



Session XII - Friday, September 4 - morning

S12-L1

DIFFUSION IN QUASICRYSTALS

Helmut Mehrer

*Retired from: Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10,
48149 Münster,
Germany*

*Private address: Berghof 3, 73635 Obersteinenberg, Germany,
mehrer@uni-muenster.de*

Quasicrystals are a form of solid matter in which the atomic positions are ordered with five-, eight- or twelve-fold rotational axes. These symmetries entail icosahedral, decagonal or dodecagonal types of quasicrystals and are incompatible with periodic, crystalline order of classical crystallography. Most quasicrystalline alloys are composed of several metallic elements and may thus be considered as complex intermetallics. With respect to diffusion properties well studied icosahedral alloys are Al-Pd-Mn and Zn-Mg-Y and the decagonal Al-Ni-Co.

Radiotracer and SIMS studies of diffusion for the above mentioned ternary quasicrystalline alloys from our laboratory and from other groups are summarized. The experiments comprise measurements of diffusion in single crystals of icosahedral and decagonal quasicrystals as functions of temperature and for the icosahedral inter-

metallic Al-Pd-Mn also as function of pressure. Diffusion in icosahedral alloys is isotropic whereas decagonal alloys have different diffusivities parallel and perpendicular to the decagonal axis. The diffusivities are usually Arrhenius activated and compare in the case of Al-based icosahedral quasicrystals well with solute and self-diffusion in aluminium. This suggests that diffusion in these quasicrystals is vacancy-mediated. The diffusion anisotropy in decagonal Al-Ni-Co is similar in size to that of uniaxial hexagonal or tetragonal metals. The influence of hydrostatic pressure on diffusion of Zn and Mn was studied for Al-rich Al-Pd-Mn icosahedral alloys. The activation volumes correlate well with activation volumes of diffusion for the same elements in pure aluminium. The latter is attributed to a vacancy mechanism as well.

S12-L2

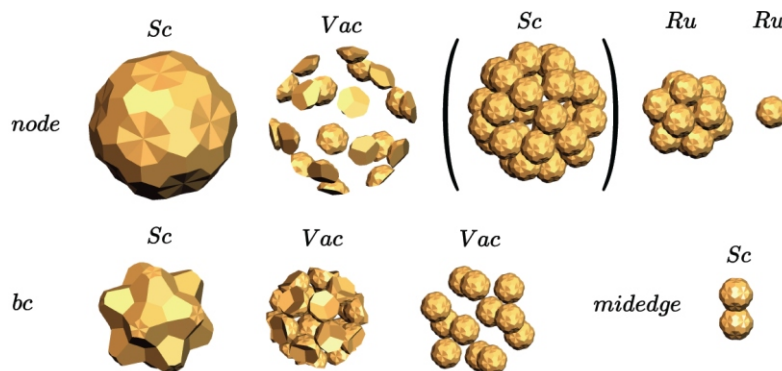
STRUCTURES IN THE (Sc, Ru) SYSTEM

Abdullah Sirindil, Loic Perriere, Philippe Vermaut, Marianne Quiquandon, Richard Portier, Denis Gratias

Paris Sciences Lettres, IRCP, ENSCP 11 rue Pierre et Marie Curie, Paris, France

The $\text{Sc}_{57}\text{Ru}_{13}$ (Sc phase has been elaborated by semi levitation melting in a copper crucible and slow solidification of the elements close to its nominal composition. X-rays powder diffraction and TEM observations confirmed the Pm3 structure of the compound as proposed by K. Cenzual, B. Chabot and E. Parthé [1] for $\text{Sc}_{57}\text{Rh}_{13}$.

Following Y. G. So, A. Shimizu et al. [2] we confirm that this structure is an almost perfect example of a 1/1 cubic approximant of a F-icosahedral structure (almost Primitive in 6D), it is made of two almost identical Mackay clusters at (0,0,0) and $1/2(1,1,1)$ of a P-cubic structure almost I. Using these data we propose a 6D model of its hypothetical parent quasicrystal and compare our model



Simple P type 6D-Model of Sc-Ru hypothetical quasicrystal.



with the experimental structure in the framework of the perpendicular shear method for generating approximant from ideal quasicrystal.

