Poster Presentation

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Structure determination of a new phase Ni_8Ti_5

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The structure of Ni8Ti5 was solved and refined from precession electron diffraction tomography data using dynamical refinement approach. It has trigonal symmetry R-3m (a = 12.24(5) Å, c = 15.33(5) Å) with a structure related to the structure of Ni4Ti3. The greatest challenge of the structure determination was the assignment of atomic types due to the proximity of scattering powers of Ti and Ni. Several approaches to determination of atom type distribution over atomic positions were used; (1) analysis of the Wyckoff position multiplicities, (2) refinement of displacement parameters, and (3) geometrical analysis of the structure and comparison with known structures. These approaches consistently pointed to one distribution, which was confirmed by a significant improvement of the refinement figures of merit.

The new phase Ni8Ti5 was studied in the Ni-48 at.%Ti alloy prepared from elemental powders by self-propagating high-temperature synthesis and subsequent annealing at 1000 °C for 12 h, followed by slow cooling to room temperature. The phase forms micrometer-sized precipitates within NiTi matrix. It was also observed in the alloy of the same composition prepared by conventional vacuum induction melting from bulk Ni and Ti metals. So its existence is not related only to the powder metallurgy preparation route.
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