Assignment Week 6 – Answers

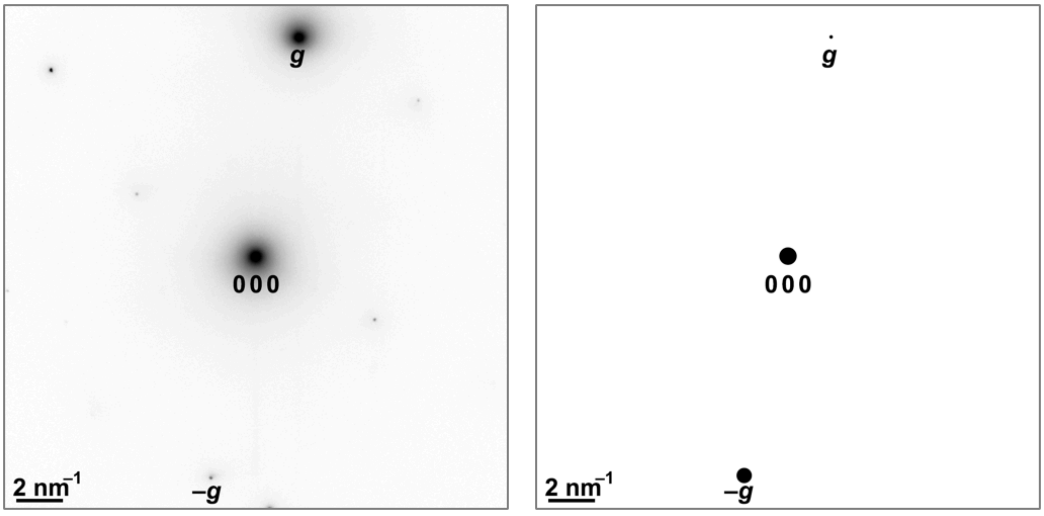
Assignment 6.1 – bend contours

a) There is bending of the nanowire along its length. Because of this bending, bright and dark bend contours are created; dark where the crystal is bent to a stronger diffraction condition and bright where it achieves a weaker diffraction condition. Because the bending axis is along the length and not the width of the nanowire, the bend contours are uniform across the nanowire width and so look like bright and dark bends bands along the length.

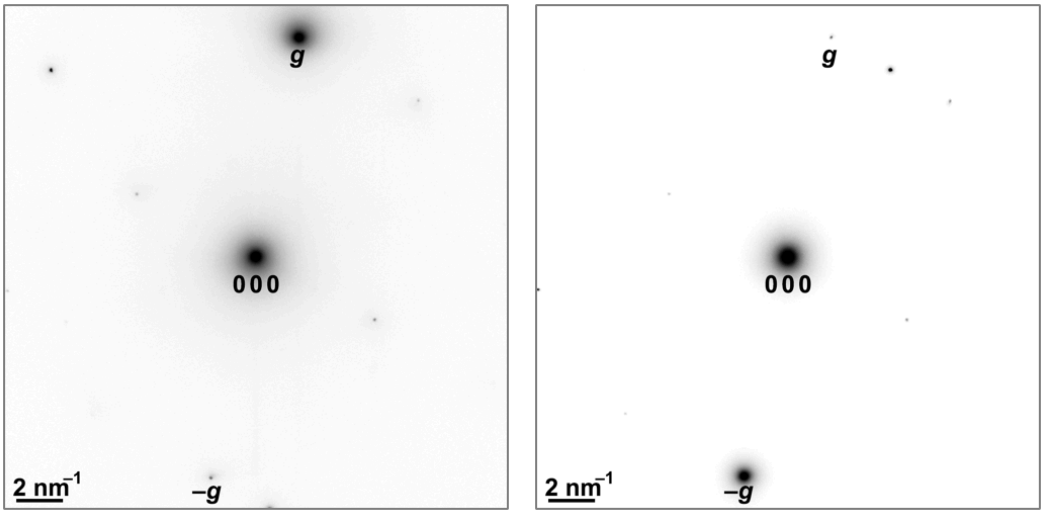
b) Each of the grains has a different crystal orientation. The dark bend contours relate to how each crystal's orientation achieves a strong diffraction condition, such as the Bragg condition. This happens at different locations in different grains because of each grain having a different orientation. Therefore, the bend contours are discontinuous from one grain to the next.

c)

i) Because of their symmetrical appearance, it can be seen that the red and blue locations on the bright-field image correspond to bend contours at the Bragg condition for a particular crystal plane, exciting either its plus ***g*** or minus ***g*** diffracted beam. Considering the red location, its corresponding strong diffracted beam can be identified on its diffraction pattern on the left; for instance, below this beam is annotated as ***g***. (Its weakly diffracting negative counterpart can also be seen.) In the diffraction pattern for the blue location, the strongly diffracting beam will instead be the ***–g*** counterpart, as shown in the sketch below right. The plus ***g*** diffracted beam will instead be very weakly diffracting.

