PHYSICAL REVIEW B

CONDENSED MATTER

THIRD SERIES, VOLUME 35, NUMBER 2 15 JANUARY 1987-I

Structure of Al-Mn-Cr-Si quasicrystals studied by pulsed neutron scattering

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(Received 22 August 1986)

The atomic structure of rapidly quenched quasicrystals, $Al_{80}Mn_{20}$, $Al_{75}Mn_{20}Si_5$, and $Al_{75}Mn_{15}Cr_5Si_5$, was studied by pulsed neutron scattering. The pair distribution function was obtained by a direct Fourier transformation of the structure factor, and by assuming isomorphous substitution of Cr for Mn the differential distribution function (DDF) was determined. The addition of Si was found to increase the medium-range order significantly. The DDF from Mn atoms indicates the presence of a quasicrystalline substructure which is occupied both by Mn and Al atoms. The atomic structure of these solids, therefore, is significantly different from that of quasicrystalline $Pd_{58.8}U_{20.6}Si_{20.6}$.

I. INTRODUCTION

The recent discovery of an icosahedral phase in a rapidly quenched Al-Mn alloy[1] has created strong interest because of the possibility that this phase may be quasicrystalline.[2] However, even though the symmetry of the solid has been specified, the actual atomic structure of this solid remains unknown,[3] while another icosahedral solid, $Pd_{58.8}U_{20.6}Si_{20.6}$, was recently found to have a quasicrystalline sublattice decorated by uranium atoms.[4] In order to investigate directly the atomic structure of icosahedral Al-Mn, we carried out a pulsed neutron scattering study of Al-Mn-Cr-Si icosahedral compounds. The use of neutrons is particularly attractive in studying the atomic structure of these solids, because the neutron scattering length of Mn is negative, while that of Cr is similar in magnitude and opposite in sign[5] ($b_{Mn}=-0.373\times 10^{-12}$ cm and $b_{Cr}=0.364\times 10^{-12}$ cm). Since Mn can be substituted by Cr without an apparent disturbance to the structure,[1] if we assume that the substitution is totally random, it is possible to determine the compositionally resolved local structure[6] by the isomorphous substitution of Mn by Cr.

However, because the icosahedral solid lacks translational symmetry, conventional methods of crystallographic data reduction cannot be applied. Instead, we used methods commonly employed to study noncrystalline solids, namely atomic pair distribution function (PDF) and differential distribution function (DDF) analyses.[6,7] The spallation pulsed neutron source is preferred since the high kinetic energies of neutrons from this source make it possible to determine the structure factor over a very wide range of scattering vector,[8] Q, typically up to 25 Å^{-1} or more, thus increasing the spatial resolution of the PDF.

II. EXPERIMENTAL METHODS

Rapidly quenched ribbons of $Al_{84}Mn_{16}$, $Al_{80}Mn_{16}Si_4$, and $Al_{80}Mn_{12}Cr_4Si_4$ were produced by melt spinning. The thickness of the ribbon was about 30 μm, and the width was typically about 2 mm. The neutron scattering measurements were carried out at the Intense Pulsed Neutron Source (IPNS) of Argonne National Laboratory, on the Special Environment Powder Diffractometer (SEPD) beamline. The samples, about 3 gm each, were enclosed in a thin-walled vanadium container in a helium atmosphere and cooled to about 10 K by a Displex closed-cycle refrigerator. The energy spectra of the scattered neutrons were collected simultaneously at five angles, 14°, 30°, 60°, 90°, and 150°, for 10 h. At each angle, from 8 to 20 detectors were placed side by side, but electronically time focussed so that the spatial spread of the detectors would not deteriorate the resolution in Q.[9] The Q resolution is dependent upon the scattering angle, but, for example, at the 90° scattering angle, it is about 0.06 Å^{-1} FWHM. The data were corrected using the GLASS program of IPNS, for the source spectrum, absorption, multiple scattering, inelastic scattering (Placzek correction[10]), incoherent scattering, and other backgrounds such as the scattering from the container, to obtain the structure factor, up to $Q=25-28\ \text{Å}^{-1}$. The corrected and normalized total (elastic and inelastic) scattering intensity, $I(Q)$, and the total structure factor, $S(Q)$, can be expressed in terms of the compositionally resolved partial structure factors, after subtracting the Laue monotonic term, as[5,6]

