Diffraction Pattern and Layer Structure of a Quasilattice

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Structure calculations are reported for a quasilattice associated with the icosahedral group. The diffraction pattern is computed in a one-center and long-range approximation and compared to experiments on Al + 14% Mn. Edge and vertex positions of the quasilattice are computed in a projection onto a plane with a layer structure.

In this note we report on computations for a quasilattice associated with the icosahedral group described in [1, 2]. For simplicity we assume that there is a single atomic center at each vertex. The diffraction pattern is computed in the long-range approximation formulated in section 5 of [2]. The δ-distributions of Eq. (5.24) have been replaced by distributions of the finite width $0.25\,\pi L^{-1}$. The position of points in $\boldsymbol{K}$-space is characterized from Eqs. (5.21, 5.22) by

$$\boldsymbol{K} = L^{-1}\, 2\pi \tfrac{1}{2} \sum_i h_i \boldsymbol{e}_i\,, \quad h_i = 0, \pm 1, \pm 2, \ldots, \qquad (1)$$

where the six vectors $\boldsymbol{e}_i$ are unit vectors perpendicular to six pairs of faces of the regular dodecahedron and where L is the edge length of the rhombohedral cells. In the long-range approximation only three of the numbers h_i are non-zero. The resulting diffraction patterns are displayed in Figures 1–3. The strong peaks result from interference between several different sublattices and are characterized by pairs of Fibonacci numbers. In Table 1 we give an index system for some peaks in the plane perpendicular to the 5-fold axis.

The icosahedral diffraction pattern observed by Shechtman et al. [3] and by Bancel et al. [4] results from Al + 14% Mn and so requires two types of centers which in general would not be located in vertex positions. Disregarding these refinements we have tentatively identified the peak c observed in [4] according to Table 1, to obtain for the edge length the value

$$L = 8.8\ \text{Å}\,. \qquad (2)$$

With the same model of a single atomic center at each vertex, the quasilattice was computed for a fixed set of parameters $\gamma_1, \gamma_2, \ldots, \gamma_6$. Figures 4 and 5 show a view through the quasilattice along the direction of the fixed vector $\boldsymbol{e}_6$. The index k_6 is varied as $k_6 = -5, -3, -1, 1, 3, 5$. Figure 4 gives the resulting edges and Fig. 5 the resulting

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Table 1. Index system for the strongest diffraction peaks corresponding to Fig. 3 and tentative comparison with experimental work of Bancel et al. [4].

Index system						Notation of [4]	Q/Å^{-1}
h_1	h_2	h_3	h_4	h_5	h_6		
0	0	3	3	0	0	c	1.876
−5	0	0	0	0	5		
0	0	5	5	0	0	d	3.043
−8	0	0	0	0	8		
0	0	8	8	0	0	f	4.928
−13	0	0	0	0	13		

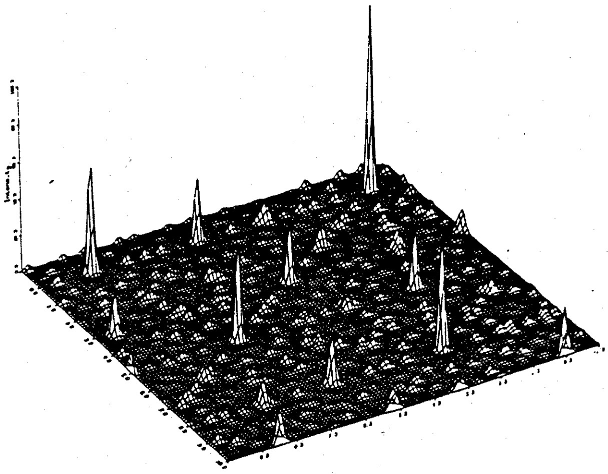

Fig. 1. Computed diffraction pattern in a plane perpendicular to the 5-fold axis. The numbers give the scale for the vector $\pi^{-1} L \boldsymbol{K}$, where L is the edge length of the rhombohedral cell.

