Science on Form: Proceedings of the First International Symposium for Science on Form,
General Editor: S. Ishizaka, Editors: Y. Kato, R. Takaki, and J. Toriwaki, 621–624.

High-resolution Electron Microscopy of Al-Mn-Si Quasicrystal

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Keywords: High-resolution electron microscopy, Al-Mn-Si quasicrystal

A high-resolution electron micrograph of a melt-quenched Al-Mn-Si quasicrystal, taken with the incident beam parallel to the fivefold symmetry zone axis, was interpreted well in terms of the projection of a three-dimensional Penrose tiling. In the observed image, there are various size pentagons formed with bright dots, which have edge lengths inflated and deflated with a scaling factor of the golden mean τ. Characteristic features of the image support that elementary golden rhombohedra in the three-dimensional tiling have an edge length of 0.46 nm. The inflation of the pentagons leads us to an atomic arrangement model of the elementary golden rhombohedra.

INTRODUCTION

High-resolution electron micrographs taken under certain conditions reproduce faithfully the topological properties of projected structures within a good approximation, although it is not easy to lead directly to an atomic structure determination from the observed images. An icosahedral quasicrystal, which was discovered in melt-quenched Al-Mn alloys by Shechtman, Blech, Gratias and Cahn (1984), is a most interesting subject for high-resolution electron microscopists; actually a number of high-resolution observations have been made for a year (Hiraga et al. (1985 a), Bursill and Lin (1985) and Portier et al. (1985)). In this paper, we present a high-resolution image of a melt-quenched Al-Mn-Si alloy, which is known to form a higher ordered quasicrystal than the Al-Mn alloy, and we aim to interpret characteristic features of the observed image in terms of a three-dimensional Penrose tiling.

RESULTS AND DISCUSSION

Figure 1 is a high-resolution image of an $Al_{74}Mn_{20}Si_6$ alloy prepared by a melt-quench method, taken with the incident beam exactly parallel to the fivefold symmetry zone axis, together with an electron diffraction pattern (b) and an optical diffractogram (c) of the image. The image is similar to that observed previously in an Al-Mn alloy (Figs. 1 and 2 of Hiraga et al. (1985 a)), but has a lower resolution than Fig. 2 of Hiraga et al. (1985 b). In the image, we notice two characteristic features on the distri-

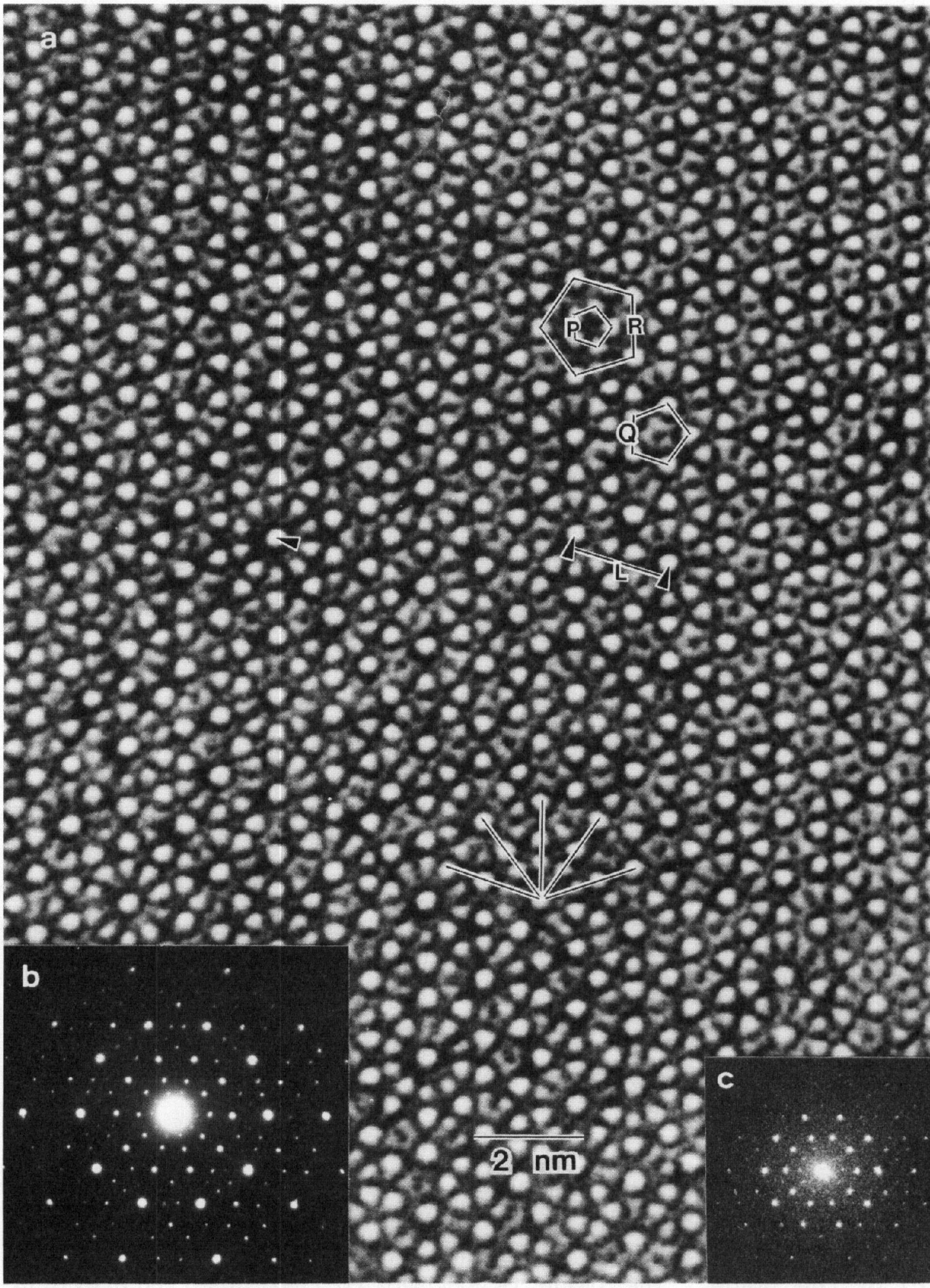

Fig. 1 High-resolution electron micrograph of a melt-quenched $Al_{74}Mn_{20}Si_6$ alloy taken with the incident beam parallel to the fivefold symmetry zone axis.