$$I(Q)=\sum_{\alpha,\beta} c_\alpha c_\beta b_\alpha b_\beta S_{\alpha\beta}(Q)\ , \tag{1}$$

$$S(Q)=I(Q)\Big/\left[\sum_{\alpha} c_\alpha b_\alpha\right]^2 , \tag{2}$$

where α and β denote elements, c_α and b_α are the concentration and the neutron coherent scattering length of the element α, and $S_{\alpha\beta}(Q)$ is the partial structure factor involving α and β,

$$S_{\alpha\beta}(Q)=\frac{1}{N}\sum_{i,j}\exp(i\mathbf{Q}\cdot\mathbf{r}_{i,j})\rho_{i\alpha}\rho_{j\beta}\ , \tag{3}$$

where $\mathbf{r}_{i,j}$ is the separation between the ith and jth atoms, and

$$\rho_{i\alpha}=\begin{cases}1, & \text{when } i\text{th atom is element } \alpha\\ 0, & \text{otherwise}\ .\end{cases} \tag{4}$$

The PDF was then obtained by the direct Fourier transformation,

$$\rho(r)=\rho_0+\frac{1}{2\pi^2 r}\int[S(Q)-1]\sin(Qr)Q\,dQ\ . \tag{5}$$

Most of the time no termination correction was applied, since the range of the Q vector was wide enough for the structure factor to converge to unity within the range observed. The PDF of fcc Al powder used as a standard is shown in Fig. 1, together with the theoretical PDF which was widened by a Gaussian function which represents the zero-point motion. For the width of the Gaussian function we chose a weak linear function of r,

$$\sigma(r)=\sigma(0)+\sigma' r\ , \tag{6}$$

where $\sigma(0)=0.086$ Å and $\sigma'=0.002$, which gives a satisfactory description of the width. The calculated PDF shows excellent agreement with the experimental results up to very high values of r, except for small ripples. The value of $\sigma(0)$ is slightly higher than the theoretically estimated value,[11] $\sigma(0)=0.056\sim0.060$, possibly due to the termination effect and lattice imperfections in the powdered sample.

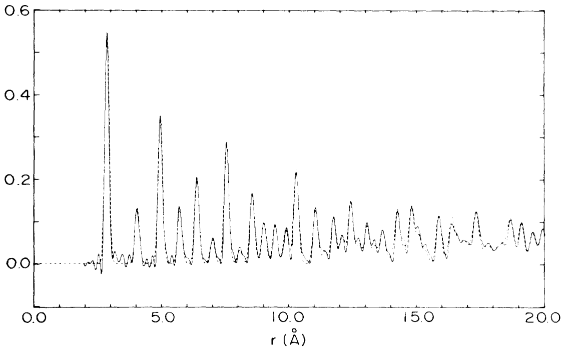

FIG. 1. Pair distribution function of fcc Al determined by the pulsed neutron scattering (solid curve) and the theoretical PDF with Gaussian broadening (dashed curve).

III. EXPERIMENTAL RESULTS

The structure factor of the three samples studied is shown in Fig. 2. All the samples contained, in addition to the icosahedral phase, grains of segregated fcc Al and a very small amount ($<1\%$) of other crystalline phases. The diffraction peaks belonging to the icosahedral phase were indexed after Bancel *et al.*[12] The peak positions in

