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Mechanical and thermodynamic properties of the some B2 rare-earth intermetallic compounds: Ab-initio study and Data mining approach

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1.1 Introduction

In this work, The full-potential linearized augmented plane wave (FP-LAPW) method have been used to examine various properties of YAg, LaAg, CeAg, DyAg, YCu, DyCu, HoCu and ErCu members of a class of fully ordered stoichiometric intermetallics with the CsCl-type B2 crystal structure. These compounds have been found to have significant polycrystalline ductility at room temperature. The calculated ground state properties such as lattice constants, bulk Modulus and elastic constants agree well with the available data. The ductility or brittleness of these materials is predicted. For ErCu and HoCu compounds. The mechanical and Debye temperature are predicted from the calculated values of elastic constants. The analysis of the density of states (DOS) gives a detailed explanation of the contribution of atomic orbital characters in the energy bands. The thermodynamic properties also are predicted by the quasi-harmonic Debye model in the temperature range 0-700 K. In addition, chemical bonding of some compounds investigate here has been investigated in the light of topological analysis approach based on the theory of atoms in molecules. The relationship between several thermo-physical and mechanical properties were discussed, and analyzed with data mining techniques. The obtained results confirm that this B2-type of rare-earth intermetallic compounds have very interesting mechanical and thermal properties for structural applications.
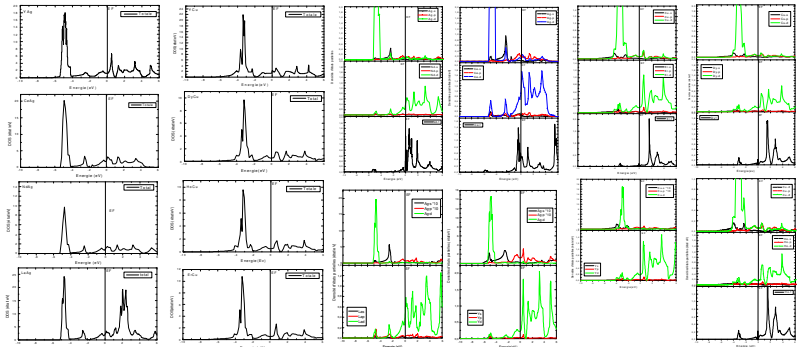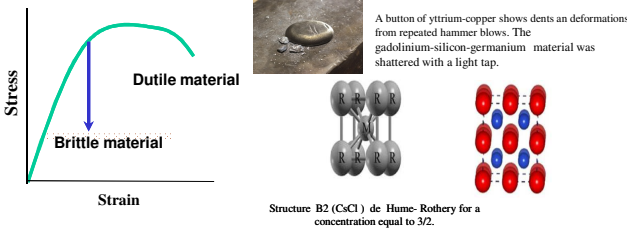
A button of yttrium-copper shows dents an deformations from repeated hammer blows. The gadolinium-silicon-germanium material was shattered with a light tap.

Structure B2 (CsCl) de Hume- Rothery for a concentration equal to 3/2.

1.2 Calculation method

- DFT & FP-LAPW
- Quasi-harmonic Debye Approximation   GIBBS
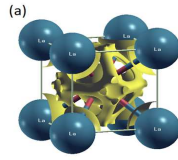- Atom in molecule   AIM
- Data Mining Techniques   PCA

Fig3.: Electron localization function plot at the value 0.8 for LaAg.

1.3 Results and discussion

1.3.1 Structural properties, elastic constants and Mechanical properties

Crystals	$a_0(A°)$	B(GPa)	B'_0	C_{11}(GPa)	C_{12}(GPa)	C_{44}(GPa)	C_{12}-C_{44}(Gpa)	G(GPa)	G[110]	B/G	A	σ	E (GPa)
YAg													
This work	3.64	65.52	3.96	97.15	49.70	32.049	17.65	28.41	23.72	2.30	1.35	0.31	74.47
Experiment	3.61	70.5	-	102.4	54.0	37.2	21.4	28.9	-	2.43	1.54	0.34	76.1
CeAg													
This work	3.69	56.86	4.46	68.98	50.53	25.26	25.27	16.87	9.22	3.36	2.73	0.36	46.06
Experiment	3.77	55.1	-	65.5	49.9	23.8	-	15.2	-	-	3.05	0.37	41.8
Theory	3.81	55.1	-	65.5	49.9	23.8	-	15.2	-	-	3.05	0.37	41.8
LaAg													
This work	3.82	52.83	3.56	62.73	47.88	22.55	25.32	14.46	7.42	3.65	3.03	0.374	39.77
Experiment	3.81	53	-	-	-	-	-	-	-	-	-	-	-
Theory	3.82	52.3	-	64.5	46.2	22.6	-	15.7	-	-	2.47	0.36	42.8
NdAg													
This work	3.66	59.70	4.09	64.02	53.06	25.89	27.17	14.06	5.48	4.24	4.72	0.39	39.11
Experiment	3.71	-	-	-	-	-	-	-	-	-	-	-	-
Theory	3.75	59.2	-	72.8	52.4	27.5	-	18.5	-	-	3.62	2.70	50.3
ErCu													
This work	3.44	52.68	4.51	104.55	35.4	26.75	8.65	29.64	34.58	1.783	0.77	0.26	74.90
Experiment	3.43	-	-	-	-	-	-	-	-	-	-	-	-
HoCu													
This work	3.45	53.43	4.05	66.56	46.86	39.24	7.61	22.69	9.85	2.35	3.98	0.31	59.63
Experiment	3.44	-	-	-	-	-	-	-	-	-	-	-	-
DyCu													
This work	3.45	55.37	4.169	74.91	40.45	36.24	4.21	26.89	17.23	2.06	2.10	0.29	69.43
Experiment	3.619	-	-	-	-	-	-	-	-	-	-	-	-
Theory	3.45	63.6	-	106.1	42.3	46.3	-	-	-	2.05	1.45	0.29	-
Theory	3.43	69.96	-	115.95	46.97	36.48	-	35.68	-	-	1.96	-	-
YCu													
This work	3.478	70.14	3.13	116.94	46.43	32.050	14.38	33.33	35.25	2.10	0.90	0.28	133.33
Experiment	3.476	70.1	-	113.4	48.4	32.3	13.50	32.38	32.5	2.16	0.99	0.28	84.18
Theory	3.18	70.7	4.6	117.7	47.2	36.1	13.40	35.25	35.25	1.97	1.02	0.28	91.80

