Simulations of Kikuchi Patterns and Comparison with Experimental Patterns

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Introduction
Since the energy filtering technique for electron microscopy was established, it has already been a common sense that rocking curves of diffraction patterns (CBED patterns) formed by elastically scattered electrons are reproduced very well by the dynamical calculations of electron diffraction. It is high time to study inelastic scattering quantitatively. There exist three major fundamental inelastic scattering processes: plasmons (5 to 30eV), core-excitations (>50eV) and phonons (thermal diffuse scattering, TDS) (<0.1eV). The cross sections of these processes cannot be taken into account. TDS is known as the thermal diffuse scattering and other terms stand for elastic scattering. T(Q,Q') is the following function

\[ T(Q,Q') = \frac{1}{V} \int \frac{d\Omega'}{d\Omega} (|\langle f(\mathbf{Q}) \rangle |^2 - |\langle W(Q) \rangle - |W(Q')||)^2 \]

which is the TDS scattering factor given by Hall and Hirsch. \( T(Q,Q') \) for MgO is shown in Fig. 1(b).

In the limiting case \( t \to \infty \), only the terms \( \lambda = \lambda' \) and \( \mu = \mu' \) remain, the TDS intensity or eq.(5) becomes

\[ \lim_{t \to \infty} \frac{d\Omega}{dt} = \sum_{p \neq 0} |a(p)|^2 \sum_{\omega} (\mathbf{g} \cdot \mathbf{h}) \Omega_{(p \omega \omega' h)} \Omega_{(00\mathbf{h})} \Omega_{(00\mathbf{h}')} \]

where

\[ T^{\omega \omega' \lambda \lambda'} = \sum_{p \neq 0} \sum_{\omega} \langle \langle g(g(p)a)T(\mathbf{Q}, \mathbf{Q}') \rangle |(h(00\mathbf{h}')(00\mathbf{h}')) \rangle \]

This is equivalent to Takagi’s expression [6]. In this expression, the cross terms of the transition probabilities (Fig. 1(c)) are omitted and the absorption effect in the elastic scattering process cannot be taken into account. As a result, the thickness dependence, the asymmetry features, the accurate intensity distribution along the band, the accurate incidence-orien-

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The thickness dependence, the incidence-orientation dependence and $B$-factor dependence of zone-axis Kikuchi patterns are displayed for MgO. The contributions from constituent elements to Kikuchi patterns are shown for the [100] and [110] incidences. Simulated Kikuchi patterns are compared with experimental patterns.

**Simulations**

**Thickness dependence**

We firstly show in Fig.2 how the [100] zone-axis Kikuchi patterns of MgO change with the specimen thickness. Kikuchi patterns are weak and vague for thin specimens. As the thickness increases, clear Kikuchi bands appear and fine interference fringes are created. The simulations were carried out at an accelerating voltage of 100kV with 357 beams for $B$(Mg) = 0.31Å$^2$ and $B$(O) = 0.34Å$^2$, the number of pixels being 281 × 281.

![Figure 2](image-url)
Incidence-orientation dependence

It is shown how the Kikuchi patterns of MgO at the [100] zone-axis incidence change with the orientation of the incident beam. The incidence orientation is changed from (a) (zone axis) to (f) in the [010] direction as shown in Fig.3. All the patterns in Fig.4 are similar but their intensities decrease with the increase of the tilt angle from the zone axis. This is understood by the fact that the excitation of branch 1 of the Bloch states, from which most part of the Kikuchi band is originated, decreases with the tilt angle.

Fig. 3. Changes of the incidence orientation in the [010] direction.

Fig. 4. Intensity changes of the simulated Kikuchi patterns of MgO with the orientation of the incident beam (in the [010] direction from the [100] zone-axis incidence).
**B-factor dependence**

It is shown how the Kikuchi patterns of MgO at the [100] zone-axis incidence change with the Debye-Waller factors ($B$ factors). Simulations were performed for five cases (a to e in Fig.5). The values of the $B$ factors and the corresponding TDS scattering factors $T(Q, Q)$ are given in the figure. It is seen in Fig.6 that the intensities of the Kikuchi patterns increase with the increase of the $B$ factors, or with the increase of the thermal motions of atoms.

