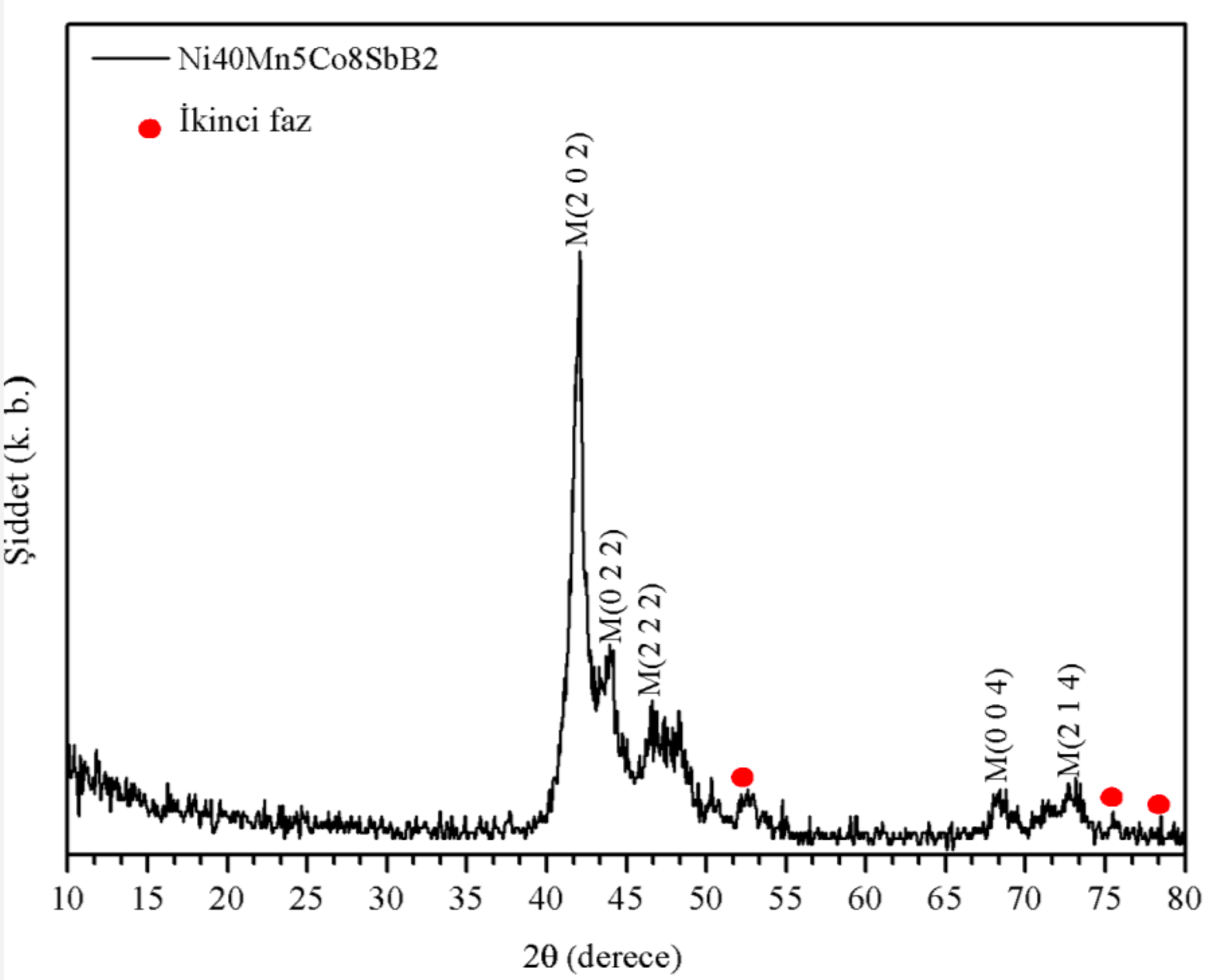
WEISS INDICES (CELL PARAMETERS), MILLER INDICES, MILLER PLANES 2

DIFFRACTION PATTERNS AND RECIPROCAL SPACE

- In the earlier sections, we have examined how X-rays interact with the crystal lattice and how this interaction can be explained by Bragg's law. In this section, we look at the consequence and results of that interaction.
- If we refer again to Fig, we see that in an X -ray diffraction experiment, the incident X-ray beam is diffracted by the crystal lattice. The diffracted X-rays are slopped by a data collection plate (previously photographic film was used. modern diffraclometers today usually use CCDs or image plates). The diffracted beams are observed on the collection plate as spots - also known as diffraction spots.

