FIRST PRINCIPLES CALCULATION STUDY OF STRUCTURAL, ELECTRONIC AND MECHANICAL PROPERTIES OF YM2 (M: Cu, Zn) LAVES PHASES

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ABSTRACT. Structural, electronic and mechanical properties of main YCu_2 and YZn_2 binary Laves phases with C14, C15, C36 and $CeCu_2$ in Cu-Y-Zn alloy are investigated by first-principles calculations. The related total energies versus occupations of nonequivalent lattice sites in all four structural forms were studied. Density functional theory is considered within framework of both pseudo-potentials and plane waves basis using VASP (Vienna ab initio Software Package).The optimized structural parameters were in very good agreement with the experimental values. Formation heat has been computed and showed that the $CeCu_2$-YCu_2 and YZn_2 Laves phases have the strongest alloying ability, structural stability and elastics properties. Electronic density of states (DOS) and charge density distribution were calculated and discussed in terms of structure stability.

KEYWORDS: *Ab initio calculations DFT, Laves phases, Intermetallics, Structural and electronic properties, CeCu2 orthorhombic structure.*