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Abstract

Ab initio study of phase stability in theCu-Cr-Zr system

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Abstract:

This work aims to study the structural, energetic and thermal properties of intermetallic compounds that precipitate in the Cu-Cr-Zr system, by an abinitio method called pseudopotential computation, as well as the quasi-harmonic model of Debye. The pseudopotential method is implemented in the Quantum Espresso code(QE) developed by S. Baroni et al [1] for the study of the physical properties of materials.

We are interested in the following compounds C15b -Cu5Zr, C11b-CuZr2, L12 -CuZr3, DO3 -CuZr3, C14-Cr2Zr, C15-Cr2 Zr and B2-CuZr.

Before undertaking the study of the different alloys, we studied the structural properties of the different structures of Cu, Cr and Zr simple metals. to start the calculation from a correct structure. Indeed, for each metal, the results found compared to those given by the literature showed a good agreement.

For each of the compounds, a minimization of the total energy with respect to the volume of the mesh was conducted. to predict the structural parameters of each compound. The results showed a good agreement with the experimental results, as well as those resulting from the theoretical studies. For the compression module, the Cu5Zr is the most rigid at 0 K in the

Cu- Zr system, while CuZr3 is the least rigid. In addition, the rigidity of the latter is independent of the type of its structure. For the Cr2Zr compound, the compression modulus inphase C 15 is more rigid than that in phase C14.

In terms of stability, the two phases L12 -Cu Zr3 and DO3 -CuZr3 are not favorable.Unlike other remaining compounds. CuZr2 in the C11b structure is the most stable,followed by Cu5 Zr then CuZr in the two structures C15b and B2 respectively. While thetwo C14 (Ⅰ) and C15 (Ⅱ) phases of the compound Cr2

Zr are stable and can coexist at low temperatures.

The quasi-harmonic model of Debye allowed us to study the evolution of the structural parameters of each of the compounds studied as a function of temperature. The volume of these phases increases linearly with increasing temperature, while the compression modulus decreases. This decrease is greater in the case of the Cu5 Zr compound. At low temperatures, this compound is the most rigid, but from 1100 K, CuZr becomes the most rigid. For volume expansion, the Cu5Zr shows a variation-parabolic depending on the temperature, while the remaining compounds the increase is linear. The specific heats of the different compounds obey the law of Debye at lowtemperatures (Variation in T3) depending on the temperature; this parameter tends towards aclassic term called Dulong and Petit.

Biography:

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Publication of speakers:

- S. Baroni, S. D. Gironcoli, A. D. Corso, Rev of modern Physics, Vol 73, (2001).

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