Professor Adam Pietraszko
Institute for Low Temperature
and Structure Research,
Polish Academy of Sciences
Okólna 2, 50-422 Wroclaw, Poland

E-mailA.Pietraszko@int.pan.wroc.pl

The Evaluation of the Thesis

Structure analysis of selected decagonal quasicrystals

by Paweł Kuczera

submitted for the Ph. D. Degree of the AGH University of Science and Technology, Faculty of Physics and Applied Computer Science

The manuscript presented herein, the volume of 134 pages, contents material related to the determination of accurate atomic structure of selected decagonal quasicrystals (QC). The quasicrystals are real crystals with sharp diffraction peaks but with a non-crystallographic symmetry. The quasicrystals can be divided into two classes: the icosahedral IQC (called also 3D QC - aperiodic in three dimensions) and the axial class of quasicrystals (with a periodic stacking of quasiperiodic layers – 2D). Decagonal quasicrystals (DQC) are an important group of the axial class of QC and the doctoral dissertation of Mr. Paweł Kuczera is devoted to study the quasicrystals, which belong to this group.

The main aim of the thesis is the determination of accurate atomic structure of DQC. It appears that the accuracy of detailed structure determination of the DQC is not high, in contrast to that of normal periodic crystals, due to the lack of proper tools of the structure refinement. Therefore the second goal of the Thesis was the elaboration of a software for refinement of the DQC structure. It should be noted that the prototype of QC structure refinement was provided by Dr B. Kozlowski also from the Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Cracow. The new software worked out by Mr. Paweł Kuczera and used in his work is based on a new method termed an Average Unit Cell concept proposed by J. Wolny (1993-2002). The method is operating in a 3D physical space, contrary to the most popular methods working in higher-dimensional space.

The work related to the Ph. D. Thesis of Mr. Paweł Kuczera has been done at the AGH University of Science and Technology in Cracow and at the ETH in Zurich. The aim of the study has been presented by the author in the *Introduction* (Chapter I) and it becomes clear throughout reading of the Thesis that **the results obtained contribute seriously to the problem the atomic structure of decagonal quasicrystals.** Chapter II entitled *Phase Problem*, chapter III *Rhombic Penrose Tilting for nD Approach* and chapter IV *Average Unit Cell (AUC) Approach* contain a survey of the problems the Thesis are dealing with, whereas the respective references are collected in chapter V entitled *Review of Literature on DQC structure refinements.*

The most important result of the doctoral dissertation of Mr. Paweł Kuczera have been published in six original papers:

i) J. Wolny, B. Kozakowski, P. Kuczera, R. Strzałka, A. Wnęk, *Real Space Structure Factor for Different Quasicrystals*, Isr. J. Chem. 51(2012)1275-1291

ii) J. Wolny, B. Kozakowski, P. Kuczera, R. Pytlik, R. Strzałka, *Periodicities in diffraction patterns of quasicrystals,* submitted to Science 2013

iii) P. Kuczera, J. Wolny, W. Steuerer, *Comparative structural study of decagonal quasicrystals in the systems Al-Cu-Me (Me = Co, Rh, Ir)*, Acta Cryst B 68(2012)578-589

iv) P. Kuczera, B. Kozakowski, J. Wolny, W. Steuerer, *Real space structure refinement of the basic Ni-rich decagonal Al-Ni-Co phase,* J. Phys.: Conf. Ser. 226(2010)-12001

v) P. Kuczera, J. Wolny, F. Fleischer, W. Steuerer, *Structure refinement of decagonal Al-Ni-Co, superstructure type I,* Phil. Mag. 91(2011) 2500-2509

vi) J. Dshemuchadse, P. Kuczera, W. Steurer, *A new cluster-based cubic phase in the Al-Cu-Ir system,* Intermetallics 32(2013)337-343

and the publications constitute an integral part of the dissertation.

Statistical approach to the description of aperiodic 1D, 2D, and 3D structures using the concept of the AUC (publication No. i) is presented in chapter VI. Chapter VII contains considerations on the periodicities in diffraction pattern of quasicrystals, and the results have been submitted for publication in Science (No. ii). The problem is related to the structure of QC which is periodic, however their diffraction patterns comprise periodic series of the peaks, that can be used to retrieve essential features of the quasicrystalline structure. Chapter VIII is devoted to a comparative structural studies of the family of decagonal Al-Cu-*Me* (*Me* = Co, Rh, Ir) quasicrystals the results of which have been published in Acta Cryst. B (publication No. iii). A decagonal cluster of ~33 Å in diameter, centred at the vertices of pentagonal Penrose tilting, was found as a basic structural building units in all three phases of the QC studied. As the atomic mass difference of constituent elements of Al-Cu-Rh and Al-Cu-Ir decagonal quasicrystals was large enough to distinguish them basing on the X-ray diffraction experiments their structures were refined as real ternary alloys. The refinement of a DQC as a ternary alloy I consider as a pioneering work in the literature of the quasicrystals. Chapter IX is dealing with publication No. iv, which describes the results of structural analysis of basic Ni-rich decagonal Al-Ni-Co phase. The authors used decorated rhombic Penrose tiling as an initial structure for the refinement process carried on with only real space parameters. The statistical approach enabled to derive the structure factor unrelated to the perpendicular space. Publication No. v), which contains the first results of the structure analysis of decagonal Al-Ni-Co superstructure of type I is the subject of chapter X. The refinement carried on with only real space parameters and based on decorated rhombic Penrose tiling resulted in a degree of a disorder within the structural unit (thin and thick rhombuses). A new cluster-based cubic phase in the Al-Cu-Ir system is described in chapter XI (publication No. vi). The structure of the system was determined by single crystal X-ray diffraction and the authors discovered that the crystal structure exhibits high degree of a disorder, in particular in the cluster centers.

I was pleased to notice that Mr. Paweł Kuczera made an effort to determine the unusual aperiodic structure of decagonal quasicrystals using the Average Unit Cell concept and **the results he obtained contribute seriously to the knowledge of the atomic structure of quasicrystals.** It seems that the nature of the crystal structure of QC is still weakly recognized and invites to clear up their detailed atomic arrangement. **There is no doubt, that the results collected in the Thesis of Mr. Pawel Kuczera present a valuable contribution to the knowledge and research into the field of atomic structure of decagonal quasicrystals.**

The Thesis of Mr. Pawel Kuczera entitled *Structure analysis of selected decagonal quasicrystals* deserves my positive opinion and the Author ought to be entitled to submit it for the Ph. D. Degree.

Wrocław, August 14, 2013

Prof. Dr hab. Adam Pietraszko

COMMENTS
to the Ph. D. Thesis of Mr. Paweł Kuczera

entitled *Structure analysis of selected decagonal quasicrystals*

i) I expected in the Thesis wider discussion of the problem of so-called "atomic displacement parameters" (ADP) since the "average displacement parameters" appear in the formula describing the structure factors (pp. 43, pp. 108, pp. 118).

ii) I noticed also typographic errors - the most frequently DCQ instead of DQC.