We describe a systematic approach to quasicrystal structure refinement on the basis of structural energy, combined with the defraction data input. We choose as an example the decagonal quasicrystal AlNiCo, for which both high-quality diffraction data, and effective ternary pair potentials needed for evaluation of energies, are available. The ensemble of structures we admit is restricted to periodic stacking of 2D rhombus tilings. The rhombi are decorated by candidate sites that are available for atoms to occupy like a lattice gas. In a finite-temperature Monte Carlo simulation, atoms may hop from one site to another, or pairs of atoms occupying different sites may swap. Simultaneously, the rhombus tilings are independently reshuffled via the standard local 'tile-flip' rearrangements. Each site is additionally assigned continuous positional degrees of freedom; these are constrained by point symmetries of the local tiling pattern, with which a site was associated. The Metropolis Monte Carlo scheme is combined with nonlinear least square fitting procedure to minimize an objective function combining structural energy with the weighted R-factor computed from the defraction data.

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References:

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