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A discussion of the influence of partial dislocations on the intensity of Bragg reflections

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Abstract. The analysis of elastic scattering experiments is considered for the case of crystals with lattice dislocations present. It is shown that some dislocations (known as partial dislocations, or Shockley partials) may give rise to a systematic change in the integrated intensities of Bragg reflections. These changes may involve additional atomic positions in the structure. A theory is developed for the description of the average intensity of a Bragg reflection for crystals with partial dislocations present. The example of Ni_3Sn in its hexagonal configuration is discussed.

1. Introduction

The investigation of a periodic arrangement of atoms in crystalline solids by coherent scattering is well established and is routinely used for structure determination. Measurements of Bragg intensities enable detailed information to be obtained concerning the arrangement of atoms. When analysing the Bragg intensities for obtaining structural parameters, deviations from perfect periodicity need to be accounted for. Effects such as the thermal motion of the atoms, chemical or isotopic (for neutron scattering experiments) disorder are easily taken into account [1–4]. Chemical disorder mainly affects the integrated Bragg intensities through the effective scattering amplitude, and if different species become chemically ordered new Bragg peaks may occur such as satellites or superlattice reflections.

In this paper attention will be focused on one particular type of non-periodicity in solids. It is concerned with the perturbation of the perfect lattice due to the presence of dislocations. The influence of dislocations on Bragg intensities is to some extent similar to the effects of stacking faults. In certain systems stacking faults occur affecting the phase relationship in the coherent scattering cross section, giving rise to a change in Bragg intensities. The question of how dislocations influence the intensity, position and the shape of Bragg reflections in structure determination experiments has been discussed in the literature [5–8]. However, since it has been generally expected that a random arrangement of dislocations in a solid does not affect the Bragg peak intensities this question has not been extensively discussed in the literature. Consequently there have been no reports of a study of dislocations by coherent Bragg reflection. However, diffuse and small-angle scattering have been used extensively [9] for the investigation of deformed solids.

Here the question is addressed of how the presence of dislocations influences experiments concerned with structure determinations. Experimentally it is the integrated Bragg intensities which form the basis for a structural refinement. Therefore it is not the primary aim to discuss the more involved question of how the shape and the position of Bragg reflections change if lattice deformations are present in the sample (this question has

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been discussed elsewhere; see e.g. Cullity [5]). Rather the discussion will be limited to the effects of dislocations on the integrated Bragg intensities. It should also be noted that experimentally only the relative intensities of Bragg reflections are of importance. This is due to the fact that experimental determinations of absolute intensities are rare, and more frequently an overall scale factor is taken as an adjustable parameter in the refinement of structural data.

After a brief introduction to dislocations it will be shown that the presence of a random arrangement of dislocations is capable of systematically modifying the intensities of Bragg reflections. The major part of changes in Bragg reflection intensities is shown to arise due to a change of the average symmetry of the unit cell. This topic will be discussed more fully below. However, lattice distortions caused by the presence of dislocations will also affect the size of those regions which are capable of coherent scattering. These effects are readily accounted for in the experimental analysis of the data, and they can thus be removed. The interest here is focused on the analysis of the integrated Bragg intensities as determined by the square of the nuclear structure factor and the intensity change brought about by the presence of partial dislocations. As shown in more detail below the partial dislocations are capable of admixing different atomic layers with the result that the symmetry of the average unit cell is changed. The theory is also illustrated with an example by applying the model to the hexagonal phase of the compound Ni_3Sn.

2. A brief introduction to dislocations and partial dislocations

The theory of dislocations is a topic which has been extensively dealt with in the literature [10–12]. A comprehensive discussion of both experimental and theoretical aspects of a wide range of dislocation phenomena is given in the series edited by Nabarro [9].

This brief introduction to dislocations is limited to illustrating those aspects of the theory of dislocations which are relevant for the discussion of their influence on the intensities of Bragg reflections. The creation of a screw or an edge dislocation is illustrated in figure 1 and figure 2. In general a dislocation will have both characteristics, but it suffices to discuss the pure screw and edge dislocations. The formation of a screw dislocation is illustrated for an A–B layered crystallographic structure in figure 1. Figure 2 shows the various steps in the formation of an edge dislocation.

