

4. DIFFUSE SCATTERING AND RELATED TOPICS

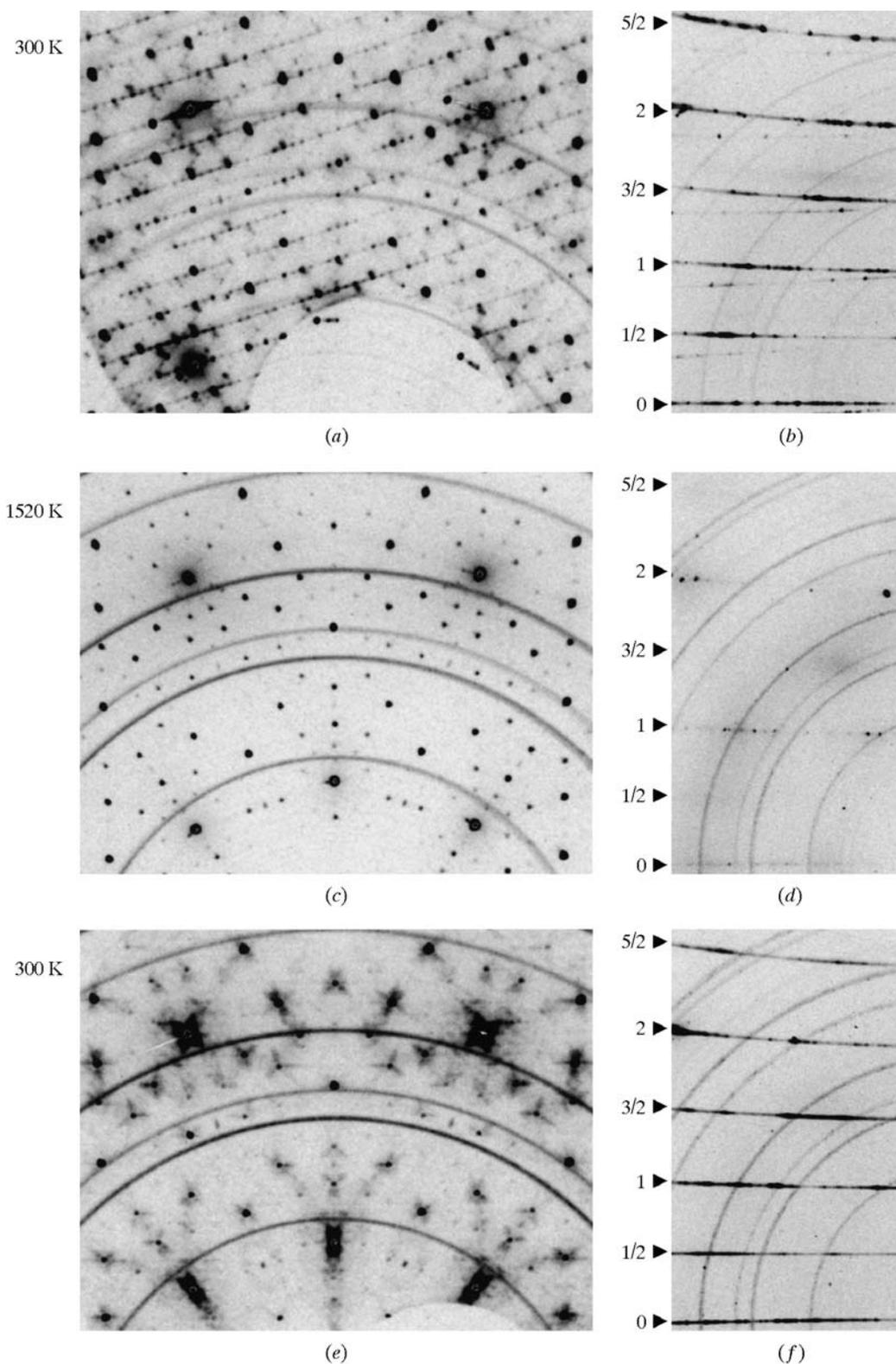


Fig. 4.6.4.2. Zero-layer X-ray diffraction patterns of decaprismatic $\text{Al}_{73.5}\text{C}_{21.7}\text{Ni}_{4.8}$ crystals taken parallel and perpendicular to the crystal axis on an image-plate scanner (Mar Research) at different temperatures. In (a) and (b), room-temperature (RT) diffraction patterns from a sample quenched after annealing at 1073 K are shown. Reflections from both a crystalline approximant and a decagonal phase are visible. The period along the unique direction in the decagonal phase and the corresponding period in the approximant phase is $\approx 8 \text{ \AA}$ (b). At 1520 K, a single-phase decagonal quasicrystal is present with $\approx 4 \text{ \AA}$ fundamental structure (c, d). In (e, f), the RT diffraction patterns of the slowly cooled sample indicate a single-phase nanodomain structure with $\approx 8 \text{ \AA}$ periodicity along the unique direction.

It turns out that 92.6% of the total diffracted intensity of 161 322 reflections is included in the 44 strongest reflections and 99.2% in the strongest 425 reflections. It is remarkable, however, that in all the experimental data for icosahedral and decagonal quasicrystals collected so far, rarely more than 20 to 50 reflections along reciprocal-lattice lines corresponding to net planes with Fibonacci-sequence-like distances could be observed. The consequences for structure determinations with such truncated

data sets are primarily a lower resolution in perpendicular space than in physical space. This corresponds to a smearing of the hyperatoms in the perpendicular space. For the derivation of the local structure-building elements (clusters) of aperiodic crystals this is only a minor problem: the smeared hyperatoms give rise to split atoms and a biased electron-density distribution. The information on the global aperiodic structure, however, which is contained in the detailed shape of the atomic surfaces, is severely