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Abstract

Ab initio study of phase stability in the Cu-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 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 in phase 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 the two C14 (□) and C15 (□) phases of the compound Cr2 Zr are stable and can coexist at low temperatures.

Publication of speakers:

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

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