In order to introduce a dislocation into an infinite, perfect crystal a cut is made along a semi-infinite plane as indicated in figures 1(*a*) and 2(*a*). Then the material at both sides of the cut is displaced in opposite directions such that the total relative displacement (known as the Burgers vector $\boldsymbol{b}$ of the dislocation) is an integer multiple of the A–B plane separation. Then the two sections are rejoined together and all atoms are allowed to relax to new equilibrium positions.

For each dislocation two different possibilities exist for joining the layers. These are shown in figures 1(*b*) and 1(*c*) for the screw dislocation and in figures 2(*b*) and 2(*c*) for the edge dislocation. However, the interface energy at the cut will be minimized if like layers are joined at both sides. Thus for an infinite lattice it is the displacement by a full lattice translation which is favoured energetically.

The matching of different layers results in a region of mismatch. The region is given by a misfit surface which is created by the cut in the crystal. The surface of mismatch between layers gives rise to a positive energy contribution and no matter how small this surface energy is, for a semi-infinite cut the total surface energy of the cut will become infinitely large and thus be energetically unfavourable. Therefore a single dislocation should always

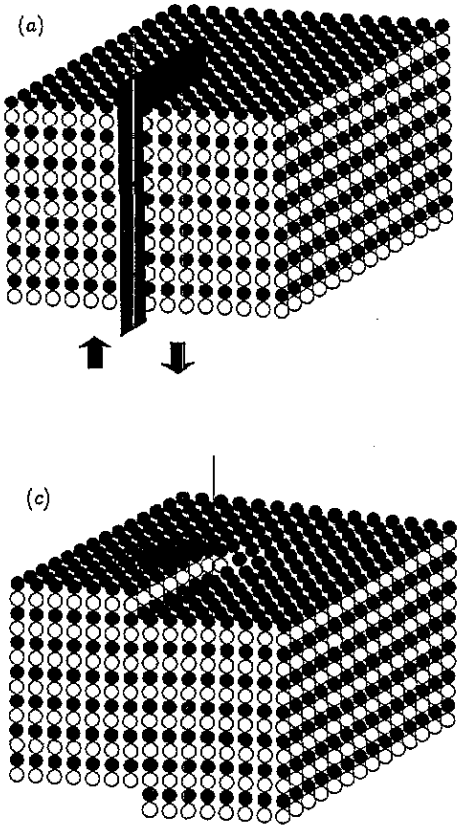

Figure 1. Various stages during the formation of a screw dislocation. (*a*) shows a section of an infinite and perfect crystal. The crystallographic structure is a sequence of A (dark spheres) and B (hollow spheres) layers. A semi-infinite cut is made in a suitable crystallographic plane as indicated by a line in (*a*). Then the material at both sides of the cut is displaced in opposite directions. Rejoining the parts at the interface one obtains the two different configurations as shown in (*b*) and (*c*).

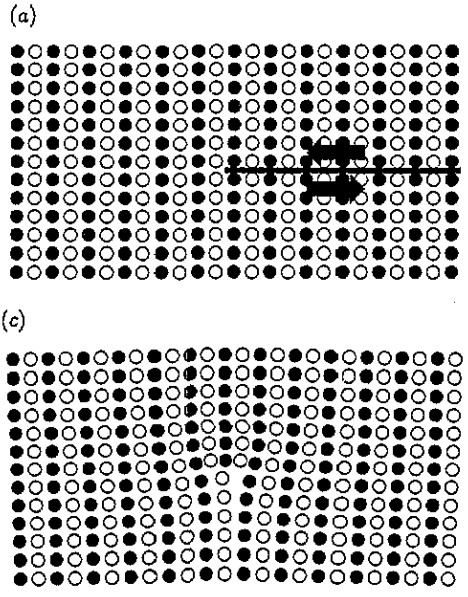

Figure 2. An edge dislocation is obtained from a perfect infinite crystal by first cutting the crystal along a semi-infinite plane as indicated in (*a*). Then the atoms at both sides of the cut are displaced in opposite directions. For a relative displacement of half a lattice vector ($\hat{=}$ A–B plane separation) the configuration in (*b*) is obtained. A full lattice translation (corresponding to twice the A–B plane separation) the arrangement shown in (*c*) is found.

be described by a Burgers vector which corresponds to a lattice translation and no regions of mismatch (i.e. an A layer linked to a B layer) should occur in the crystal.