bution of bright dots lying along the fivefold directions; the first is the existence of various size pentagons formed with bright dots, and the second is the appearance of double rings, each of which consists of ten bright dots surrounding a central dot as marked by arrows. The three pentagons P. Q and R in the image have edge lengths of 0.42, 0.68 and 1.1 nm, respectively, which have approximately a ratio of τ (golden mean).

Similar pentagons can be seen in the projection of a three-dimensional Penrose tiling along the fivefold symmetry axis as shown in Fig. 2. This is a balls and sticks model based on a Penrose skeleton formed by Ogawa (Fig. 4(a) of Hiraga et al. (1985 **b**)). In the model, we notice that many pentagons with various sizes are formed with balls which correspond to vertices of the elementary golden rhombohedra, and the pentagons labeled as M, N, O, P, Q and R are expanded with the scaling factor of τ in linear dimension. The edge length of the pentagons P, Q and R in the model are estimated respectively to be 0.41, 0.66 and 1.07 nm, if the edge length of the elementary rhombohedra is a= 0.46 nm as was proposed by comparison between calculated and experimental diffraction patterns (Elser (1985)). These values coincide very well with the edge lengths of P, Q and R pentagons in the image of Fig. 1. Also the double rings in the observed

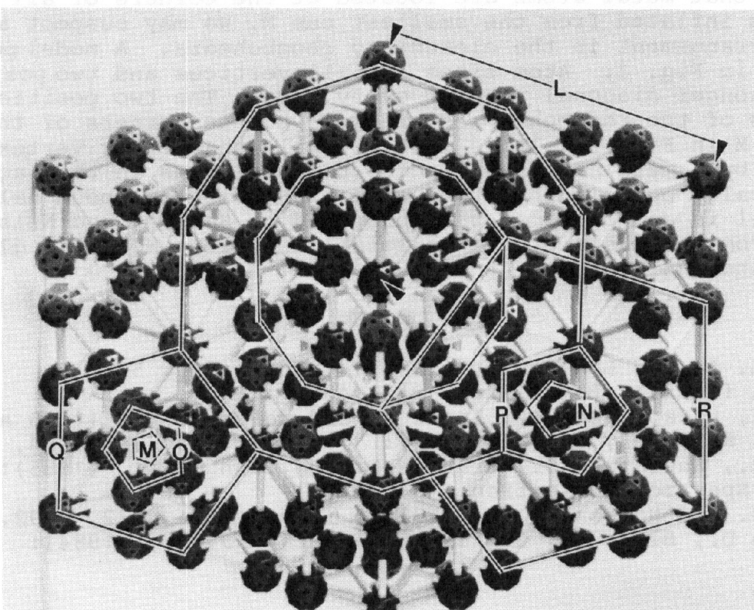

Fig. 2 A three-dimensional Penrose tiling projected along the fivefold axis. Balls correspond to the vertices of elementary rhombohedra. Pentagons P, Q and R, and a distance L correspond to those in Fig. 1. Double decagonal rings surrounding a vertex of expanded rhombohedra correspond to double rings of bright dots surrounding the bright dot marked by an arrow in Fig. 1. Pentagons M, N and O are those deflated with a factor of τ.

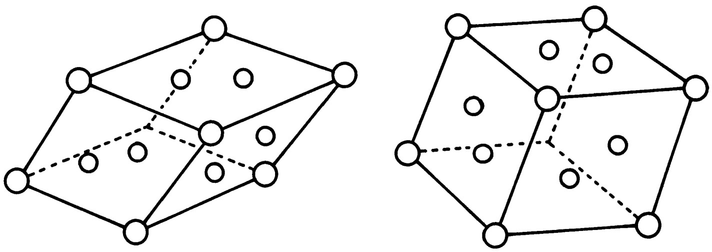

Fig. 3 Atomic sites in the elementary rhombohedra. Small circles indicate the sites with occupation probability of about half. Only the sites on three faces are shown.

image correspond well with double decagons surrounding a vertex of the extended rhombohedra marked with an arrow in Fig. 2.

The inflation and the deflation of the pentagons in the observed image and consequently of reflection spots in the electron diffraction pattern lead us to the existence of smaller pentagons such as O, N and M in Fig. 2 dwindling with the scaling factor of τ, although they may not be resolved in the present experiment. Provided that metal atoms are located at the corners of all the pentagons inflated from the smallest one M, we may suspect an atomic arrangement in the elementary rhombohedra. A model poposed is shown in Fig. 3. Atom sites are all vertices and two positions along a longer diagonal line of every face. The two positions in the faces of the rhombohedra correspond to the corners of the pentagon M in Fig. 2. It is most probable that every vertex is occupied by a metal atom, while the two positions in the faces are statistically occupied by atoms with a fraction of about half. This model is analogous to that proposed by Sachdev and Nelson (1985) from the basis of the correlation between metallic glasses and icosahedral crystals.

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