Crystal structure of the $Al_{78}Mn_{17.5}Pt_{4.5}$ phase as revealed by electron crystallography

Louisa Meshi[1], Rimon Tamari[1], Benjamin Grushko[2,3]

[1]*Department of Materials Engineering, Ben Gurion University of the Negev, Beer Sheva, Israel*

[2]*MaTecK GmbH, 52428 Jülich, Germany*

[3]*Peter-Grünberg-Institut, Forschungszentrum Jülich, 52425 Jülich, Germany*

louisa@bgu.ac.il

Structure of high temperature "Al_3Mn" (T) phase was investigated numerously. Studies of binary and ternary extensions of T-phase resulted in many published atomic models [1-8]. Until today, exact space group and atomic positions of transition metals in this structure is a matter of dispute. In current research, atomic model of the $Al_{78}Mn_{17.5}Pt_{4.5}$ phase (quenched from 800 °C) was successfully derived using a combination of electron crystallography methods. This structure was regarded as ternary extension of the "Al_3Mn" T–phase. The lattice parameters of the $Al_{78}Mn_{17.5}Pt_{4.5}$ T-phase were found to be a = 14.720(4) Å, b = 12.628(2) Å, c = 12.545(3) Å (as refined against X-ray diffraction data). Using convergent beam electron diffraction (CBED), the space group of this ternary composition was proved to be non-centrosymmetric P$na2_1$, instead of Pnam - which describes the symmetry of the binary T-phase. Atomic model was determined applying direct methods, utilized in SIR2011 [9], on electron diffraction tomography data and refined using ShelXL [10]. At the $Al_{78}Mn_{17.5}Pt_{4.5}$ composition, the Pt atoms were not distributed randomly in the Mn/Al sublattices, but adopted two specific Wyckoff sites, therefore, this composition should be regarded as an ordered variant of the T-structure. On the other hand, CBED study of the T-phase samples with a bit different stoichiometry ($Al_{71.3}Mn_{25.1}Pt_{3.6}$) allowed attribution of the structure to the original T-phase structure type, i.e. centrosymmetric. Using Barnighausen tree [11], these two structures (centrosymmetric and non-centrosymmetric) were found to be related.

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