THE CRYSTAL STRUCTURE OF $(Ni, Co)_3Al_4$ IN THE Al-Ni-Co TERNARY SYSTEM ——A NEW VACANCY CONTROLLED ALLOY PHASE

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ABSTRACT

$(Ni, Co)_3Al_4$ is a ternary phase in the Al-Ni-Co system, the homogeneous range at room temperature being 55—58.5 A/0 Al, 26—35 A/0 Ni, and 10—15.5 A/0 Co. It belongs to the cubic system with space group O_h^{10}—$Ia3d$. There are 112 atoms per unit cell, the lattice spacing at room temperature being $a = 11.3962$ Å.

This structure may be considered as a superlattice built up by stacking together 64 CsCl type fundamental structural units. Among these structural units, there are 16 'Centre' positions left vacant in order. They occupy the $16(b)$ equivalent positions forming 16 octahedral voids. The 'Corner' positions $16(a)$ and $48(f)$ are all occupied by Al atoms, while the 'Centre' positions $48(g)$ are occupied at random by Ni and Co. Due to the existence of the voids, the positions originally at cube corners and centres are displaced somewhat, the parameters being $x_f = 0.010$, $x_g = 0.369$.

From the homogeneous range of this alloy phase and the distribution of the various atoms in the structure, the ideal stoichiometric formula of this alloy phase may be written as $(Ni, Co)_3Al_4$. There are 16 formula weights per unit cell.