

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  $\delta$ -distributions of Eq. (5.24) have been replaced by distributions of the finite width  $0.25 \pi L^{-1}$ . The position of points in  $K$ -space is characterized from Eqs. (5.21, 5.22) by

$$K = L^{-1} 2 \pi \frac{1}{2} \sum_i h_i e_i, \quad h_i = 0, \pm 1, \pm 2, \dots, \quad (1)$$

where the six vectors  $e_i$  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

$$L = 8.8 \text{ \AA}. \quad (2)$$

With the same model of a single atomic center at each vertex, the quasilattice was computed for a fixed set of parameters  $\gamma_1, \gamma_2, \dots, \gamma_6$ . Figures 4 and 5 show a view through the quasilattice along the direction of the fixed vector  $e_6$ . 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

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]	$Q/\text{\AA}^{-1}$
$h_1$	$h_2$	$h_3$	$h_4$	$h_5$	$h_6$		
0	0	3	3	0	0	c	1.876
−5	0	0	0	0	5	d	3.043
0	0	5	5	0	0		
−8	0	0	0	0	8	f	4.928
0	0	8	8	0	0		
−13	0	0	0	0	13		

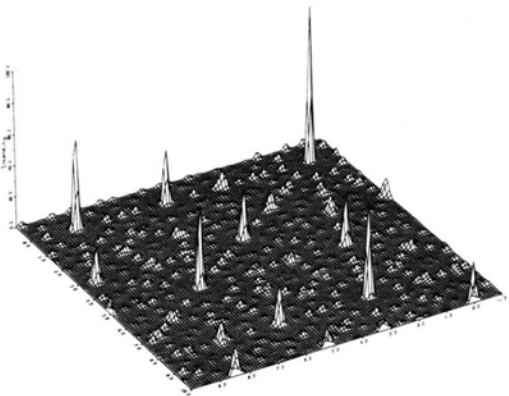


Fig. 1. Computed diffraction pattern in a plane perpendicular to the 5-fold axis. The numbers give the scale for the vector  $\pi^{-1} L K$ , where  $L$  is the edge length of the rhombohedral cell.

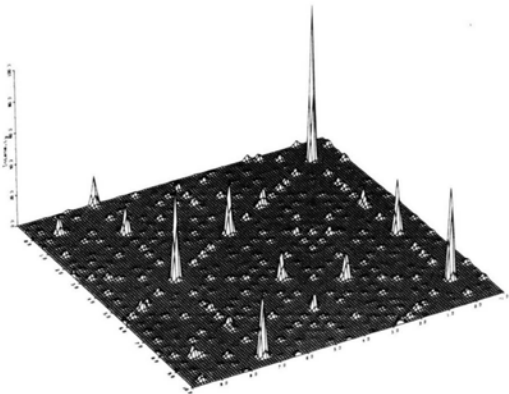


Fig. 2. Computed diffraction pattern in a plane perpendicular to the 3-fold axis.

