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# Direct confirmation of the quasicrystalline structure of a *T*-phase quasicrystal by ion channeling combined with Rutherford backscattering

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The channeling properties of a *T*-phase $Al_{62}Cu_{20}Co_{15}Si_3$ quasicrystal are investigated in a Rutherford-backscattering study using 2-MeV He ions. Besides axial channeling along the decagonal axis, planar channeling is observed in planes having the decagonal axis in common and showing the decagonal symmetry of the quasicrystal. Besides a system of main planes, various planes exhibiting only weak channeling properties are observed; they correspond to linear arrangements of vertices in a two-dimensional Penrose grid, demonstrating the close relationship between *T*-phase quasicrystals and Penrose pattern.

Up to the present time many binary and ternary alloys have been synthesized which exhibit axes of fivefold or tenfold symmetry in x-ray or transmission-electron diffraction patterns. Since an axis of fivefold or tenfold symmetry is strictly forbidden in ordinary periodic structures, many suggestions have been made to explain the observed diffraction pattern, such as twinned periodic crystals,[1] randomly stacked oriented icosahedral clusters of atoms,[2] and others. Perhaps the most striking was the concept of icosahedral Amman tiling of space[3] (a three-dimensional generalization of the two-dimensional Penrose pattern[4]), since it proposed a completely different class of crystalline structures, the so-called icosahedral quasicrystals. The special type of quasicrystal with which we will be dealing in this paper is the *T*-phase quasicrystal. It is periodic along one axis, but quasiperiodic in the plane perpendicular to this axis.

During the last few years more and more evidence for the existence of such quasicrystalline structures has been collected. Primarily the detailed analysis of x-ray-diffraction patterns yielded strong support for this model; we mention in particular the thorough work of Steurer[5] and Steurer and Kuo[6] who used the method of high-dimensional embedding to derive electron-density distributions and the positions of the individual atoms from x-ray-diffraction patterns.

Among the various experimental methods known to provide information on the structural properties of a crystal, fast ion channeling has not been used up to now for the investigation of quasicrystals. In contrast to the diffraction methods, which sample reciprocal space, ion channeling is able to give direct information about the structure of a crystal in real space. However, the observation of channeling requires the existence of linear and planar arrangements of the atoms in a crystal. Until very recently it was unknown whether such atomic strings or planes also exist in a quasicrystal. In a computer study on icosahedral quasicrystals Kupke *et al.*[7] showed that (i) the atoms of a quasicrystal also form strings and planes, although in contrast to ordinary crystals the occupation of these strings and planes by atoms is not uniform, and that (ii) fast ion channeling should be feasible in quasicrystals. So far only the experimental realization was missing.

In the present Rutherford-backscattering spectroscopy (RBS) we show, to our knowledge for the first time, that ion channeling is indeed possible in quasicrystalline structures and is useful in confirming their structure. For this purpose we used a $0.8\times0.8\times0.8$ mm$^3$ *T*-phase $Al_{62}Cu_{20}Co_{15}Si_3$ quasicrystal grown by one of us (R.W.) at the crystal laboratory of the Institut für Festkörperforschung (IFF) at the Forschungszentrum Jülich. A detailed description is found in Ref. 8.

The RBS measurements were performed using a beam of 2-MeV $^4He^+$ ions (beam size at the target, $0.5\times0.5$ mm $^2$; angular spread of the ion beam, $\pm0.05°$). For the recording of the channeling profiles, the backscattering rate of these ions was measured during angular scans across several axes and planes of the quasicrystal.

Figure 1 shows typical backscattering spectra obtained from this quasicrystal for ion incidence along a "random"

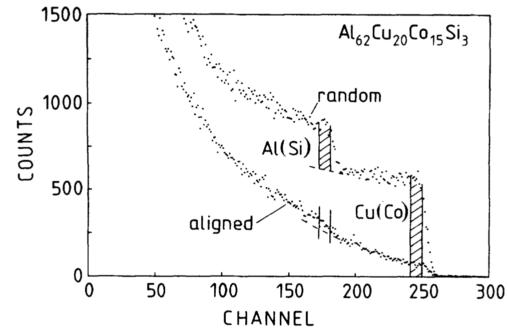

FIG. 1. Rutherford-backscattering spectra of 2-MeV He ions as obtained from a $T$-phase $Al_{62}Cu_{20}Co_{15}Si_3$ quasicrystal for ion incidence along a "random" direction and along the decagonal axis. For the channeling measurements presented in the subsequent figures two energy windows were set at about channel 175 and channel 245 in order to obtain the Al (Si) and Co (Cu) yield.