![Fig.5. Dependence of TDS scattering factors for MgO on $B$ factors.](image_url)

![Fig.6. Intensity changes of the simulated Kikuchi patterns of MgO with the $B$ factors (at the [100] zone-axis incidence).](image_url)

**MgO [100]**

(a) $B$(Mg):0.10Å$^2$, $B$(O):0.12Å$^2$
(b) $B$(Mg):0.20Å$^2$, $B$(O):0.23Å$^2$
(c) $B$(Mg):0.31Å$^2$, $B$(O):0.34Å$^2$
(d) $B$(Mg):0.40Å$^2$, $B$(O):0.45Å$^2$
(e) $B$(Mg):0.50Å$^2$, $B$(O):0.56Å$^2$

Accelerating voltage : 100kV  
Thickness : 70nm  
Number of beams : 357  
Number of pixels : 281 × 281
Contributions from constituent elements

\( T(\mathbf{Q}, \mathbf{Q}') \) contains the sum of atom species. If summation is carried out only for a definite atom species, the contributions from different atom species can be separately calculated. A similar simulation can also be carried out by selecting a certain branch of the initially excited Bloch states because a Bloch state often forms its intensity maximum at the rows consisting of atoms of one kind.

In the case of the [100] incidence for MgO, Mg atoms are located on top of O atoms (Fig.7). Thus, the Kikuchi patterns produced by both atoms are the same but their intensities are different according to the difference of their atomic scattering factors (Fig.8). In the case of the [110] incidence for MgO, the branches 1 and 2 form high electron concentrations on Mg and O atom rows, respectively (Fig.9). The Kikuchi bands running in the upper-right direction have different intensity distributions between the patterns of Mg and O (Fig.10). That is, owing to the difference of the excitations of the branches (the sites of inelastic scattering) concerned, the innermost band is weaker than the next band in the pattern of O but the innermost band is stronger than the next band in the pattern of Mg.

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**Fig. 7.** (a) Crystal structure of MgO. (b) Projected potential of MgO. (c) Bloch states for branches 1 and 2. (d) Excitation ratios of branches 1 and 2.

**Fig. 8.** Intensity changes of the simulated Kikuchi patterns of MgO with the specimen thickness for (a) branch 1 and (b) branch 2 (at the [100] zone-axis incidence).
Fig. 9. (a) Crystal structure of MgO. (b) Projected potential of MgO. (c) Bloch states for branches 1, 2, 4 and 8. (d) Excitation ratios of the branches.

<table>
<thead>
<tr>
<th>Branch</th>
<th>Excitation ratio</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>0.54</td>
</tr>
<tr>
<td>2</td>
<td>0.23</td>
</tr>
<tr>
<td>4</td>
<td>0.22</td>
</tr>
<tr>
<td>8</td>
<td>0.01</td>
</tr>
</tbody>
</table>

Accelerating voltage: 100kV
$B$(Mg): 0.31Å$^2$, $B$(O): 0.34Å$^2$
Number of beams: 315
Number of pixels: 279 $\times$ 281

Fig. 10. Intensity changes of the simulated Kikuchi patterns of MgO with the specimen thickness for (a) branch 1 and (b) branch 2 (at the [110] zone-axis incidence).
Comparison Between Experimental and Simulated Patterns

Simulated zone-axis Kikuchi patterns are compared with experimental patterns for MgO [100]. The experimental diffraction patterns are energy-filtered zero-loss patterns taken with the JEM-2010FEF at an accelerating voltage of 100kV. The simulations agree very well with the experiments (Fig. 11). That is, not only the Kikuchi lines and bands at high angles but also the detailed patterns at the central area are reproduced very well. It is seen that the thickness dependence (Fig. 12) and incidence-orientation dependence (Fig. 13) are also reproduced well by the simulations.

Conclusion

To carry out computer simulations of Kikuchi patterns, we derived a comprehensive theoretical expression for inelastic scattering of fast transmission electrons from a perfect crystal. The simulations for MgO based on this expression showed good agreement with experimental CBED patterns taken with the JEM-2010FEF energy-filtering TEM.

The results presented here have brought us to a first step for studying TDS intensities quantitatively. We will continue this study aimed at quantitative analysis of inelastic scattering in electron microscopy.

Detailed studies of Kikuchi patterns are referred to in our latest book “Convergent-Beam Electron Diffraction IV” published in 2002 by JEOL.

References:


Fig. 11. Experimental Kikuchi pattern of MgO taken with the JEM-2010FEF (left) and its simulated pattern (right) (at the [100] zone-axis incidence).

Fig. 12. Thickness dependence: Experimental and their simulated patterns (right).
Fig. 13. Incidence-orientation dependence: Experimental patterns (left) and their simulated patterns (right).

patterns (left)

$B$(Mg): 0.31Å$^2$, $B$(O): 0.34Å$^2$
Number of beams: 277
Number of pixels: $281 \times 281$

Incidence-orientation dependence

$B$(Mg): 0.31Å$^2$, $B$(O): 0.34Å$^2$
Number of beams: 277
Number of pixels: $281 \times 281$