The 6D primitive model shows three atomic surfaces located on n, bc and mid-edge sites that generate in the physi-

cal space identical Mackay clusters connected by octahedra oriented along ternary directions.

1. K. Cenozual, B. Chabot and E. Parthé, *Acta Cryst.* (1985), **C41**, 313-319.
2. Y. G. So, A. Shimizu, K. Edagawa and S. Takeuchi, *Philos. Mag.* **86** n°3-5 (2006), 373-379.

S12-L3

DETERMINING THE PRINCIPAL CLUSTERS IN COMPLEX ALLOY PHASES

D. D. Dong, C. Dong

*Key Laboratory for Materials Modification by Laser, Ion and Electron Beam
(Dalian University of Technology), Ministry of Education, Dalian 116024, China
dandan3006@126.com*

The most striking feature of short-range orders, either in crystalline or in non-crystalline structures, is the characteristic nearest-neighbor coordination polyhedral clusters (called clusters for short in the following) of various types, as the result of the strongest nearest-neighbor atomic interaction. Clusters in complex alloy phases are especially important for the influence from periodic long-range ordering is weak or even absent in the case of non-crystalline solids such as quasicrystals and amorphous phases. We have developed a so-called 'cluster-plus-glue-atom' model which suits for the local cluster-based structural description of such phases, and any structure can be expressed by cluster-plus-glue-atom formulas. This approach has provided an easy and simple way towards their structural as well as

compositional interpretations. However, ambiguities arise in defining multi-shelled nearest neighbours and more importantly the principal clusters that enter into the cluster formulas. In this talk, the cluster formation is correlated to Friedel oscillation: the 1st-neighbor multi-shells of a cluster are confined within the first Friedel oscillation valley, with the outermost-shell distance falling below the upper limit of 1.5 times the innermost-shell distance. Hard-sphere atomic dense packing is further introduced to narrow down this limit for clusters with different facet capping geometries. Principal clusters are further determined via cluster isolation and packing efficiency criteria. Examples in Cu-Zr binary alloy phases are analyzed in detail to illustrate the use of this cluster-based approach.

SL12-L4

CHARACTERIZATION OF NANOINDENTATION-INDUCED DEFORMATION STRUCTURE IN AN Al-Pd-Fe CRYSTALLINE APPROXIMANT

W. Sun, L. L. Zhou

*Institute of Microstructure and Property of Advanced Materials, Beijing University of Technology, China
weisun@bjut.edu.cn*

Crystalline approximants belong to a kind of complex alloy phases whose basic structural units and mechanical properties are similar to those of corresponding quasicrystalline phases. It is well known that quasicrystals and their crystalline approximants are usually very brittle at room temperature and can undergo a brittle-to-ductile transition at elevated temperatures. In comparison with ordinary crystalline phases with a small unit cell, those structurally complex crystalline approximants can have a quite large unit cell consisted of hundreds or even thousands of atoms, and therefore their deformation properties have been attracted great interest since their structures can be described on the basis of arrangement of atom clusters and novel deformation mechanisms can occur. So far deformation studies of crystalline approximants are mostly concentrated on determining their deformation behaviours and structures at high

temperatures where these complex alloy phases are ductile, however the information about those at room temperature is still lacking. In the present study, the deformation behaviour of an Al-Pd-Fe crystalline approximant (α_{16}) at room-temperature was examined by nanoindentation testing and the corresponding deformation structure investigated by using a combination of FIB cross-section fabrication technique and transmission electron microscopy. Well-defined impressions without microcracking and typical loading-depth curves obtained from single grains of the Al-Pd-Fe α_{16} phase indented under various loading conditions indicate an apparent plasticity. TEM observations show that the deformation structure below the indent is characterized by distribution of scattering deformation bands of different density. Deformation is localized



in these deformation bands, and their density and width increase during the indentation process through which local distortion and fragmentation will take place to accommodate deformation strain. There is no clear evidence showing that the deformation is mediated by movement of dislocations. On the basis of HREM observations, the detailed structural characteristics of deformation bands will

be presented and the effect of pre-existing phason defects in the Al-Pd-Fe₁₆ phase on the evolution of the deformation structure during the indentation will be discussed.

This work was supported by the Beijing Natural Science Foundation (No.2132019) and by National Natural Science Foundation of China (No. 11274027).