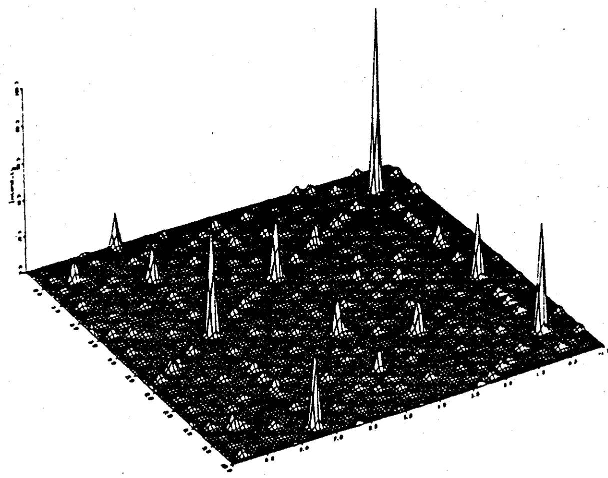

Fig. 2. Computed diffraction pattern in a plane perpendicular to the 3-fold axis.

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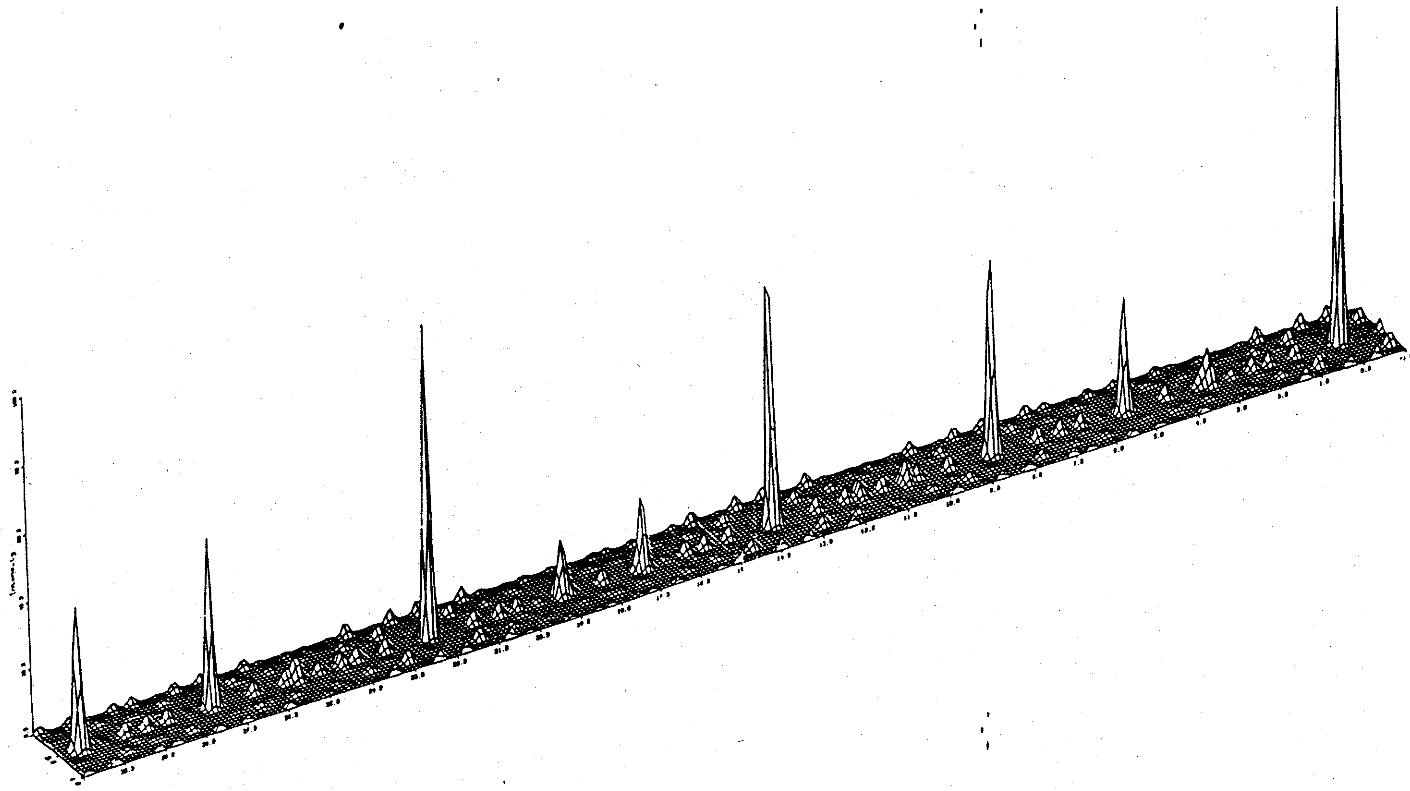

Fig. 3. Computed diffraction pattern along a line in the plane as in Figure 1.

