Modelling of τ-phase in Al-Cu-Zn system

S. Kovaříková Oweis [a,1], J. Pavlů [a], O. Zobač [b]

[a] Department of Chemistry, Faculty of Science, Masaryk University,
Kotlářská 2, 611 37 Brno, Czech Republic
[b] Institute of Physics of Materials, Academy of Sciences of the Czech Republic,
Žižkova 22, 616 62 Brno, Czech Republic

[1] 394665@mail.muni.cz

We present a detailed theoretical study of intermetallic τ-phases in the Al-Cu-Zn system. This study is focused on the modelling of the region of existence and properties of the τ-phase, which does not appear in binary systems. The τ-phase exists in two modifications: cubic and rhombohedral. The goal of our work was to comprehensively describe the equilibrium between these two important structures. The complex thermodynamic model was proposed, based on the knowledge of the energies of formation of corresponding end-members (configurations with occupations of sublattices exclusively by one element). These energies were obtained by *ab-initio* calculations in the frame of the density functional theory using the Vienna Ab initio Simulation Package (VASP) [1–3] with projector-augmented plane wave (PAW) potentials [4, 5]. The *ab-initio* calculated structural and thermodynamic properties of the τ-phase are discussed and compared with literature data where available. The phase diagram calculated using these data is also presented.

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