

STRUCTURE OF EMBEDDED NANODOMAINS IN INTERMETALLICS

Ni-Te system is possible applied in thermoelectric generators converting heat into electrical power

Ni-Te is an intermetallic compound with possible applications in thermoelectric generators (TEGs) that convert heat into electrical power by exploiting a temperature gradient. Ni_{1-x}Te_{1+x} system is a two-solid phase mixture where nanodomains of modulated (layered) unknown phase (phase β) were found inside the NiTe matrix. Despite many attempts to solve this unknown Ni-Te phase β, its structure and stoichiometry was revealed only using 3D diffraction tomography

The challenge: Embedded nanodomains with size up to 70nm, two Ni-Te phases

Solution: Automated 3D Diffraction Tomography combined to Precession electron diffraction

coupled to precession electron diffraction (PED).

3D diffraction tomography data were collected on the edge of a milled particle, revealed the presence of two phases, the matrix Ni₁Te₁ (phase α) and the superstructure Ni₅Te₄ (phase β). Structure determination of the modulated β phase was hampered by the small dimensions of the domains and the fact that most of them are embedded into the Ni₁Te₁ matrix. Reflections coming from the superstructure were recognized and showed a doubling of both c and a parameters, leading to a monoclinic. It is found out that is locally similar to NiTe, but there is a shift of one Te layer by (1/3, 1/3, 0) every two c-periods referred to the initial hexagonal NiTe-type structure.

The analysis of the experimental data confirms that Ni₁Te₁ (phase α) has a hexagonal structure, of NiAs type, where the Te atoms form a BCBC... hexagonal sequence. The remaining Ni atoms are distributed over octahedral sites between the Te Layers (figure 2).

The new Ni₅Te₄ (phase β) has a monoclinic structure where the Te

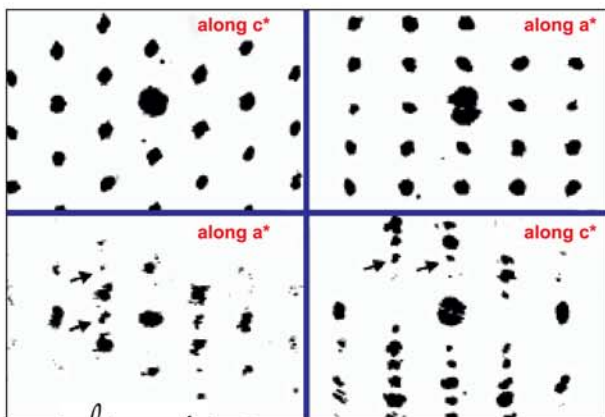


figure 1
PROJECTIONS OF THE RECONSTRUCTED 3D DIFFRACTION OF PHASE α ALONG THE C* & THE A* AXIS; (TOP, HEXAGONAL) PHASE β ALONG THE C* & THE A* AXIS (DOWN, MONICLINIC) SUPERSTRUCTURE REFLECTIONS ARE MARKED WITH BLACK ARROWS.



atoms form a sublattice with BABCA... hexagonal sequence, while the Ni atoms occupy deformed octahedral sites with a ...c₀c₀a₀a₀c₀... sequence and tetrahedral sites with a ...c₁b₁c₁... sequence. It is found out that is locally similar to NiTe, but there is a shift of one Te layer by (1/3, 1/3, 0) every two c-periods referred to the initial hexagonal NiTe-type structure.

Crystal Structure

Ni ₁ Te ₁ (α-phase)	Ni ₅ Te ₄ (β-phase)
Hexagonal P6₃/mmc	Monoclinic Pm
a= 3.85 Å	a= 6.95 Å
b= 3.85 Å	b= 4.02 Å
c= 5.22 Å	c= 11.96 Å
α= 90°	α= 90°
β= 90°	β= 90°
γ= 120°	γ= 90°

ADT together with PED allowed the structure determination of the nickel-rich phase superstructure Ni₅Te₄ (phase β) for the first time.

Experimental data
Ni₁Te₁ / Ni₅Te₄
tilt range: ±50° / ±40° step: 1°
No ind. reflections 47 / 411
No ind. atoms 2 / 11
R = 22.3% / 24.6%

figure 2