However, it was first demonstrated by Shockley [13] that a dislocation with a full lattice translation Burgers vector may separate into two partial dislocations according to the equation

$$b \Rightarrow b_1 + b_2. \tag{1}$$

In this dissociation of one dislocation into two single ones the Burgers vector is a conserved quantity. Thus the equation $b = b_1 + b_2$ must hold. When a screw or edge dislocation with the smallest possible lattice translation dissociates into two separate dislocations, the Burgers vectors b_1 and b_2 will not correspond to full lattice translations. For this reason the two resulting dislocations are called partial dislocations.

The interaction between the two partial dislocations is usually repulsive, driving both dislocations apart. The point of interest for the following discussion is the fact that in the process of separating two partial dislocations, an area of misfit is created. This misfit interface is bounded by the partial dislocations. The region of misfit has the appearance locally of a translation twin (see figures 3 and 4). The relative displacement is given either by the Burgers vectors of the partial dislocations, i.e. either b_1 or b_2.

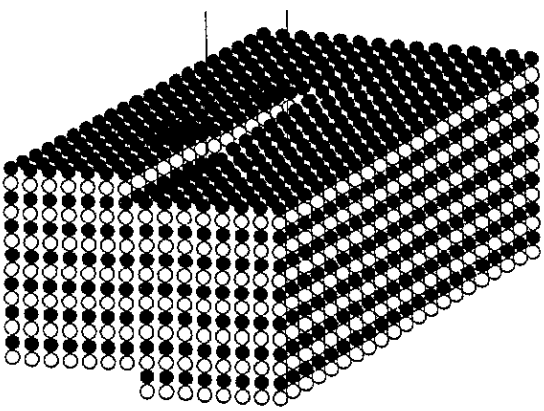

Figure 3. The dissociation of a screw dislocation which is characterized by a full lattice translation vector results in two dislocation lines with Burgers vectors which do not correspond to a full lattice translation. The dislocation lines repel one another, creating an area of mismatch as they separate. The area of mismatch is bound by the two partial dislocation lines.

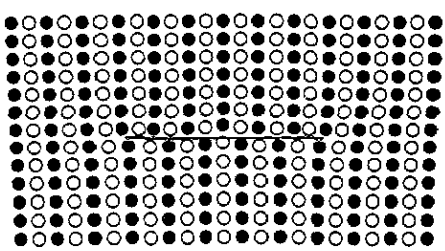

Figure 4. The dissociation of an edge dislocation results in two Shockley partials which are joined by an interface where A and B layers are joined to one another. In equilibrium, the energy reduction due to the separation of the partial dislocations is balanced by the surface energy needed for the creation of the surface of mismatch, where A and B layers are joined to one another.

It is thus appropriate to describe the effect of the misfit interface on the average nuclear structure factor in terms of a translational twinning operation. This translation symmetry is not a proper symmetry operator of the crystallographic space group, because the Burgers vectors of the partial dislocations are not lattice translations. But the admixture of such a symmetry element into the average crystallographic structure will change the overall symmetry and thereby also the intensity of Bragg reflections. The twinning translation is not a proper symmetry operation of the lattice, and in order to make this distinction it will be referred to as a pseudosymmetry operation.

3. Bragg scattering

An introduction to the theory of x-ray scattering can be found in Warren [3], and for an exposition of the theory of neutron scattering the books by Squires [1] or Lovesey [2] can be consulted.

Bragg scattering is by its very nature elastic scattering without an energy transfer between the probing particle and the system under investigation. The elastic scattering cross section can be written as

$$\frac{d\sigma}{d\Omega} = N \sum_{\tau} |F(k)|^2 \delta(k - \tau). \tag{2}$$

Here τ is a reciprocal lattice vector, N the total number of unit cells in the target and $F(k)$ is known as the nuclear structure factor defined as

$$F(k) = \sum_{j} b_j \exp(-W(k)k^2) \exp(ik \cdot R_j) \tag{3}$$

where $\exp(-W(k) \cdot k^2)$ is the Debye–Waller factor, which may be anisotropic. The summation in (3) is carried out over all atoms of the unit cell.