Table 1: The lattice constant a_0, the bulk modulus B and its first order pressure derivative (B'_0), elastic constants and C_{ij}, of the R-Ag (R= Y, Ce, La and Nd) and R-Cu (R= Y, Dy, Ho and Er) compounds. Calculated from them: shear modulus (G) in the Voigt-Reuss-Hill approximation, shear modulus ($G_{(110)}$)the Young modulus (E) , the anisotropy factor (A), the B/G ratio and Poisson ratio (σ),and Cauchy's pressure C_{12}–C_{44}. Our FP-LAPW results using the PBE-GGA functional are compared to the theoretical and experimental values.

1.3.2 Electronic properties: Density of State and bonding feature:

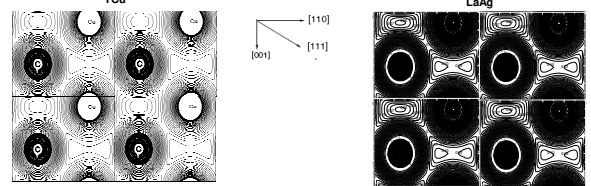Fig.1: Calculated total DOS of R-Ag (R= Y, Ce, La and Nd) and R-Cu (R= Y, Dy, Ho and Er) compounds

Fig. 2. Bonding charge distribution (BCD) on B2 {1 1 0} plane for Ycu and LaAg intermetallic compounds
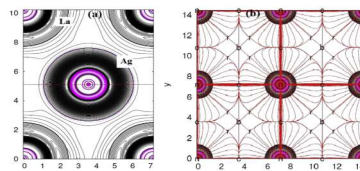

Fig.4. (a) Electron density of the LaAg and it: (b) topological analysis in the [111] plane. This plane contains all the CPs of the structure: the three nuclei, the La–Ag bond Cp's, a single ring Cp's, and two different cage Cp's. the down trajectories from the bcp's and the up trajectories from the rcp show the limits of the central ionic basin. Thick red lines correspond to ∇ρ trajectories, black (magenta) lines are positive (negative) contours of ρ and ∇^2 ρ.

	Volume anion	Volume cation	Charge anion	Charge cation	Ionicity (ξ)
YAg	125,867	201,289	1,432	-1,432	0,955
CeAg	159,866	181,598	1,158	-1,158	0,724
LaAg	174,916	203,743	1,214	-1,214	0,810
HoCu	131,063	148,102	1,001	-1,001	0,417

Table2. Atomic properties in column order, it shows the cationic and anionic volume, the integrated charge Q, and the degree of ionicity (x) for YAg, CeAg, HoCu and LaAg compounds.

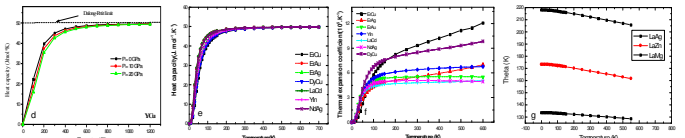### 1.3.3 Thermodynamic properties:

Fig. 5: (d) The heat capacity versus temperature at pressure of 0, 10 and 20 GPa, respectively, for YCu; (e) The heat capacity versus temperature for ErCu,ErAg,DyCu and NdAg;(f) Evolution of thermal expansion of ErCu, ErAg,DyCu and NdAg compounds with temperature;(g) The relationship between Debye Temperature and temperature for LaAg, LaMg and LaZn compounds at 0 pressure.
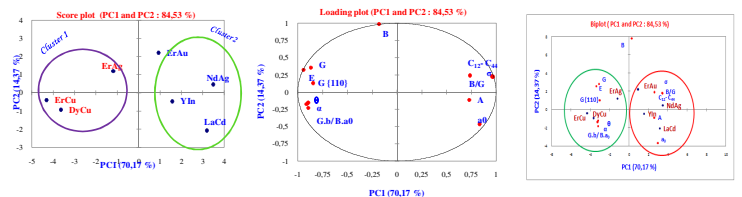
1.3.4 Data mining results:

Fig.6: PCA score plots, PCA loading and PCA Biplot of different rare-earth intermetallic compounds