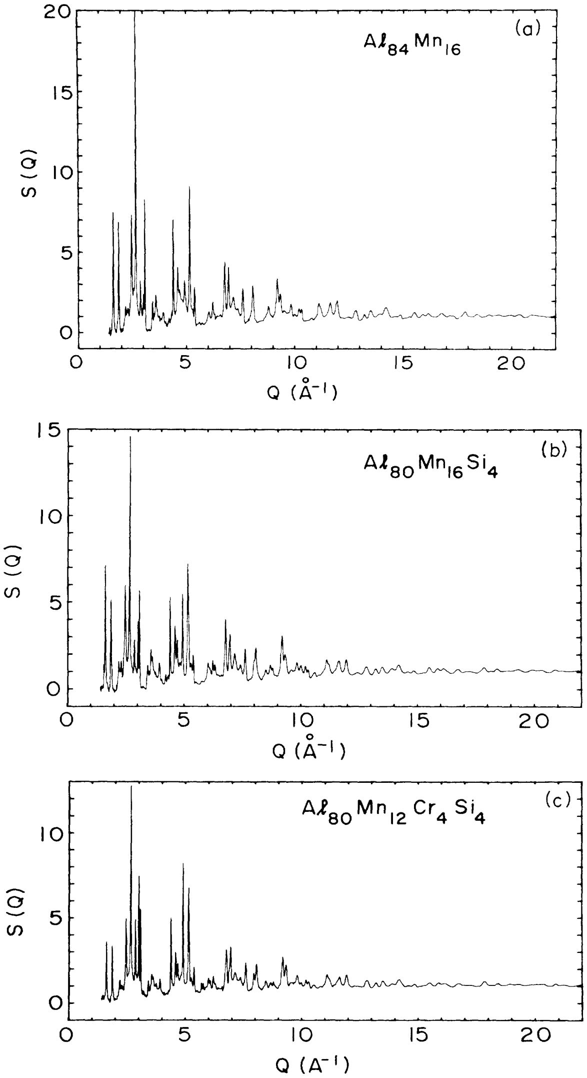

FIG. 2. Neutron structure factor of rapidly quenched (a) $Al_{84}Mn_{16}$, (b) $Al_{80}Mn_{16}Si_4$, and (c) $Al_{80}Mn_{12}Cr_4Si_4$.

TABLE I. Calculated compositions of the icosahedral phases and amounts of Al precipitates.

Nominal composition	fcc Al (at. %)	Approximate composition of the icosahedral phase
$Al_{84}Mn_{16}$	18	$Al_{80}Mn_{20}$
$Al_{80}Mn_{16}Si_4$	20	$Al_{75}Si_5Mn_{20}$
$Al_{80}Mn_{12}Cr_4Si_4$	19	$Al_{75}Si_5Mn_{15}Cr_5$

the structure factor of the I phase match those of the x-ray structure factor, but the intensities are significantly different. As shown in Fig. 2, compared to the x-ray diffraction pattern[12] the intensities of the (100000) and (110000) peaks are generally weaker, while those of $(11\bar{1}00\bar{1})$ and $(2\bar{1}\,\bar{1}0\bar{1}0)$ peaks are much stronger. The diffraction peaks due to crystalline Al were subtracted from the total structure factor using the experimental structure factor for Al. By this subtraction process the relative amounts of Al precipitates were determined to be about 19 at. %, and the compositions of the icosahedral phases were calculated as shown in Table I. The amount of the additional crystalline phases was small enough not to produce significant effects on the analysis below. Since Mn atoms carry a magnetic moment[13] the diffraction intensity includes magnetic contributions. A preliminary study of the temperature dependence, however, shows that the magnetic contributions are negligibly small.

The PDF of $Al_{80}Mn_{20}$ is shown in Fig. 3. We used the atomic number density ρ_0 of 0.0628 $Å^{-3}$, which was calculated from the result of the physical density measurement[14] by correcting for the Al inclusion. It should be noted that peaks due to Al-Mn pairs appear as *negative* peaks, because b_{Mn} is negative. For instance the strong negative peak at around 2.5 Å is due to the Al-Mn nearest neighbors. The atomic correlation becomes weak beyond 10 Å, almost as in glasses. As shown in Fig. 2, replacing a part of Al (5%) by Si produced relatively small changes in the peak intensities, except for (110000) at 3.045 $Å^{-1}$ and (101000) at 4.928 $Å^{-1}$ which became noticeably higher. However, these changes resulted in significant changes in the PDF. As shown in Fig. 4 the magnitudes of the Al-Mn peak at 2.5 Å and the first peak at around 2.9 Å are reduced, while the medium-range order in the 5–20 Å range is markedly increased by the Si addition. Shown in Fig. 5 is the difference PDF due to the addition of Si, which is the Fourier transformation of the difference structure factor,