The nuclear structure factor reflects the symmetry of the crystallographic structure. Following the notation of Rae [15] let (Θ, t) denote a symmetry element. This operator is composed of a point group operation Θ and a translation t. The action of (Θ, t) on a position vector r will result in $(\Theta, t)r = \Theta r + t$ and thus the structure factor will be transformed according to the equation

$$(\Theta, t)F(k) = F_{\Theta,t}(k) = \exp(ik \cdot t)F(\Theta^{-1}k). \tag{4}$$

For (Θ, t) being a symmetry element of the crystallographic space group the transformed atom positions will coincide with the original location of atoms in the crystallographic structure. As a result $F(k) = F_{\Theta,t}(k)$.

However, for an operator (Θ, t) which is not a symmetry element of the space group the transformed atomic positions are expected to be different from the original ones. For such a case $F(k) \neq F_{\Theta,t}(k)$ and in general (Θ, t) transforms atoms from location r to new positions in the average unit cell as determined by $\Theta r + t$.

For a translational twinning operation the operator (Θ, t) simplifies to $\Theta = \mathbf{1}$ where $\mathbf{1}$ is the identity operator of the crystallographic point group and t is equal to one of the partial Burgers vector b_1 or b_2. As pointed out above $(\mathbf{1}, b_1)$ and $(\mathbf{1}, b_2)$ are not symmetry operations of the crystallographic lattice. Rather they have to be thought of as forming a cyclic group of partial translations (modulo a lattice translation) of order n with elements

$$(\mathbf{1}, \mathbf{0}), (\mathbf{1}, b_1), \ldots, (\mathbf{1}, (n-1)b_1). \tag{5}$$

In general $(\mathbf{1}, b_1) = (\mathbf{1}, b_2)^{-1}$ (up to a lattice translation) and the translation element of the Burgers vector b_1 or b_2 can be considered as the inverse operator of the other.

Combining these operators with the group G of crystallographic symmetry operations one obtains the total symmetry group G_{tot} as

$$G_{tot} = G + (\mathbf{1}, b_1)G + (\mathbf{1}, 2b_1)G + \cdots + (\mathbf{1}, (n-1)b_1)G. \tag{6}$$

As a result of the increase in the number of symmetry elements of the crystal the nuclear structure factor is changed according to

$$F_{\text{tot}}(\boldsymbol{k}) = F(\boldsymbol{k}) + \exp(i\boldsymbol{k}\cdot\boldsymbol{b}_1)F(\boldsymbol{k}) + \cdots + \exp(i(n-1)\boldsymbol{k}\cdot\boldsymbol{b}_1)F(\boldsymbol{k}). \tag{7}$$

The effect of the twinning on the average structure factor of the crystal will depend on the details of the splitting of a full dislocation into partial dislocations, which in turn determines the size of the misfit region and the extent of the stacking fault. In order to discuss the effects of these stacking faults the cases of a large and a small separation of the partial dislocations are discussed in turn.

First the partial dislocations are taken to be far apart from one another. Under these circumstances the effects due to the finite size may be neglected and an average structure considered which is characterized by stacking faults.

The twinning which occurs in crystals due to the presence of dislocations is essentially restricted to displacements by $\boldsymbol{b}_1$ and $-\boldsymbol{b}_1$. As both displacements occur with the same probability one is led to consider a structure factor of the average structure given by

$$F_{\text{dis}}(\boldsymbol{k}) = (1-2p)F(\boldsymbol{k}) + p((\mathbf{1}, \mu\boldsymbol{b}_1) + (\mathbf{1}, -\mu\boldsymbol{b}_1))F(\boldsymbol{k}) = (1-2p)F(\boldsymbol{k}) + 2p\cos(\boldsymbol{k}\cdot\boldsymbol{b}_1)F(\boldsymbol{k}). \tag{8}$$

Here p determines the degree of admixing the various layers due to the presence of partial dislocation induced stacking faults.