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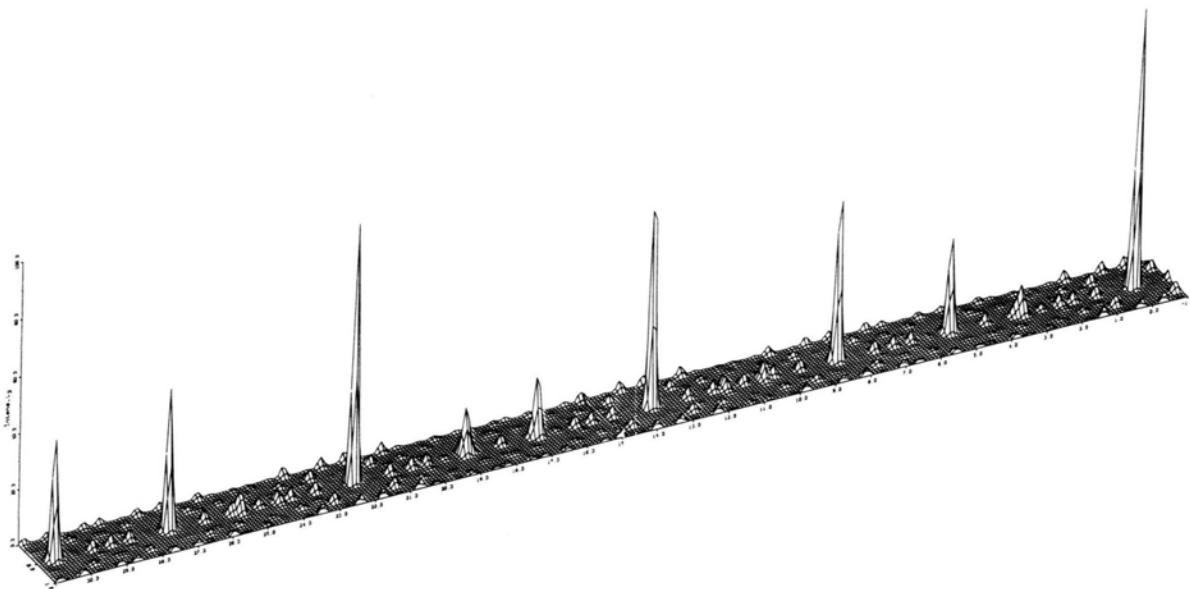


Fig. 3. Computed diffraction pattern along a line in the plane as in Figure 1.

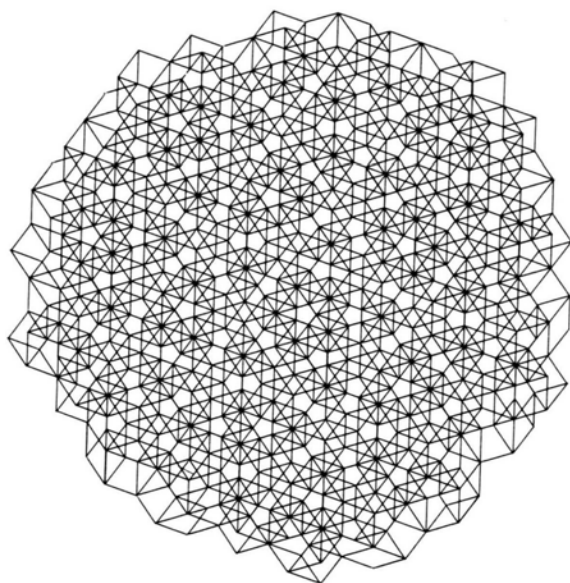


Fig. 4. Edge lines of the quasilattice seen along the direction of the vector  $e_6$ .

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

$$L \cdot 2\theta = L \cdot 0.89442. \quad (3)$$

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

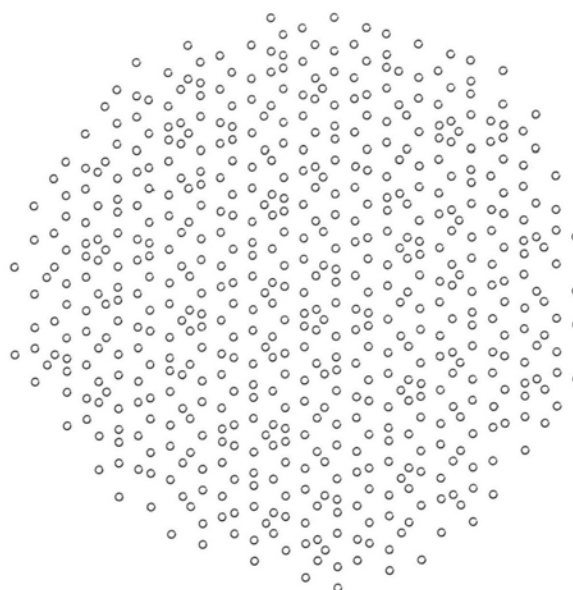


Fig. 5. Vertex positions of the quasilattice marked as circles seen along the direction of the vector  $e_6$ .

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