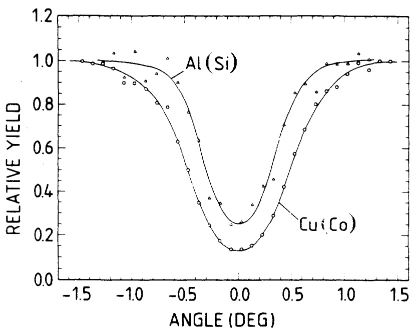

FIG. 2. Rutherford-backscattering profiles as obtained from an angular scan through the decagonal axis of a $T$-phase $Al_{62}Cu_{20}Co_{15}Si_3$ quasicrystal. The lines are drawn to guide the eyes.

direction, i.e., an arbitrary direction, and along the decagonal axis. According to the stoichiometry of the crystal, the backscattering spectrum consists of two parts: the scattering by the two light elements Al and Si superimposed on the scattering by the two heavy elements Co and Cu. Because of the 15-keV energy resolution of the detector, neither the Co and Cu scattering nor the Al and Si scattering can be resolved. For the recording of the Co (Cu) yield, an energy window was set on the Co (Cu) spectra as indicated in Fig. 1. In order to obtain the Al (Si) scattering, an appropriate second window was set (see Fig. 1) and the Co (Cu) scattering was subtracted. The latter was obtained from the extrapolation of the high-energy scattering data by a fit function.

Figure 1 further shows that the backscattering rate for ion incidence along the decagonal axis is strongly suppressed due to axial channeling along this axis. This can be seen more clearly from Fig. 2 where the Co (Cu) and the Al (Si) scattering rates are plotted versus the angle of ion incidence. Both yield profiles show pronounced channeling minima with minimum yields $\chi_{\min}$ of 0.13 and 0.25, and angular half widths $\psi_{1/2}$ (half width at half minimum) of 0.51° and 0.37°, respectively. If we use these values in Barrett's formula[9] for ion channeling in periodic, monatomic structures [see Eq. (2) of Ref. 7], with $E=2.0$ MeV and $\bar{u}=7.0$ pm, we find a mean atomic charge per unit string length of $\langle Z_2/d\rangle=41.4$ per nm. Since the mean atomic charge of the atoms of this quasicrystal is $\langle Z_2\rangle=18.3$, one then finds an interatomic distance of $d=0.44$ nm. This is close to the values found in other investigations, which are in the range 0.408–0.428 nm (cf. e.g., Ref. 6). Channeling computer simulations[10] based on the structure model derived by Steurer and Kuo[6] for this system show that full agreement is obtained between calculated and experimental angular half widths when a proper treatment is adopted. These calculations also show that the difference between the Co (Cu) and Al (Si) profiles is almost completely explained by the different thermal vibration amplitudes of the atoms.

The existence of axial channeling along the decagonal axis is, however, nothing spectacular, since $T$-phase quasicrystals are periodic along this axis with the lattice atoms forming strings of a fixed interatomic distance $d$. Thus axial channeling along this row should exist; only the arrangement of the strings in the transverse plane and the shapes of the channels formed by these strings are quasiperiodic. Nevertheless, the relatively deep minimum in the Cu (Co) scattering of $\chi_{\min}=0.13$ indicates that the quasicrystal is of relatively good quality.

In a further series of experiments, the planar structure of this quasicrystal was examined. Figure 3 shows the Co (Cu) yields obtained from various angular scans in the (angular) neighborhood of the decagonal axis. In these scans the quasicrystal was rotated with respect to the ion beam (which is incident horizontally on the target) about a vertical axis (angle of rotation $\theta_x$) at fixed tilt angles $\theta_y$ of the sample (rotation about a horizontal axis) and the scattering yield measured as a function of $\theta_x$. The yield profiles shown in Fig. 3 pertain to scans exactly through the decagonal axis ($\theta_y=-4.5°$) and scans at short ($\theta_y=-5.8°$ and $-6.9°$) and somewhat larger angular distances ($\theta_y=0°$, 1.1°, and 2.2°) from this axis. Besides the deep minimum observed for the scan through the decagonal axis, several shallow minima are seen in the other scans. They apparently are due to channeling in planes which have the decagonal axis in common. Because of the great number of equivalent planes in the neighborhood of the decagonal axis the planes are partially overlapping. This is particularly pronounced for the scans close to the decagonal axis; for the larger distances (upper part of figure) they are well separated. In Fig. 4 the angular positions of the more pronounced minima are plotted in a $\theta_x,\theta_y$ graph as is commonly used for crystal orientation purposes in ion-beam experiments[11] (we want to note that these positions are not well defined in the very neighborhood of the decagonal axis due to the overlapping mentioned above). As the figure shows, these minima mark planes which have the decagonal axis in common; the stronger planes, i.e., planes that show the deeper minima (indicated by thick lines in Fig. 4), meet at angles of 36° with each other, thus proving the decagonal symmetry of the quasicrystal, while a set of weaker planes (thin lines) is found halfway between the main planes.