For the intensity of Bragg reflections this results in an additional scattering vector dependence and in a modulation of the scale factor. However, it is pointed out that only those Bragg reflections with a non-zero structure factor are affected. Thus the scattered intensity may be written as

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = N\sum_{\tau} |F_{\text{dis}}(\boldsymbol{k})|^2\delta(\boldsymbol{k}-\boldsymbol{\tau}) = \sum_{\tau} N(\boldsymbol{k})|F(\boldsymbol{k})|^2\delta(\boldsymbol{k}-\boldsymbol{\tau}) \tag{9}$$

with $N(\boldsymbol{k}) = ((1-2p) + 2p\cos(\boldsymbol{k}\cdot\boldsymbol{b}_1))^2$.

In order to illustrate finite size effects consider a structure which is given by a sequence of A and B layers. Let the A and B layers be related to one another by inversion symmetry: with the structure factor $F(\boldsymbol{k}) = F_{\text{A}}(\boldsymbol{k}) + F_{\text{B}}(\boldsymbol{k})$ the inversion symmetry will ensure that $F(\boldsymbol{k})$ is real (due to $F_{\text{A}}(\boldsymbol{k}) = F_{\text{B}}^*(\boldsymbol{k})$). The inversion symmetry element will also link the displacements in the average structure of the A and B layer, i.e. it will link $\exp(i\boldsymbol{k}\cdot\boldsymbol{b}_1)F_{\text{A}}(\boldsymbol{k})$ with $\exp(-i\boldsymbol{k}\cdot\boldsymbol{b}_1)F_{\text{B}}(\boldsymbol{k})$ (type I) and $\exp(-i\boldsymbol{k}\cdot\boldsymbol{b}_1)F_{\text{A}}(\boldsymbol{k})$ with $\exp(i\boldsymbol{k}\cdot\boldsymbol{b}_1)F_{\text{B}}(\boldsymbol{k})$ (type II). In general both configurations will have different energies at the interface, as a result of which the probability of their occurrence in the interface will differ. As the partial dislocations separate in order to minimize their interaction energy the mismatch interface created by this separation is found to be composed of alternating layers of type I and type II. The interface energy is minimized if the lower energy configuration is the end configuration of the mismatch area. Thus an unequal number of type I and type II configurations are found in the interface. While this difference is unimportant for a large separation of the partial disclocations its effect is more significant for a small separation of the partial dislocations. Writing

$$\exp(i\boldsymbol{k}\cdot\boldsymbol{b}_1)F_{\text{A}}(\boldsymbol{k}) + \exp(-i\boldsymbol{k}\cdot\boldsymbol{b}_1)F_{\text{B}}(\boldsymbol{k}) = \cos(\boldsymbol{k}\cdot\boldsymbol{b}_1)(F_{\text{A}}(\boldsymbol{k}) + F_{\text{B}}(\boldsymbol{k})) + \mathrm{i}\sin(\boldsymbol{k}\cdot\boldsymbol{b}_1)(F_{\text{A}}(\boldsymbol{k}) - F_{\text{B}}(\boldsymbol{k})) \tag{10a}$$

$$\exp(-i\boldsymbol{k}\cdot\boldsymbol{b}_1)F_{\text{A}}(\boldsymbol{k}) + \exp(i\boldsymbol{k}\cdot\boldsymbol{b}_1)F_{\text{B}}(\boldsymbol{k}) = \cos(\boldsymbol{k}\cdot\boldsymbol{b}_1)(F_{\text{A}}(\boldsymbol{k}) + F_{\text{B}}(\boldsymbol{k})) - \mathrm{i}\sin(\boldsymbol{k}\cdot\boldsymbol{b}_1)(F_{\text{A}}(\boldsymbol{k}) - F_{\text{B}}(\boldsymbol{k})) \tag{10b}$$

it is seen that an equal number of type I and type II configurations makes the $(F_A(k)-F_B(k))$ part cancel on the left hand side of the sum of $(10a)$ and $(10b)$. For an unequal number of type I and type II configurations a net contribution proportional to $(F_A(k)-F_B(k))$ remains.