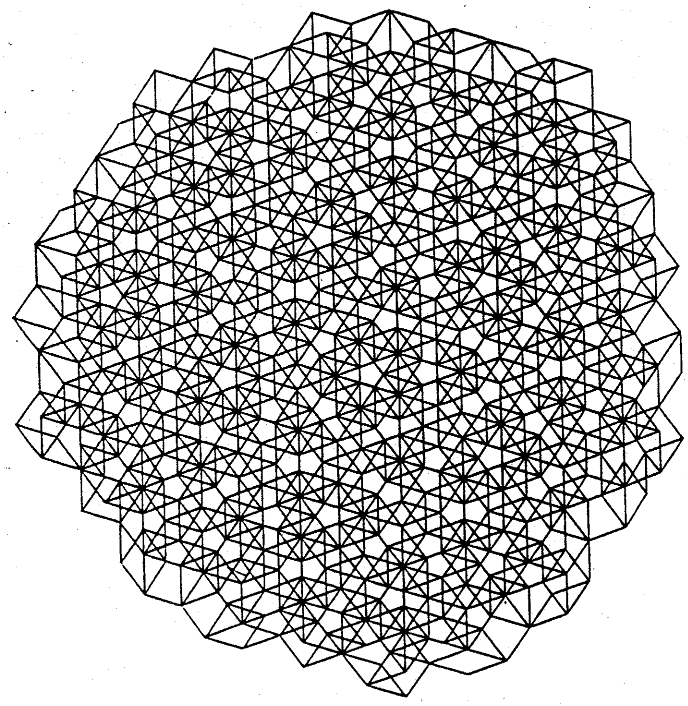

Fig. 4. Edge lines of the quasilattice seen along the direction of the vector e_6.

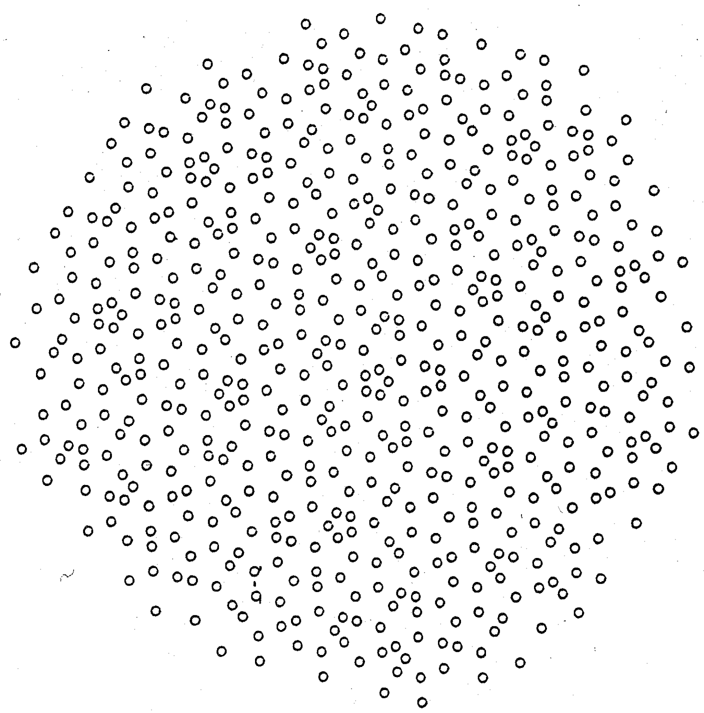

Fig. 5. Vertex positions of the quasilattice marked as circles seen along the direction of the vector e_6.

projected vertex positions. Note that the projected edge length in this plane is

$$L \cdot 2\theta = L \cdot 0.89442. \tag{3}$$

The projection includes six layers of the type described in Sect. 8 of [2].

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[4] P. Bancel, P. A. Heiney, P. W. Stephens, A. I. Goldman, and P. M. Horn, Phys. Rev. Lett. **54,** 2422 (1985).