$$\Delta S_{Si}(Q)=[I_{Al_{75}Mn_{20}Si_5}(Q)-I_{Al_{80}Mn_{20}}(Q)]/\langle b\rangle^2 , \quad (7)$$

where $\langle b\rangle$ is the average between the compositional averages for these two compositions. It is observed that the effect of Si is to replace some of the Al-Al distances at around 2.8 Å with shorter Si-Al distances of about 2.46 Å, in addition to improving the medium range order.

The substitution of Cr for Mn produces more significant changes in the peak intensities of $I(Q)$. If we assume a perfect isomorphous substitution, which means that each partial structure factor remains unchanged by substitution of Cr for Mn, and,

$$S_{\alpha Cr}(Q)=S_{\alpha Mn}(Q) , \quad (8)$$

then the difference in the normalized scattering intensity caused by substituting Cr for Mn,

$$\Delta I_{Cr}(Q)=I_{Al_{75}Mn_{15}Cr_5Si_5}(Q)-I_{Al_{75}Mn_{20}Si_5}(Q) , \quad (9)$$

becomes,

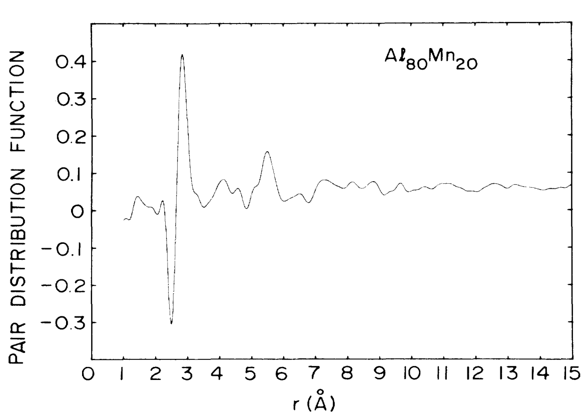

FIG. 3. Pair distribution function of icosahedral $Al_{80}Mn_{20}$ determined by neutron scattering. Note that the Al-Mn pairs appear as negative peaks since the scattering length of Mn is negative.

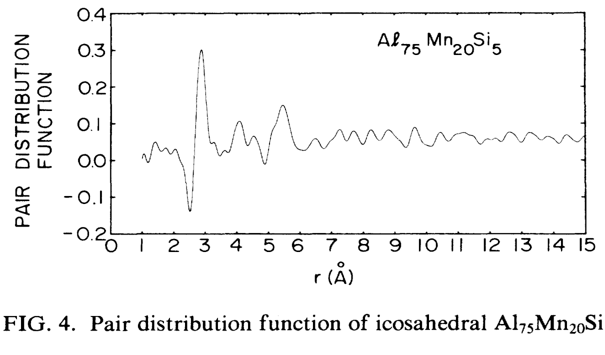

FIG. 4. Pair distribution function of icosahedral $Al_{75}Mn_{20}Si_5$.

$$\Delta I_{\mathrm{Cr}}(Q)=2c_{\mathrm{Cr}}(b_{\mathrm{Cr}}-b_{\mathrm{Mn}})[c_{\mathrm{Al}}b_{\mathrm{Al}}S_{\mathrm{Al\text{-}Mn}}(Q)+c_{\mathrm{Si}}b_{\mathrm{Si}}S_{\mathrm{Si\text{-}Mn}}(Q)+c_{\mathrm{Mn}}b_{\mathrm{Mn}}S_{\mathrm{Mn\text{-}Mn}}(Q)]+c_{\mathrm{Cr}}^2(b_{\mathrm{Cr}}^2-b_{\mathrm{Mn}}^2)S_{\mathrm{Mn\text{-}Mn}}(Q)\ , \qquad (10)$$

