MS23 Quasicrystals and complex intermetallic materials

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(3+3)D incommensurately modulated structure of the τ phase in the Al-Cu-Zn system
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Abstract
Dural alloys based on the Al-Cu-Zn system are of great technological importance for superior mechanical properties. They also exhibit shape-memory effect [1]. Recently, phase equilibria in this system were experimentally studied [2]. At 400 °C, a single-phase field was found, containing three structural modifications of the ternary phase τ: cubic CsCl structure (τC), related rhombohedral structure type (τR), and an unknown structure with incommensurate modulation (τi), which is the topic of this study.

A sample was prepared from pure elements in the 40Al:45Cu:15Zn ratio (at%), i.e. in the region of the phase τi. It was then melted in evacuated quartz-glass ampoules, annealed at 400 °C for 648 hours and quenched in water. Overall composition was measured by SEM-EDX and the structure was analyzed by powder XRD, which confirmed the ternary phase τi.

More detailed structural evaluation of the incomensurate structure τi was done by electron diffraction (3D ED) [3]. A thin lamella cut out with FIB as well as a crushed sample prepared under liquid nitrogene were investigated. Data were collected on an FEI Tecnai G2 20 transmission electron microscope operated at 200 kV with LaB6 cathode, equipped with an ASI Cheetah direct detection camera (512x512 pixels) using the continuous rotation approach (tilt range +/-50deg, step 0.25deg). The data were processed in the PETS software [4]. Structure solution and refinement were performed in the computing system Jana2020 [5]. The structure was solved by the charge flipping algorithm using the program Superflip [6].

The basic structure has cubic symmetry and it is of the CsCl type with lattice parameter a = 2.91(1) Å. The modulation is quite complex (Fig. 1a) consisting of three independent modulation vectors and a non-standard centring, which only effects the satellite reflections. The centring vectors are (0,0,0,0.5,0.5,0), (0,0,0,0.5,0,0.5) and (0,0,0,0,0.5,0.5). The corresponding (3+3)D superspace group is Xm-3m (a,0,0) (0,a,0) (0,0,a) with a=0.386. The simple CsCl-type structure, in this case with the sites occupied by Al and Cu, is modified by the addition of Zn on the Al-site and vacancies on the Cu-site. The number of the vacancies increases from 4at% in τC to 17at% in τR and it is likely the cause of the modulation. The modulation (Fig. 1b) is mostly occupational even though slight deviations from the average atomic positions are also visible (Al shown in grey, Cu in green, electrostatic potential in yellow).

References
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(a) Reciprocal space sections, (b) structure model