The existence of such planes and the observation of ion channeling in the channels formed by these planes is by no

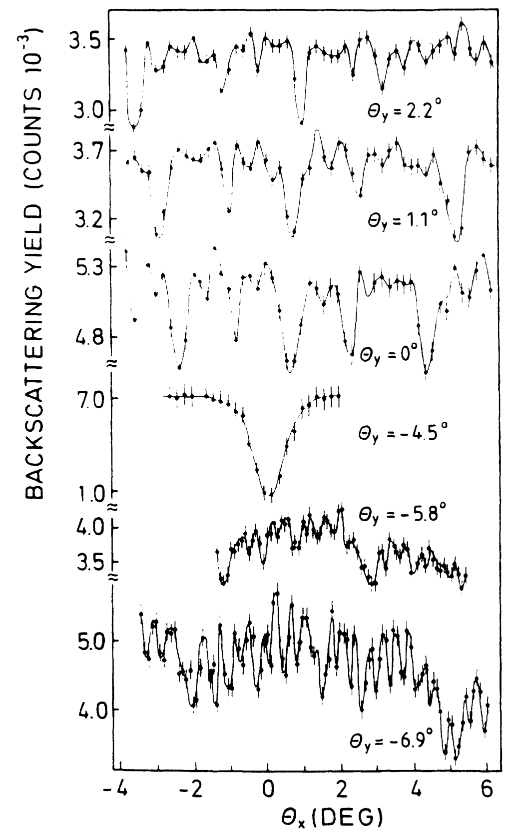

FIG. 3. Rutherford-backscattering yield profiles [Co (Cu) scattering] as obtained from angular scans in the (angular) neighborhood of the decagonal axis of a *T*-phase $Al_{62}Cu_{20}Co_{15}Si_3$ quasicrystal. During the scans (rotation about a vertical axis, angle $\theta_x$) the quasicrystal was kept at various fixed tilting positions $\theta_y$. Channeling in the decagonal axial channel and in various planar channels is clearly visible. For short angular distances from the decagonal axis ($\theta_y = -6.9°$ and $-5.8°$) the planar channeling dips are partially overlapping, while they are well separated for larger distances (upper part of figure). The lines are drawn to guide the eyes.

means trivial. It requires the existence of *linear atomic arrangements* in the quasiperiodic layers of (locally) decagonal symmetry in the crystal which, stacked together periodically, form the planes observed in the channeling experiment. Thus, the observation of channeling by these planes may be considered as an independent proof of the quasicrystalline structure of this crystal. This proof is somewhat more straightforward than that by diffraction experiments since ion channeling directly images the real structure of the crystal.

Besides the pronounced dips arising from channeling along the decagonal axis and in the system of planar channels discussed above the yield profiles shown in Fig. 3 also exhibit additional smaller dips. They are due to channeling in crystal planes that apparently are less densely occupied by lattice atoms and, therefore, exert only weaker steering forces on the motion of channeled ions. These planes are indicated by dashed lines in the orientation diagram of Fig. 4 (because of the overlapping effect only dips from the scan at large distance from the decagonal axis, i.e., for $\theta_y = 2.2°$ are used for this purpose). In Table I the angular positions of these planes as derived from Fig. 4 (counted from the main planes) are listed together with the angles obtained from the evaluation of corresponding linear arrangements of vertices in a two-dimensional Penrose pattern. As the table shows, there is close agreement between these values, once more proving the quasicrystalline nature of the crystal.