The contribution $F_A(k) - F_B(k)$ is proportional to twice the imaginary part of the structure factor of a layer. While the perfect lattice has systematic absences for all Bragg reflections with $F_A(k)+F_B(k)=0$, the contribution proportional to $F_A(k)-F_B(k)$ will in general not be equal to zero. Thus as a result of the difference contribution of the structure factors of the layer a non-zero Bragg intensity may be obtained for Bragg reflections with systematic absences in the perfect crystal.

4. The effect of partial dislocations on Bragg intensities in Ni_3Sn

In order to illustrate the above discussion an example is investigated. The structure chosen here for illustration is the hexagonal Ni_3Sn structure with the space group $P6_3/mmc$. This arrangement of atoms within the unit cell is illustrated in figures 5 and 6. The lattice parameters (Pearson [14]) are given as $a = 5.386$ Å and $c = 4.243$ Å. The position of the Sn atoms is fixed at $(\frac{1}{3}, \frac{2}{3}, \frac{1}{4})$ and $(\frac{2}{3}, \frac{1}{3}, \frac{3}{4})$. The six Ni positions within the unit cell are determined by one positional parameter x_{Ni} with $x_{Ni} \simeq \frac{5}{6}$.

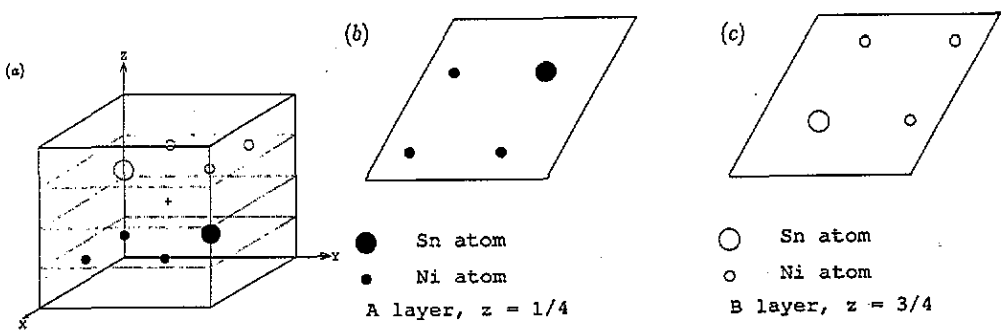

Figure 5. Crystallographic structure of Ni_3Sn. (a) shows the three dimensional unit cell of Ni_3Sn with atoms in the A and B layers at $z = \frac{1}{4}$ and $z = \frac{3}{4}$, respectively. The plane with $z = \frac{1}{2}$ contains the point of inversion symmetry $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and this plane is also indicated in (a). (b) and (c) show cuts through the unit cell for constant values of z. The A plane (obtained for $z = \frac{1}{4}$) is shown in (b), while the atom positions in the B plane $(z = \frac{3}{4})$ are shown in (c).

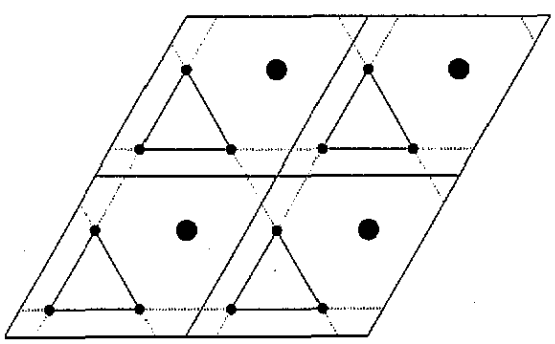

Figure 6. Position of atoms in the A plane showing four unit cells. The Ni atoms are arranged in equilateral triangles. One triangle (full line) is located within a unit cell, while the second triangle (dotted line) connects Ni atoms in different unit cells. The crystallographic positions of the Ni atoms are characterized by a free parameter x. For the special choice of $x = \frac{5}{6}$ the two triangles are of equal size.