where $c_{\mathrm{Mn}}=0.15$. If we neglect the last term which is smaller than the other terms by two to three orders of magnitude, $\Delta I_{\mathrm{Cr}}(Q)$ is proportional to the weighted average of the partial structure factors involving Mn, an equivalent of the differential structure factor obtained by the differential anomalous x-ray scattering measurement.[4,7] Therefore we may normalize the intensity by

$$\Delta S(Q)=\Delta I(Q)/[2c_{\mathrm{Cr}}(b_{\mathrm{Cr}}-b_{\mathrm{Mn}})\times(c_{\mathrm{Al}}b_{\mathrm{Al}}+c_{\mathrm{Si}}b_{\mathrm{Si}}+c_{\mathrm{Mn}}b_{\mathrm{Mn}})] \qquad (11)$$

to obtain the differential structure factor. By the Fourier transformation of (11), similar to Eq. (5), we obtained the differential distribution function (DDF), which is shown in Figs. 6 and 7. The DDF is a pair distribution function with a particular element at the origin, in this case Mn, and describes the local environment of this element. Since the peaks are weighted by the scattering length of each element, Mn-Al and Mn-Si pairs appear as positive peaks, while Mn-Mn pairs produce negative peaks.

IV. DISCUSSION

The most salient feature of the neutron structure factor of the icosahedral phase of the $\mathrm{Al_{80}Mn_{20}}$ compound is that the two most intense peaks of the x-ray structure factor, namely the (100000) and (110000) peaks, are quite weak. This indicates, since the neutron scattering length of Mn is negative, that the Al-Al contribution and the Al-Mn contribution to these peaks are about equal and canceling each other. This fact is rather surprising because the scattering lengths of Al and Mn are similar in magnitude though opposite in sign, while the concentration of Mn in this compound is only 20%. Therefore, such a good cancellation suggests a stronger correlation of Al-Mn positions than the Al-Al positions. A consequence of this will be discussed later.

In the absence of translational symmetry, however, it is practically impossible to reconstruct the three-dimensional structure based upon the knowledge of the structure factor alone without any phase information. Therefore as an intermediate step toward such a goal, we employed noncrystallographic methods of PDF and DDF analyses. The total PDF itself was already quite informative, and revealed, for instance, a significant difference in the medium range order between $\mathrm{Al_{80}Mn_{20}}$ and $\mathrm{Al_{75}Mn_{20}Si_5}$. But far more important was the DDF, which describes the local structure around a particular element. The result shown in Figs. 6 and 7 indicates that the nearest neighbors of Mn atoms are predominantly Al atoms, and the maximum of the nearest-neighbor peak is located at about 2.62 Å, with a small shoulder at around 3.04 Å. This observation is in good agreement with the extended x-ray-absorption fine structure (EXAFS) results,[15–19] except that the height of the shoulder observed here is lower than that of the EXAFS results. The apparent coordination number of the first peak, obtained by integrating the DDF times $4\pi r^2$ from 2.2 to 2.9 Å, is 12.2, while that of the shoulder (2.9 to 3.26 Å) is 2.8. The total coordination number, 15.0, is rather high, but this is primarily the consequence of assuming no compositional short-range order (CSRO) and assigning the average scattering length $\langle b\rangle$ for each neighbor. If we assume that all the nearest neighbors of Mn are Al, however, the total coordination number is reduced to 8.9. Therefore, as suggested by Elser and Henley[20] and Guyot and Audier[21] and by the EXAFS measurement by Marcus *et al.*,[16] it is most likely that the local environment of the Mn atom is similar to that in the α-AlMnSi in which Mn atoms have either 9 or 10 Al nearest neighbors.[22]

A recent EXAFS measurement also suggested Mn-Mn distances of 4.46 and 5.04 Å.[19] The comparison of the total PDF in Fig. 3 and the Mn DDF in Fig. 6 shows that the sharp valleys at 4.5 Å and at 5.1 Å in Fig. 6 correspond to positive peaks in Fig. 3, indicating that they indeed represent the Mn-Mn distances. On the other hand, as shown in Fig. 6, many of the pronounced peaks due to Mn-Al correlations in the Mn DDF agree in position with the vertex-vertex distances of the quasicrystal-

