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Computational modelling of structural, electronic and thermodynamic properties of Cu-In intermetallic phases: *ab-initio* and phase diagram calculations

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Abstract – We study structural, electronic and thermodynamic properties of the recently proposed $Cu_{10}In_7$ phase as well as the ideal hexagonal NiAs/$InNi_2$ type structures of the Cu-In system. The latter represents a first step towards the understanding of the more complex equilibrium superstructures proposed for the Cu-In η-phase field. We perform ab-initio calculations employing density-funcional theory, projector augmented wave potentials and the generalized gradient approximation for the exchange-correlation energy. Using the CALPHAD method we postulate the new phase as a stoichiometric one and we analize the range of enthalpy an entropy of formation to assess its stabilty within the equilibrium phase diagram.

This work is part of an investigation of the phase equilibria of the Cu-In-Sn system, in connection to the application of In-Sn alloys as a lead free micro-soldering alloy. The aim is to understand aspects of the phase formation between the common Cu contact element and the Sn-In solder alloy involved in the process of diffusion soldering [1]. In the present study we focus on the phase equilibria of one of the three constituent binaries, Cu-In. This system contains five distinct binary phases, the two high temperature phases: the β Cu_4In with BCC structure and the γ Cu_9In_4 phase with Cu_9Al_4 type structure; the δ Cu_7In_3 phase with a unique structure type connected to NiAs and γ-brass structures; the η-phase field and the compound $Cu_{11}In_9$ with CuAl type structure. The η-phase field is rather complex and has not yet been resolved. This phase field is composed of at least two different but closely related superstructures of the NiAs/Ni_2In (hP4/hP6) type: the high temperature (η') phase and the low temperature (η) phase. The η-η' transition temperature is composition dependent and lies between 310-389°C [2]. The crystalline structure of η' corresponds to an hP6 lattice with random parcial occupation of Cu sites at symmetry Wyckoff positions 2d. The η crystalline structure would correspond to modulated superstructures based on the hP6 structure with ordered distribution of Cu vacancies at sites 2d [3]. The phase field has a range of stability extended in both composition (33-37 at.% In) and temperature (T < 667 °C). During an investigation of this η-phase field, Piao *et. al* [4] has recently found a new binary $Cu_{10}In_7$ phase. This compound crystallizes in the monoclinic space group C2/m, with a structure closely related to the $Cu_{11}In_9$ structure type.

In the present work we perform ab-initio calculations to characterize structural, electronic and thermodynamic properties of some intermetallic phases of the Cu-In system: the recently proposed binary $Cu_{10}In_7$ phase as well as the ideal hexagonal B8 NiAs/$InNi_2$ type structures which represent the basic lattice underlying the more complex superstructures proposed for the η-phase field. We calculate equilibrium lattice parameters, cohesive and formation energies of the phases considered. The calculations performed here are based on the electronic density-functional theory (DFT) carried out using the Viena ab-initio simulation package (VASP) [5] employing electronic density-funcional, *PAW* (projector augmented wave) potentials and the generalized gradient approximation (GGA) for the exchange-correlation energy.

Using the CALPHAD method we postulate the new phase as a soichiometric one and we analize the range of enthalpy an entropy of formation in order to assess its stabilty within the equilibrium phase diagram.

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