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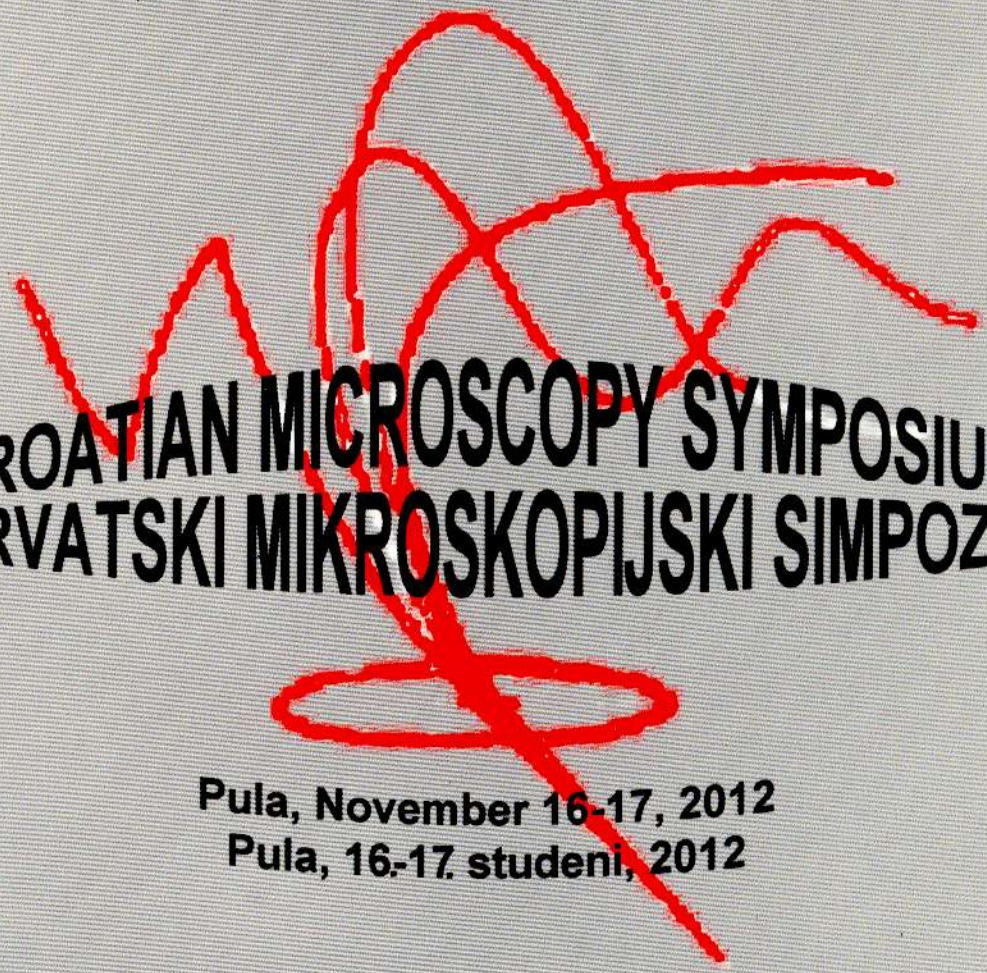

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Order and disorder in AlCuCo quasicrystal; an electron diffraction study

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Here, we present our recent electron diffraction study on $Al_{.63}Cu_{.24}Co_{.13}$ decagonal quasiperiodic crystal (QC); type, range, and degree of structural order and disorder.

Nobel price in Chemistry 2011. (Dan Shechtman for the discovery of quasicrystals), has recently resumed our interest in this matter and these materials. Namely, twenty years ago one of us (OM) had encountered these "exotic" materials for the first time, and performed some electron microscopy studies[1]. Seven years ago, one of us (IM) published numerical study on magnetic order and spin dynamics using model of finite approximants of the octagonal tiling, in two-dimensional quasicrystal[2]. Nowadays, one has to familiarize with structure of quasicrystals in relation to their functional properties.

Traditional definition of crystalline state was based on a concept of ordered unit cell with anticipation of its infinite repetition on three-dimensional lattice [3]. However, crystal ordering can be compromised by additional parameters; it can be incommensurately modulated and perfectly ordered on extended scale with no strict periodicity in three-dim. direct space. Such order is prominently revealed in reciprocal space, so that the contemporary definition of crystal refers to "... an essentially discrete diffraction diagram". These crystal structures, as well as their diffraction patterns is to be considered in terms of higher-dimensional crystallography, by using more then 3 lattice parameters. i.e. the space with 3+d dimensions[4]. Periodicity in higher-dimensional space is revealed (projected) as quasiperiodicity in real three-dim space; consequently one can consider two categories: periodic (PC) and quasiperiodic (QC) crystals.

