**Ab initio Simulations on the W-phase of the Al-Co-Ni System**

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The W-phase [1] is the highest stable approximant of the decagonal quasicrystal known in the system Al-Co-Ni. Its structure contains the so-called “20 Å-cluster", which is a characteristic building unit of decagonal Al-Co-Ni.

The Co/Ni ratio determines which modification of decagonal $Al_{72}Co_{28-x}Ni_x$ ($8 \leq x \leq 20$) is formed. Therefore, we studied the influence of the Co/Ni ratio on the structure of the W-phase, starting from binary compositions Al-Co and Al-Ni with idealized positions. From these results a realistic ternary model was derived.

The structure models were optimized using the VASP code [2,3]. Our calculations are based on the generalized gradient approximation and utilized PAW potentials [4] supplied with VASP. The band structure, electron density districution and electron localization function were calculated.

These calculations help to get insight into the factors governing formation and stability of this kind of complex intermetallic alloy. They also corroborate the results of the single-crystal X-ray structure analysis, from which a significantly distorted and disordered structure model was obtained.

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