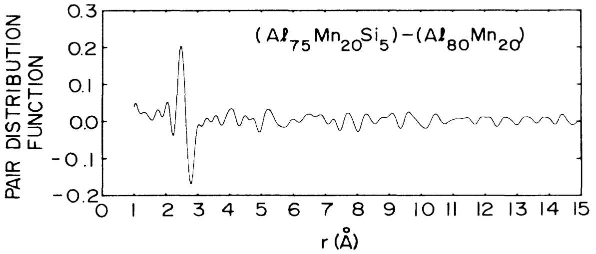

FIG. 5. The difference PDF between $\mathrm{Al_{80}Mn_{20}}$ and $\mathrm{Al_{75}Mn_{20}Si_5}$. See the text for the definition.

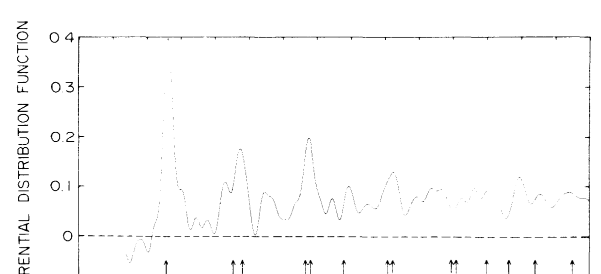

FIG. 6. Differential distribution function around Mn obtained by comparing the scattering intensities from $\mathrm{Al_{75}Mn_{20}Si_5}$ and $\mathrm{Al_{75}Mn_{15}Cr_5Si_5}$, by assuming a random substitution of Mn for Cr. The arrows indicate the quasicrystalline vertex-vertex distances with the quasicrystalline lattice parameter of 4.60 Å.

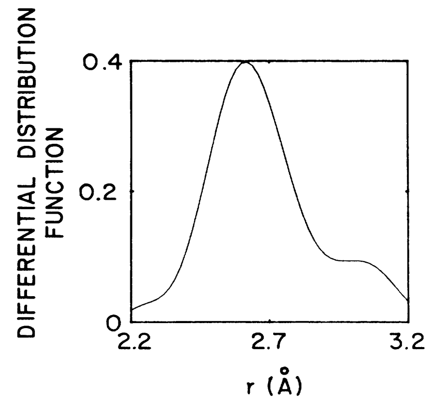

FIG. 7. Differential distribution function around Mn, in the region of the first peak.

line lattice, strongly suggesting the presence of a quasicrystalline substructure. The vertex-vertex distances of the quasicrystalline lattice were calculated using the quasicrystalline lattice constant of 4.60 Å, from the model generated by the generalized dual method[23] and supplied to us by Steinhardt. In Fig. 6 some of the distances with low occurrences are omitted. A similar substructure was observed in the U-DDF in the icosahedral phase of $Pd_{58.8}U_{20.6}Si_{20.6}$, by anomalous x-ray scattering,[4] and in that case the sublattice was mostly decorated by U. In the present case, however, the agreement is less satisfactory than the case of Pd-U-Si, and the substructure is not occupied by the minority atoms, in this case Mn, since the quasicrystalline distances are observed in the Mn-Al correlation, rather than in the Mn-Mn correlation. This result is consistent with the observation discussed earlier that the two main peaks in the structure factor contain strong contributions from the Al-Mn correlation. Such a substructure, however, is at variance with the structure proposed by Elser and Henley[20] and Guyot and Audier,[21] in which the vertex positions of the quasicrystalline lattice are either occupied by Mn or vacant. In fact the Mn-Mn distance of 5.1 Å predicted by Guyot and Audier is actually seen in Fig. 6, but their model calls for the quasicrystalline lattice constant, or the edge length of the rhombohedra, to be 4.85 Å, which is by 5% larger than 4.60 Å deduced from the diffraction data.[20] Therefore even though a structure similar to the Mn icosahedra present in the α-AlMnSi may also be found in the icosahedral phase, the way in which the icosahedra were decomposed into a collection of rhombohedral units by these authors may be incorrect. An alternative assignment of the quasicrystalline cell to the Mackay polyhedron is to take one of the Mn-Al distance on the surface of the Mackay polyhedron (a Mn atom at a corner of a triangle with the edge length of 5.1 Å, and an Al atom near the edge center of the opposing edge of the triangle) to be the edge of the rhombohedron. This assignment would require the Mackay polyhedron to be slightly deformed in the quasicrystalline structure, but such a deformation may be a natural consequence if the icosahedral phase were to be obtained by some martensitic or sheared transformation from the α phase, as can be conjectured from the observation of the direct orientational correlation between these two phases.[24]