The structure of Ni_3Sn consists of a sequence of A and B layers. Both layers are connected by inversion symmetry to one another with the centres of inversion being the origin and the point (0.5, 0.5, 0.5) within the unit cell. As a result of the inversion symmetry the structure factor of the unit cell is a real entity.

For this structure a full dislocation with a Burgers vector (0, 0, 1) may dissociate into two partial dislocations according to $(0,0,1) = \boldsymbol{b}_1 + \boldsymbol{b}_2$ with $\boldsymbol{b}_1 = \frac{1}{6}(-2,2,3)$ and $\boldsymbol{b}_2 = \frac{1}{6}(2,-2,3)$. According to the Frank criterion this dissociation is energetically favourable. As noted above, for the discussion here $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ may be considered to be the inverse of one another. Thus by using (8) and denoting the layer structure factors by $F_A(\boldsymbol{k})$ and $F_B(\boldsymbol{k})$ for A and B layers, respectively, one may obtain for a crystal with partial dislocation induced stacking faults

$$F_A(\boldsymbol{k}) \longrightarrow F_A(\boldsymbol{k})(1-2p) + p\exp(i\boldsymbol{k}\cdot\boldsymbol{b}_1)F_A(\boldsymbol{k}) + p\exp(-i\boldsymbol{k}\cdot\boldsymbol{b}_1)F_A(\boldsymbol{k})$$

$$F_B(\boldsymbol{k}) \longrightarrow F_B(\boldsymbol{k})(1-2p) + p\exp(i\boldsymbol{k}\cdot\boldsymbol{b}_1)F_B(\boldsymbol{k}) + p\exp(-i\boldsymbol{k}\cdot\boldsymbol{b}_1)F_B(\boldsymbol{k}). \tag{11}$$

The effect of the displacements is essentially to project down an A (B) layer onto a B (A) layer and translate it by $\pm(\frac{1}{3}, -\frac{1}{3}, 0)$ within the B (A) layer. The arrangement of atoms is depicted in figures 7 and 8. It is noticeable that the projection of one layer onto the neighbouring one may result in an almost perfect match (figures 7(*a*) and 8(*b*)) while for a layer translated in the opposite direction the translated atoms occupy intermediate positions within the plane. Thus one may set

$$F_A(\boldsymbol{k}) \simeq \exp(i\boldsymbol{k}\cdot\boldsymbol{b}_1)F_B(\boldsymbol{k}) \tag{12a}$$

$$F_B(\boldsymbol{k}) \simeq \exp(-i\boldsymbol{k}\cdot\boldsymbol{b}_1)F_A(\boldsymbol{k}). \tag{12b}$$

Equation (12) becomes an identity for $x = \frac{5}{6}$, while for positional values of the Ni atom close to this value the above equivalence is only fulfilled approximately (see figure 8(*b*)). Using (12) the identity

$$(-1+\cos(\boldsymbol{k}\cdot\boldsymbol{b}))(F_A(\boldsymbol{k}) + F_B(\boldsymbol{k})) = i\sin(\boldsymbol{k}\cdot\boldsymbol{b})(F_A(\boldsymbol{k}) - F_B(\boldsymbol{k})) \tag{13}$$

may be obtained.

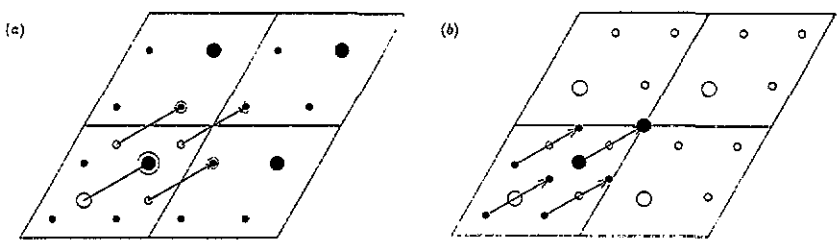

Figure 7. Effect of the partial dislocation vector $\boldsymbol{b}_1$. (*a*) shows the B layer projected down onto the A layer. The translations of the projected atoms within the plane are indicated by the arrows. The effect of $\boldsymbol{b}_1$ for an A layer projected down onto a B layer with subsequent translation within this layer is shown in (*b*).

