Atomic Models of ε_n Structural Variants - Overview

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Abstract. The present work is focused on the overview of atomic models of ε_n decagonal quasi crystalline approximants in the Al-Pd-Co system. Atomic structural models of the structural variants ε_6, ε_{16}, ε_{22}, ε_{28} and ε_{34} were created using ab-initio calculations and/or Monte Carlo simulation. Atomic models were calculated based on the experimental results obtained by X-ray diffraction and scanning transmission electron microscopy. Good agreement was obtained between calculated and experimentally observed atomic structures of the ε_n phase. The calculated data for the structural variant ε_{28} are available in the appendix, as CIF file in text format.