Figure 2.5 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

- Each diffraction spot is the sum result of the diffraction from a Miller plane, thus each spot can be identified with an hkl value corresponding to the Miller indices. Each spot also has an intensity value, depending on how strong or weak the resulting diffracted X- ray is. In some cases, a spot may be absent when the intensity corresponds to zero. These are known as absences.
- Each set of diffraction spots produced and collected is known as a frame of data. In the course of a typical experiment, several thousand frames may be collected. These frames of data can then be reconstructed to produce a diffractioll map. and subsequently an electron density map of the crystal lattice. This diffraction map in essence consists of the reciprocal form of the crystal lattice under study.



Ni40Mn5Co8SbB2
İkinci faz
M(2 0 2)
M(0 2 2)
M(2 2 2)
M(0 0 4)
M(2 1 4)
Şiddet (k. b.)
2θ (derece)
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80

THE RECIPROCAL LATTICE

$$2d\sin\theta = n\lambda,$$

the equation can be rearranged as

$$\sin\theta = \left(\frac{n\lambda}{2}\right)\left(\frac{1}{d}\right).$$

We can also say that sine is directly related to the reciprocal of d, that is, 1/d. If we recall that d represents the spacing between the sets of Miller planes, then we see that the resultant diffraction pattern is in units of 1/d, this is known as reciprocal space. If we assume that for each set of Miller planes (each value of hkl) in real space there is a point in reciprocal space, then the collection of all of these points can be referred to as the reciprocal lattice.

This relationship is illustrated in Figure

Figure 2.7 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

$$a.a^* = b.b^* = c.c^* = 1; \alpha = \alpha^*; \beta = \beta^*; \gamma = \gamma^*.$$

Table 2.3 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

STEREOGRAPHIC PROJECTİON

- To display the angular relationships between planes and directions in a crystal distributed over three dimensions, various methods are employed. For this purpose, the stereographic projection based on spherical projection is very common in crystallography, because this projection method enables us to permit graphical solution of angular problems between planes.

- In spherical projection, the direction of a plane when placing the crystal at the center of the sphere is represented by a point that the straight line drawn in the direction that passes through the center of the sphere intersects the surface of the sphere. The sphere is called a reference sphere or a projection sphere. The direction of any plane can be represented by the inclination of the normal to that plane. Then, all the planes in a crystal can be described by a set of plane normals radiating from one point within the crystal. If a reference sphere is placed about this point, the plane normals intersect the surface of the sphere in a set of points called poles. The pole position on the sphere represents the direction of the corresponding plane. The plane can also be represented by the trace (line) the extended plane makes in the sphere surface.

- The spherical projection can accurately represent the symmetry of the angular relationships between planes and directions as well as zone, but the use of sphere is not always convenient, because the measurement of angles on a flat sheet is more convenient in comparison with measurements on the surface of a sphere. For this purpose, the stereographic projection is widely used. The method is similar to that used by geographers who want to transfer a world map from a terrestrial globe to a sheet of an atlas. Particularly, the equiangular stereographic projection is preferred in crystallography, because it preserves angular relationships faithfully, although area is distorted.

Figure 2.11 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

- If a certain plane of the crystal has its pole at P, the stereographic projection of P. can be obtained as P0, by drawing the line NP, and it will intersect the projection plane. Alternatively stated, if a pole P is located in the southern hemisphere, its stereographic projection P0 is made from the arctic (north pole) N being the point of perspective and P0 corresponds to the intersection of a straight line NP with a projection plane. If a pole Q is in the northern hemisphere, consider the intersection Q0 with the straight line SQ which makes the Antarctic (south pole) S the point of perspective. It may be added that the stereographic projection of the pole Q is the shadow cast denoted by Q0 on the projection plane when a light source is placed at S.

- As shown in Fig. 2.12, a line for each of the poles in the northern hemisphere is projected to the south pole and its intersection with equatorial plane of the equator can be marked with a point.

Figure 2.12 Principles of Xray Crystallography, L.Ooi, Oxford Uni. Press

- By this method, all poles can be depicted inside an equatorial circle (basic circle). In this case, it is required to distinguish the projecting point with N being the point of perspective and the projecting point with S being the point of perspective. Such issue is easily resolved by using different symbols, for example, for the former and ı for the latter. Great circles on the reference sphere project as circular arcs, whereas small circles project as circles, but their projected center does not coincide with their projection center. One can also select any arbitrary plane perpendicular to NS besides the equatorial plane as a projection plane. In this case, only the diameter of the basic circle changes but the relative positions of projections are unchanged.

- The net graphics obtained by projecting meridian circles and latitude circles at every 1ı or 2ı on the equatorial plane is called polar net. Polar net is used for obtaining the projecting point on the equatorial plane with respect to a point on a projection sphere. When considering a terrestrial globe, the longitudinal lines correspond to great circles, whereas the latitude lines are small circles, except the equator. The net graphics obtained by projecting the meridian circles and latitude circles on one meridian circle is called Wulff net.

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