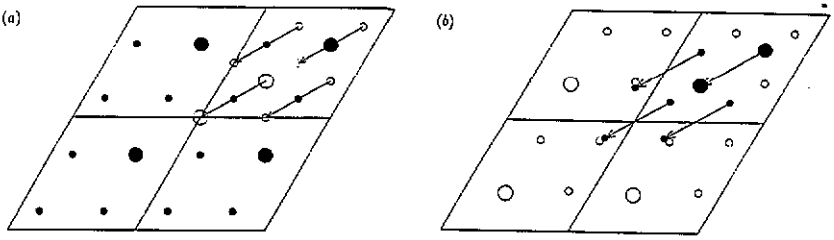

Figure 8. (*a*) shows a projection of a B layer onto an A layer using the vector b_2 with the arrows indicating the translations within the A plane. In (*b*) the equivalent projection is shown for an A layer onto a B layer. The positional parameter x of the Ni atoms has been changed to a value of $x = 0.82$ in (*b*) in order to show that for x value with $x \neq \frac{5}{6}$ the projected and translated Ni atom positions do not superimpose onto the Ni atom positions of the layer onto which the projection was carried out.

Inserting (12) into (11) results in an average structure factor of the unit cell given by

$$F_{\text{average}}(\boldsymbol{k}) = F_{\text{A}}(\boldsymbol{k}) + F_{\text{B}}(\boldsymbol{k}) + 2\mathrm{i}p \sin(\boldsymbol{k} \cdot \boldsymbol{b})(F_{\text{A}}(\boldsymbol{k}) - F_{\text{B}}(\boldsymbol{k})). \tag{14}$$

The intensity of a Bragg reflection is determined by the square of the modulus, resulting in an intensity proportional to

$$|F_{\text{A}}(\boldsymbol{k}) + F_{\text{B}}(\boldsymbol{k})|^2 + 4\mathrm{i}p \sin(\boldsymbol{k} \cdot \boldsymbol{b}_1)(F_{\text{A}}(\boldsymbol{k}) + F_{\text{B}}(\boldsymbol{k}))(F_{\text{A}}(\boldsymbol{k}) - F_{\text{B}}(\boldsymbol{k})) + 4p^2 \sin^2(\boldsymbol{k} \cdot \boldsymbol{b}_1)|F_{\text{A}}(\boldsymbol{k}) - F_{\text{B}}(\boldsymbol{k})|^2. \tag{15}$$

As seen in (14) it is the imaginary part of the layer structure factor that determines additional terms for the average structure factor. In deriving (14) use has been made of the centrosymmetry of the Ni_3Sn structure by using $F_{\text{A}}(\boldsymbol{k}) = F_{\text{B}}(\boldsymbol{k})^*$. However, due to (13) no additional Bragg reflections occur for Ni_3Sn. Using (13) the intensity is given by

$$(1 - 4p(1 - \cos(\boldsymbol{k} \cdot \boldsymbol{b}_1)) + 4p^2(1 - \cos(\boldsymbol{k} \cdot \boldsymbol{b}_1)^2)|F_{\text{A}}(\boldsymbol{k}) + F_{\text{B}}(\boldsymbol{k})|^2. \tag{16}$$

The scattered intensity of a crystal with stacking faults induced by partial dislocations is proportional to the structure factor of the perfect crystal combined with a modulation of the scaling factor. This modulation is brought about because of the presence of the displaced atoms within the average unit cell.

5. Conclusions

An analysis has been given of the effect of partial dislocations and the resulting stacking faults on the average structure factor of the unit cell. It has been shown that a systematic change of the intensity of Bragg reflections may occur. The changes include the modulation of the intensities of Bragg reflections with a non-zero structure factor for the ideal structure as well as the possibility of non-zero intensities for systematic absences.

The example of Ni_3Sn has been considered in some detail. It was demonstrated that at least for this crystallographic structure the effect of stacking faults may result in the occurrence of additional atoms at intermediate atomic positions within the average unit cell. The analysis as given here applies equally well for neutron as well as x-ray scattering. The results of the present analysis will be tested by experiment and the results published elsewhere.

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