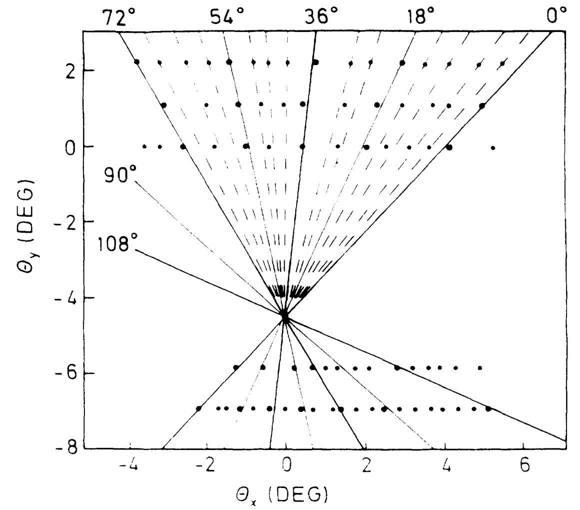

FIG. 4. Orientation diagram of a *T*-phase quasicrystal as obtained from the channeling results of Fig. 3. Besides the decagonal axis at $\theta_x = 0°$, $\theta_y = -4.5°$, various strong, intermediate, and weak planes (thick, thin, and dashed lines, respectively) are indicated which show the tenfold symmetry of the quasicrystal. The numbers indicate the azimuthal angles of the various planes. The azimuthal angles of the planes indicated by dashed lines are listed in Table I.

Figure 5 finally shows backscattering yield profiles from an angular scan across the main planar system of the quasicrystal for scattering by the Co (Cu) atoms and Al (Si) atoms. Both profiles exhibit minima of about equal depths and angular widths: $\chi_{\min} = 0.79$ and 0.77, $\psi_{1/2} = 0.112°$ and 0.104° for Co (Cu) and Al (Si) scattering. This indicates that the Co (Cu) and Al (Si) atoms are well aligned in planes that are common to all the atom species. Perhaps the most striking feature is the presence

TABLE I. Comparison of the angles included by linear arrangements of vertices in a two-dimensional Penrose grid and angles between planes parallel to the decagonal axis (counted from the main planes) of a *T*-phase quasicrystal as derived from the present channeling measurements.

| Penrose | Channeling | Penrose | Channeling |
|---|---|---|---|
| 0° | 0° | 9.732° | · · · |
| 2.491° | 2.5° | 10.925° | · · · |
| 4.386° | 4.1° | 13.614° | 13.9° |
| 5.554° | 5.6° | 15.017° | · · · |
| 6.645° | · · · | 15.510° | 15.5° |
| 7.563° | 7.8° | 18° | 18.0° |

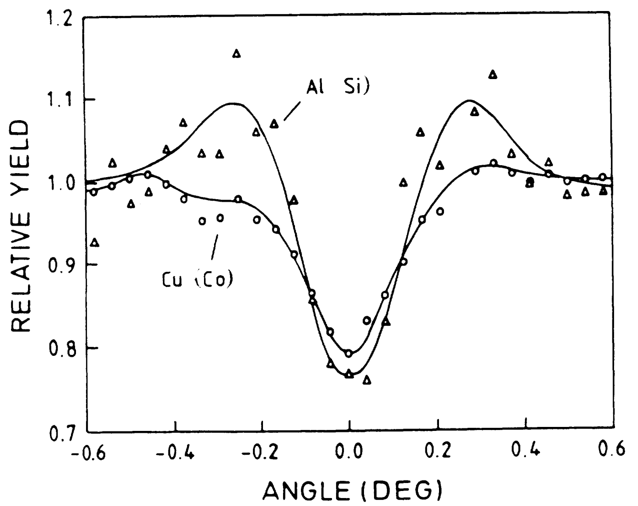

FIG. 5. Backscattering profiles from an angular scan across the main planar system parallel to the decagonal axis of an $Al_{62}Cu_{20}Co_{15}Si_3$ $T$-phase quasicrystal.

of high shoulders in the Al (Si) scattering; they indicate that at least part of these atoms are slightly displaced from the planes. For a more detailed analysis of the channeling data, however, a comparison with calculations is needed, which will be presented in a subsequent paper.

This study has verified that real-space atomic strings and planes having the correct $T$-phase quasicrystal symmetry exist in an $Al_{62}Cu_{20}Co_{15}Si_3$ alloy by observing both planar and axial channeling patterns having these symmetries. It has also been shown that ion channeling is very well able to provide structural information on the individual atom species present in a sample, information which is hardly obtainable by other methods (with perhaps the exception of neutron scattering). Hence channeling in particular should yield valuable information on the decoration of a quasicrystalline structure with the different atoms of the sample. A more detailed study which takes advantage of these possibilities will be published in a subsequent paper. Perhaps the most useful application of ion channeling will be its use for the localization of foreign atoms and the study of lattice imperfections, subjects which have been investigated by this method with great success on ordinary crystals in the past.

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