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 (5.24) have been replaced by distributions of the finite width $0.25 \pi L^{-1}$.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

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

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

$$L = 8.8 \text{ Å}. \quad (2)$$

With the same model of a single atomic center at each vertex, the quasilattice was computed for a fixed set of parameters $\gamma_1, \gamma_2, \ldots, \gamma_5$. Figures 4 and 5 show a view through the quasilattice along the direction of the fixed vector $e_5$. The index $k_5$ is varied as $k_5 = -5, -3, -1, 1, 3, 5$.

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.

<table>
<thead>
<tr>
<th>Index system</th>
<th>Notation of [4]</th>
<th>$Q/\text{Å}^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$h_1$ $h_2$ $h_3$ $h_4$ $h_5$ $h_6$</td>
<td>$c$</td>
<td>1.876</td>
</tr>
<tr>
<td>$-5$ $0$ $0$</td>
<td>$d$</td>
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<td>$f$</td>
<td>4.928</td>
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<tr>
<td>$-13$ $0$ $0$ $0$ $0$</td>
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<td></td>
</tr>
</tbody>
</table>

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

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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

$$L \cdot 20 = L \cdot 0.89442.$$  \hspace{4cm} (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 $e_6$.