(GGA+S+L.S) : Fermi Energy Ef = 18.9342 67 (eV).

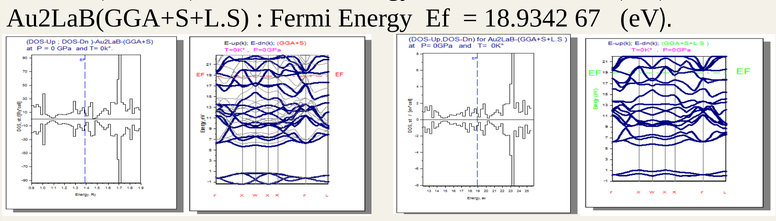
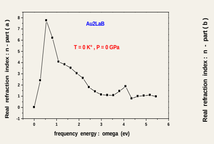


Fig.11.DOS ,Spin polarization (GGA+S) **Fig.12.DOS ,Spin polarization (GA+S+L.S)**

4.Optical properties.



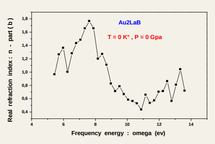


Fig.13.Real refraction part (a ,b)

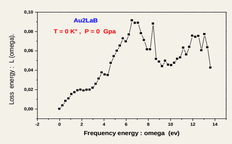
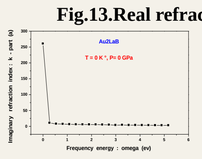


Fig.14 .Loss energy L(ω)



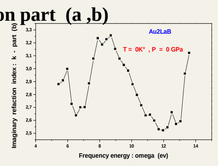


Fig.15.Imaginary refraction part (a , b)

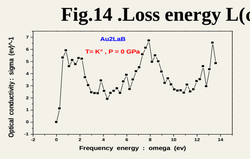


Fig .16. Conductivity σ(ω)

Reflectivity R (ω) : $R(\omega) = \frac{n + ik - 1}{n + k + 1} = 0$

Conclusion

A predicted New Regular Full Heusler (Au2LaB) identity is revealed , using FP-LMTO methods based on (DFT) tools, extended to LDA, then to GGA .Calculus take account of spin polarization (S) and spin-orbit coupling interaction (L.S) . Material (Au2LaB) is found a good thermal conductor according to calorific capacities values. It can be artificially elaborated as confirmed by entropy and free enthalpy .For sound wave, it will be a perfect transducer, or an acoustic fiber. When undergo others types of strains stationary linear perturbations , permits to understand mechanical instability relative to : crystallographic Bravais net work ? Range interval linear strain values ? Tensors categories? Time depending strain functions, especially sinusoidal case? We wonder if cubic structure and symmetry are exactly adapted and preserved ? Material (Au2LaB) may develop a possible Piezoelectric efects ? Pyroelectric ? Ferroelectric ? properties . Magnetic moment is too low ? So may be the material is paramagnetic after checking its magnetic susceptibility ? Boron concentration contributes to enhance: elastic, mechanic, magnetic properties. Optical complex properties are related to dielectric also complex functions, as responses to an external uniform electromagnetic field excitation , proof that : (Au2LaB) material is a crystal quantum well, where no reflective wave , only absorption-evanescence. Lanthanum concentration contribute to enhance: magnetic, pyroelectric and optical properties. Quantum effects must be more investigated in future, much precisely : Transport Phenomena, Phase Transition , Tunneling effects, Scatterings by RX or Neutrons . In the other side ,this alloy is a metallic electronic superconductor with increasing density of states and Fermi energy according to (P ,T) increasing . Parameters , properties are all related directly to atoms positions and chemical concentration. Many applications result from this materials as a super metal optoelectronic devices as its 100% spin polarization, dielectric - optical complex parameters , with no reflectivity, so 100% transmission, gives technical importunities in : Renewable energies process : energy storage , harvesting , efficiency , distribution , solar optic cones, solar photovoltaic cell ,microelectronic: transport polarized , support data storage, tunnelling spin junction ,Radars , antennas, captors, sensors , screens , probes .We suggest more research for temperature T (K°) > 1600 and pressure P (GPa) > 50.Quantum behaviour need to be more detailed on Beam-Matter interactions, even variations in components ‘s concentrations ‘s and changing atoms ‘s positions.

Literature Cited

[1]Parr, Robert G; Yang, Weitao (1994). Density-Functional Theory of Atoms and Molecules. Oxford: Oxford University Press.
[2] P . Chaquin Pratiques -Chimie Theorique methodes DFT.
[3] Savrasov .S , Savrasov .D .Full potential linear Muffin-Tin in orbital method for calculating total energy and forces. Phys .Rev.B.46.121816-12195. 1992.
[4]Savrasov.S . Y. Linear response theory and lattice dynamics : a Muffin-Tin orbital approach . Phys .Rev.B.16470-6486. 1992.
[5]Perdew.J.P.Density functional approximation for the correlation of the inhomogenous electro gaz . Phys .Rev.B.33. 8822-8824. 1986.
[6]Perdew.J.P,Wang.Y. Pain distribution function and its coupling constant average for the spin polarized electron gaz Phys .Rev.B.46. 12947. 1992.
[7]Pankaya Singh , tanveer ahmad Wain ..An applicability aspect of quasi harmonic Debye model . J App and Ind Phys. Vol 1(20).107-113.2011. India.
[8] M. Ameri, K. Boudia, R. Khenata, B. Bouhafs, A. Rais, S. Bin Omran, B. Abidri, Y. Al-Douri . Structural, elastic, electronic and thermodynamic properties of the filled skutterudite $CeOs_4Sb_{12}$determined by density functional theory, Materials Science in Semiconductor Processing no -16 , 2013 , 1508–1516..
[9] C. Chappert, A. Fert, F.N.V. Dau. The emergence of spin electronics in data storage Nature Materials , 6 . 813–823. 2007.
[10]A. De Freitas, P. Martín, E. Castro, J.L. Paz. Physics Letters A, Volume 362, 2007. Pages 371-376.
[11] Greaves, G. N., Greer, A. L., Lakes, R. S., and Rouxel, T., "Poisson's Ratio and Modern Materials", *Nature Materials*, 10, 823-837 Nov. (2011).

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