Structural disorder and aperiodicity in direct space of PC is revealed in reciprocal space by additional intensity in between the basic spots of ordered structure. The same holds for QC, as seen in electron diffraction patterns of $Al_{.63}Cu_{.24}Co_{.13}$, in Fig.1. Sharp discrete spots of Fig.1(a), with the 10-fold symmetry, have to be assigned by four indexes; the in-plane quasiperiodicity of this decagonal structure is based on the 4-dim pentagonal lattice. The out of plane regular periodicity of the decagonal structure is displayed in Fig.1c&d, indicating double and quadruple layer stacking with lattice parameter 0.42 and 0.84 nm. Slight tilting in Fig.1b discloses average first-neighbour correlation within the double layer structural unit with $q^* \approx 4$ nm^{-1}. Higher or lower compositional in-plane order was observed locally in the variable spot intensity of Fig.2a&b, so that indexing on primitive or centred pentagonal lattice cell can be used.

References:

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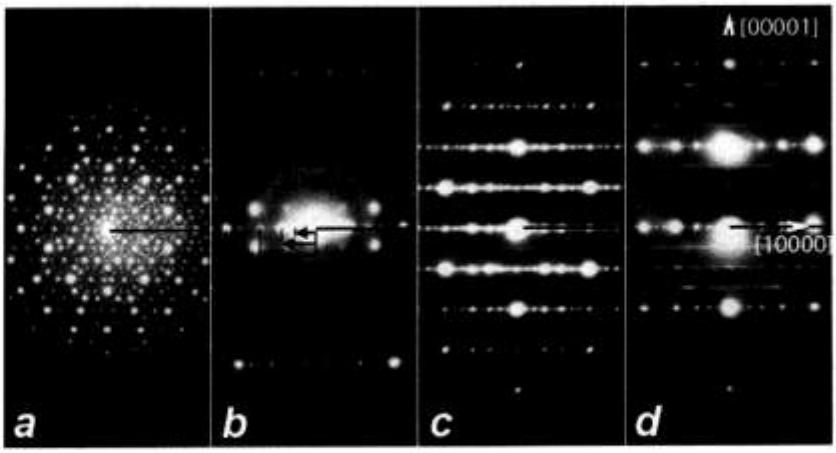

Figure 1. ED Patterns of $Al_{63}Cu_{24}Co_{13}$ quasicrystal; 5-fold zone -(a); oblique zones - (b), (c), (d); tilt axis [10000] -central line. Sharp discrete spots in (a) reveal long range planar order. Diffuse hallo (arrow-heads) in (b) indicates first neighbour correlation, while arrows indicate linear quasiperiodic $(1,\tau)$ spacing; diffuse streaks (arrow-heads) in (c) and (d) indicate disorder in 2- and 4-layer stacking.

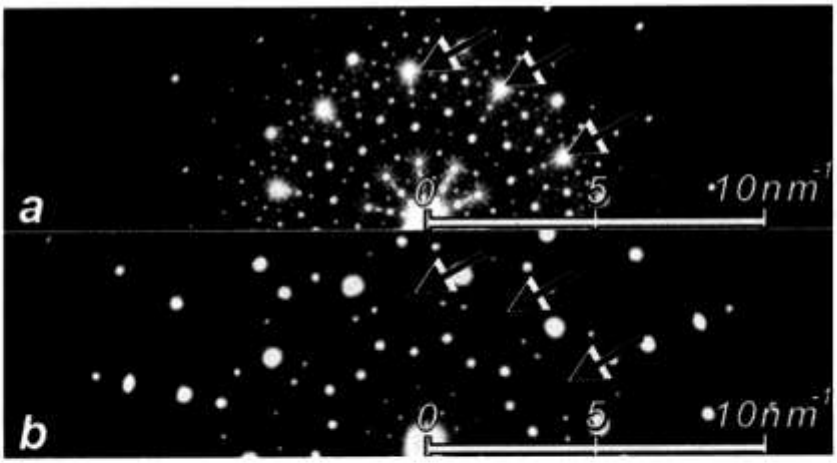

Figure 2. ED Patterns of the same $Al_{63}Cu_{24}Co_{13}$ quasicrystal along 5-fold axis revealing different degrees and ranges of local QC order: (a) low level of compositional order with primitive planar decagonal 4-dim lattice cell; (b) high compositional order with centred decagonal cell. Arrows indicate basic spots which are strong in (a) and weak in (b); presence and absence of diffuse intensity around basic spots in (a) and (b) corresponds to short and long range of correlation length (crystallite size), respectively. Diffraction information is more extended in (b) than in (a) disclosing higher level crystal perfection, correspondingly.