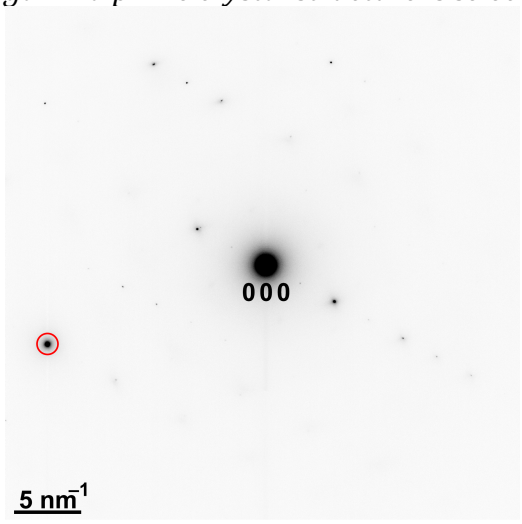


For comparison, the two actual experimentally recorded patterns are shown beside each other below, confirming the correctness of this answer:



ii) If a dark-field image is made by selecting the strongly diffracting beam in the pattern on the left (reflection ***g*** as annotated above), then the dark, curving bend contour selected by the red aperture position in the bright-field TEM image will appear as a bright contour in this dark-field image. (Specifically, the dark fringes of this bend contour will become bright and vice-versa.) The rest of the image will be very dark.

d) As for part c), the red circle for the TEM image in part d) indicates a bend contour for a certain (but different) crystal plain tilted to its Bragg diffraction condition. However, compared to the bend contour in part c), the bend contour in part d) has a much sharper/narrower contrast and has fewer fringes extending away from it. This corresponds to the plane having a narrower peak in its curve of diffracted beam intensity versus excitation error *s*. (Remember that in the 2-beam condition the bright-field image will have the opposite intensity to this.) The reason for this is that the Bragg diffracting plane for the bend contour in part d) has a much greater extinction distance than that of the diffracting plane in part c).
Ungraded remarks: for reference the diffraction pattern acquired from the selected area aperture location of part d) is shown below. The diffraction spot corresponding to the plane which is diffracting at the 2-beam condition is indicated by the red circle. Note the different scale of the pattern compared to the pattern shown in part c): this confirms that the scattering angle of the diffracting plane and hence the index of diffracting plane are much higher for d) than c). It is also commented that, as well as the extinction distance being greater for a higher index plane than a lower index plane, for this crystal structure extinction distance also increases if a superlattice type reflection of the ordered Ni3Al gamma prime crystal structure is selected. That may be the case in part d).

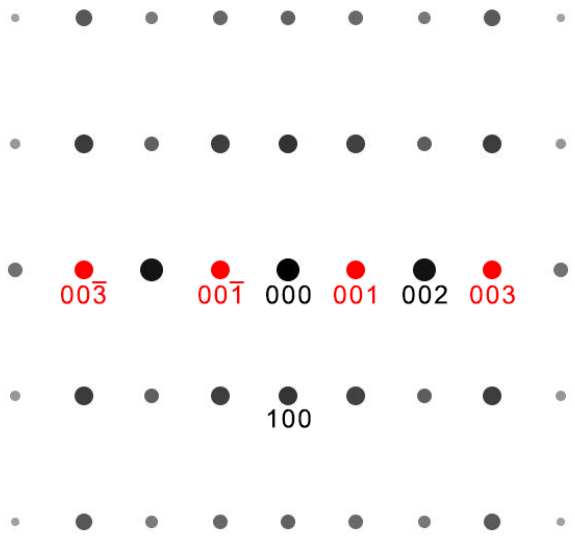


Assignment 6.2 – double diffraction

a)

i) This is a zero order Laue zone diffraction pattern. Therefore, the Weiss zone law applies:
$hU + kV + lW = 0$
Given the that the pattern has planes indexed with (h k l) of (1 0 0) and (0 0 2) then the zone axis [U V W] consistent with the Weiss zone law is [0 1 0] (or equivalently [0 –1 0]).

ii) The updated diffraction pattern with indexing should look like this:



iii) The double diffraction created spots closest to the direct beam correspond to $\boldsymbol{g}$ vectors of either:

$\boldsymbol{g}_{0\,0\,1}$

or:

$\boldsymbol{g}_{0\,0\,\bar{1}}$

The most direct $\boldsymbol{g}$ vector equations for obtaining either of the above $\boldsymbol{g}$ vectors from the kinematical diffracted beams are the following:

$\boldsymbol{g}_{1\,0\,1} + \boldsymbol{g}_{\bar{1}\,0\,0} = \boldsymbol{g}_{0\,0\,1}$

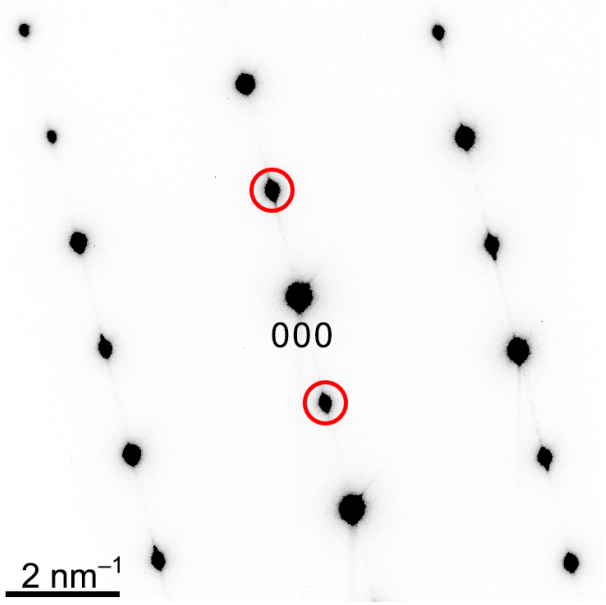
$\boldsymbol{g}_{\bar{1}\,0\,1} + \boldsymbol{g}_{1\,0\,0} = \boldsymbol{g}_{0\,0\,1}$

$\boldsymbol{g}_{1\,0\,\bar{1}} + \boldsymbol{g}_{\bar{1}\,0\,0} = \boldsymbol{g}_{0\,0\,\bar{1}}$

$\boldsymbol{g}_{1\,0\,\bar{1}} + \boldsymbol{g}_{\bar{1}\,0\,0} = \boldsymbol{g}_{0\,0\,\bar{1}}$

b)

i) By comparing the experimental diffraction pattern to the simulated pattern in part a) it can be seen that the diffraction spots that are exclusively present by double diffraction are the ones circled in red below:



The intensity of these spots is similar to many of the other diffracted beams. This confirms how dynamical scattering can make it difficult to interpret the intensities of diffracted beams in a zone axis diffraction pattern.

ii) To verify that these spots are created by double diffraction, the sample should be tilted away from the zone axis in order to excite a systematic row including the (0 0 2) and (0 0 –2) planes. (That is, these planes are parallel to the electron beam, but planes such as (1 0 0) are far from parallel to the electron beam.) In this way, the ***g*** vector mechanism to create the extra spots should be cut out, and these extra spots should disappear.

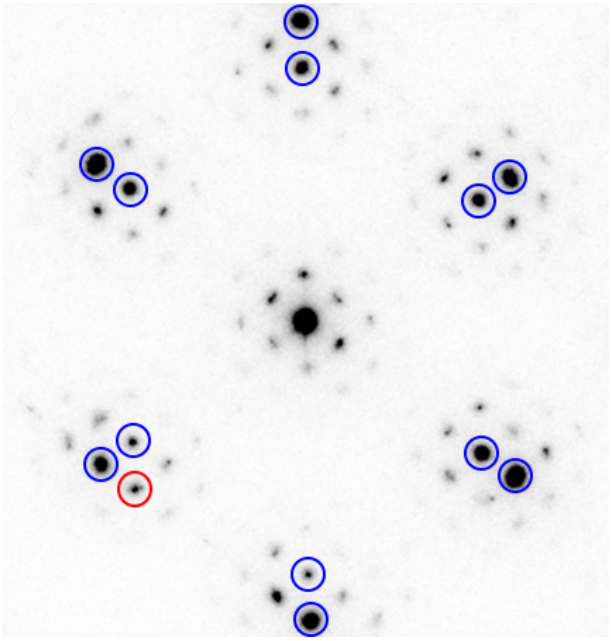
c)

i) Around both the direct beam and the kinematically-predicted diffracted beams, extra spots are seen because of double diffraction between the NiO and the Ni crystals. These extra spots are called "satellite spots". Is this term correctly given?

ii) The spots which do not require double diffraction to be present are those corresponding to:

- those of the NiO zone axis pattern on the left
- those for the equivalent Ni zone axis pattern, which are similarly oriented but a factor of about 0.418/0.368 = 1.14 further away from the direct beam.

These various diffracted beams are indicated with blue circles below:



iii) The possible solution is:

$\boldsymbol{g}_{1\,\bar{1}\,1\ (\mathrm{NiO})} + \boldsymbol{g}_{0\,0\,\bar{2}\ (\mathrm{Ni})}$