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

Methods

Equilibrium point stable state \( (E_g, E_f) \) fitted data are taken in ideal conditions investigations for Husserl’s alloy. Seeking through iterations by Minim Lab Metal 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 Murnaghan’s equation non linear fit implemented in code Djoin 5.0, when external stationary fixed feeble positive mechanical strain \( \delta \) is applied on variable compressed lattice parameters \( \sigma \text{ (Ry)} \). (0.0-2.0) assuming orthorhombic tensor for (C11, C12), and monoclinic Tensor for (C44), shows different intervals slopes (positives negatives) that proved the instability. The elastic coefficients relative to mechanical strains \( \delta \) are not constants and not always positive. Characteristic mechanic parameters can not be deduced as recommended: Bulk modulus (B), Shear modulus (G), Young modulus (E), anisotropy elastic parameter (\( \lambda \)), Ratio ductility (B/G). Degree temperature (0-D), mean sound velocity, Poison Ratio (\( \nu \)), Poisson ratio function \( f (\nu) \) for static ideal conditions, Gibbs code simulation gives parameters related to thermo elasticity like: \( \sigma = 0.25 \) .

\[ \gamma = \frac{1}{J} \]

Results

1. Structural parameters

2. Thermodynamic parameters

3. Electronic properties

4. Optical properties

Conclusions

A predicted Regular Full Heusser (Au2LaB) identity is revealed - using FP-LMTO methods based on (DFT) full, extended to LDA, then to GGA. Calculate take account of spin polarization (S) and spin-orbit coupling interaction (L,S). Material (Au2LaB) is found a good thermal conductor according to calculated, capacities values. It can be artificially elaborated as confirmed by entry and free enthapy. For sound wave, it will be a promising conductor on the acoustic fiber. When undergo other types of strains stationary linear perturbations permits to understand mechanical instability relative to crystallographic Bravais net work ? Range internal strain values ?

Tensors categories? Time depending strain functions, especially sinusoidal case? We wonder of cubic structure and symmetry are exactly adapted and preserved? Material (Au2LaB) may develop a possible Piezoelectric effects ? Pyroelectric ? Ferroelectric properties. Magnetic moment is too low? Is it possible the material is paramagnetic after checking its magnetic susceptibility?

Boron concentration contributes to enhance: elastic, mechanic, magnetic properties. Optic complex properties are related to dielectric also complex functions, as responses to an external uniform electromagnetic field excitation, proved that (Au2LaB) material is a crystal quantum well, where no reflective interferences are observed, evanescent. Lanthanum concentration contribute to enhance: magnetic, pyroelectric and optical properties. Quantum effects must be more investigated in future. Nonlinear sensors, Phenomena, Phase Transition, Tunneling effects, Scattering by RX or Neutrons. In the other side this alloy is a metallic resonator-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 - optic complex parameters, with no reflection loss; TDS, transmission, gives technical implications in Renewable energies process: energy storage , harvesting, efficiency , distribution , solar optic cones, solar photovoltaic cell , microelectronics, thin film , spin polarized , support data storage, tunnelling spin junction Radars , antennas captures, sensors, etc. We suggest the reader when research for temperature T (K°) > 1600 and pressure P (GPa) = 50 Quantum behaviour need to be more detailed on Brain-Matter interactions, every various components ‘concentrations ‘ and changing atoms ‘positions.

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