As we mentioned earlier, the agreement of the Al-Mn distances with the quasicrystalline lattice vertex-vertex distances is less satisfactory than the case of the icosahedral phase of Pd-U-Si.[4] In addition the PDF of $Al_{80}Mn_{20}$ suggests a higher degree of disorder in this compound. Therefore, not only the structure of the Al-Mn-Si compound is fundamentally different from that of Pd-U-Si, as shown by the different decoration of the quasicrystalline lattice vertices, but also there may be a significant difference in the density of defects between these two compounds. Interestingly, however, even if such a difference exists, it is not directly reflected in the diffraction peak widths. For instance, even though the addition of Si is known to reduce the peak widths considerably and improve the correlation,[25] the correlation length in $Al_{80}Mn_{20}$ deduced from the diffraction peak widths[12] is more than 100 Å, while Fig. 3 shows that the correlation beyond 10 Å is rather weak. A possible explanation of this discrepancy is that the nature of disorder is primarily chemical rather than topological.

In obtaining the DDF we assumed that Cr atoms randomly substitute Mn atoms in $Al_{75}Mn_{20}Si_5$. In crystalline alloys such an assumption can be checked by examining the superlattice diffraction or diffuse scattering. But in the quaiscrystalline structure the diffraction peaks are densely populated,[2] and a superlattice can only modify the intensity rather than create new diffraction peaks. Therefore the assumption of random substitution cannot be easily checked. Even when the Cr substitution is not random, however, the DDF in Figs. 6 and 7 can be interpreted as suggesting the presence of a quasicrystalline substructure viewed from the Cr atoms in the icosahedral phase of $Al_{75}Mn_{15}Cr_5Si_5$.

V. CONCLUSION

The pulsed neutron scattering experiment was carried out on rapidly quenched alloys of several compositions, $Al_{84}Mn_{16}$, $Al_{80}Mn_{16}Si_4$, and $Al_{80}Mn_{12}Cr_4Si_4$. The samples contained about 80% of icosahedral phase and 20% of fcc Al. The structure factor, after subtracting the contribution from the Al phase, was directly Fourier transformed to obtain the pair distribution function. It was found that the atomic correlations in the icosahedral $Al_{80}Mn_{20}$ are rather weak beyond 10 Å, while the correlations are much improved by substituting 5 at. % of Al by Si. By assuming a random substitution of Mn for Cr, the differential distribution function around Mn, or the PDF with Mn atoms at the origin, was obtained. The Mn DDF showed good agreement with the vertex-vertex distances of a quasicrystalline lattice, suggesting the presence of a quasicrystalline substructure. Unlike the icosahedral Pd-U-Si alloy, however, the substructure is not decorated with the minority component alone, in this case Mn, but both by Al and by Mn, and the quasicrystalline distances are clearly seen in the Al-Mn correlation. This result apparently is not in agreement with the models proposed recently based upon the structure of the α phase AlMnSi.

ACKNOWLEDGMENTS

The authors are grateful to D. D. Kofalt and Yu Wu for technical assistance, and to D. L. Price, P. J. Steinhardt, P. A. Heiney, P. A. Bancel, S. J. Poon, and J. A. Leake for useful comments and discussions. The research was sponsored by the National Science Foundation through Grants No. DMR-83-18816 and DMR-82-16718. The Intense Pulsed Neutron Source at Argonne National Laboratory is operated as a user facility by the U.S. Department of Energy, Basic Energy Science Program (Division of Materials Sciences), under Contract No. W-31-109-Eng-38.

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