*Acta Cryst.* (1989). A45, 320-325

# Systematic Determination of Coincidence Orientations for all Hexagonal Lattices with Axial Ratio $c/a$ in a Given Interval

By Hans Grimmer

*Paul Scherrer Institute, Laboratory of Materials Science, CH-5232 Villigen PSI, Switzerland*

(*Received* 10 *June* 1988; *accepted* 1 *December* 1988)


## Abstract

Two neighbouring grains of the same phase with a lattice of hexagonal Bravais type are considered which have a three-dimensional lattice of symmetry translations in common, called the coincidence site lattice or CSL. The volume ratio of unit cells for the CSL and the original lattice is called the multiplicity $\Sigma$. The $\Sigma$-hex theorem gives $\Sigma$ in terms of four integral parameters that describe the axis and angle of the rotation connecting the hexagonal lattices of the two neighbouring grains and in terms of their axial ratio $c/a$. Two types of rotations generating CSL's may be distinguished, *viz* common rotations, which generate CSL's with the same $\Sigma$ for every value of $c/a$, and specific rotations, which generate CSL's with a low value of $\Sigma$ only for a few values of the axial ratio. The $\Sigma$-hex theorem makes it possible to determine a lower and an upper bound for $\Sigma_{\min}$, the minimum value of the multiplicity of specific rotations for a given axial ratio. The lower bound can serve to determine systematically all specific rotations with $c/a$ in a given interval and $\Sigma$ not larger than some given value $\Sigma_c$. The bound is used to complete published tables. The upper bound is stronger than a similar bound given by Delavignette.


## 1. Introduction

In experimental investigations and computer simulations of the structure and properties of grain boundaries, the results are frequently discussed with reference to the special case of coincidence boundaries, where the two neighbouring grains have a three-dimensional lattice of symmetry translations in common.

Consider two neighbouring grains of the same phase with a primitive hexagonal lattice. One of the factors determining the structure and energy of the boundary between the two grains is the relative orientation of their lattices. It can be described by a rotation transforming the symmetry translations of lattice 1 into those of lattice 2. It has often been observed that low-energy boundaries have a large portion $1/\Sigma$ of symmetry translations in common.

A coordinate system defined by a basis of lattice 1 is used to express the rotation by a $3\times3$ matrix **R**. Grimmer (1976) showed that the two lattices have symmetry translations in common if and only if **R** is rational and that $\Sigma$, called the *multiplicity*, is the smallest integer such that $\Sigma\mathbf{R}$ and $\Sigma\mathbf{R}^{-1}$ are integral matrices. These results are valid for arbitrary symmetry of lattice 1. They have been applied to lattices of hexagonal symmetry by Grimmer & Warrington (1983, 1985).

Rotations by 180° around a lattice vector perpendicular to the sixfold axis and rotations around the sixfold axis such that $3^{1/2}\tan(\Theta/2)$ is rational are represented by rational matrices **R** that do not depend on $c/a$. It also follows that $\Sigma$ is independent of $c/a$. Such rotations are called *common* rotations. If and only if $(c/a)^2$ is rational then there are also other rotations that give rise to rational matrices. They are called *specific* rotations because they are associated with specific values of $c/a$ in contrast to the common rotations. The matrix and the multiplicity of these rotations depends on $c/a$.

Bonnet, Cousineau & Warrington (1981) undertook to determine for seven elements with hexagonal structure all the specific rotations with $\Sigma\leq25$ that can be relevant for the description of the structure of grain boundaries. Usually there are no values of $c/a$ that admit small values of $\Sigma$ and lie within the uncertainty of the experimentally measured value of $c/a$. The above-mentioned authors considered therefore approximate coincidence of lattices with the experimental value of $c/a$. They restricted attention to the cases where a strain of one of the lattices by less than 1% was sufficient to turn approximate into exact coincidence. Delavignette and co-workers undertook instead to determine all the specific rotations with low values of $\Sigma$ for $c/a$ values in certain intervals around the experimental value of $c/a$. They considered the same seven elements, *i.e.* $\alpha$-Be, $\alpha$-Ti, $\alpha$-Zr and Mg in Bleris, Nouet, Hagège & Delavignette (1982), Zn and Cd in Delavignette (1982) and graphite in Delavignette (1983). All these authors were aware that their methods did not guarantee completeness of their tables.

Hagège & Nouet (1985) found rules that show the dependence of $\Sigma$ on the axis and angle of the rotation and, in case of specific rotations, on the axial ratio of the lattice. However, their rules do not always give $\Sigma$ correctly. Grimmer & Warrington (1987) showed

0108-7673/89/050320-06$03.00

how the rules have to be modified in order to obtain a rigorous theorem. This theorem is presented here in a more elegant form under the name of $\Sigma$-hex theorem. The theorem is applied to derive for each value of the axial ratio a lower bound on the multiplicity of specific rotations. This bound makes it possible to determine the finite number of axial ratios $c/a$ that may give rise to specific rotations with $\Sigma$ less than or equal to a given value $\Sigma_c$. A computer program which determines the specific rotations for a given value of $c/a$ and for $\Sigma \leq \Sigma_c$ may then be used to determine these rotations systematically for all values of $c/a$ in a given interval. It has been used to complete the above-mentioned tables of specific rotations.

## 2. The $\Sigma$-hex theorem and its applications

A basis of the hexagonal lattice is given by two vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ both of length $a$ and perpendicular to the sixfold symmetry axis, and a vector $\mathbf{e}_3$ of length $c$ and parallel to the sixfold axis. The angle between $\mathbf{e}_1$ and $\mathbf{e}_2$ is 120°. A rotation with axis $[U, V, W]$ in this coordinate system and with angle $\Theta$ given by

$$\tan \Theta/2 = \{[a^2(U^2 - UV + V^2) + c^2W^2]/3c^2m^2\}^{1/2} \quad (1)$$

is denoted by the hexagonal quadruple $(m, U, V, W)$. The theorem of Grimmer & Warrington (1987) can be written as:

*Theorem* 1 (*$\Sigma$-hex theorem*)

The rotation $(m, U, V, W)$ of the hexagonal lattice with

$$c^2/a^2 = \mu/\nu, \quad (2)$$

where

$$\gcd(m, U, V, W) = 1^* \quad (3)$$

and

$$\gcd(\mu, \nu) = 1 \quad (4)$$

generates a CSL with multiplicity

$$\Sigma = F/F_1^2F_2F_3F_4F_5, \quad (5)$$

where

$$F = \mu(3m^2 + W^2) + \nu(U^2 - UV + V^2) \quad (6)$$

$$F_1 = \gcd(2, U, V, m + W) \quad (7)$$

$$F_2 = \gcd(3, U + V, W) \quad (8)$$

$$F_3 = \gcd(2/F_1, \nu, m + W) \quad (9)$$

$$F_4 = \gcd(\nu/F_3, 2W/(F_1F_2), m + W) \quad (10)$$

$$F_5 = \gcd(\mu, 3U/(F_1F_2), (U + V)/F_1). \quad (11)$$

* gcd $(u, v, \ldots)$ denotes the greatest common divisor of the integers $u, v, \ldots$.

Table 1. *Lattice parameters of seven elements with hexagonal structure [according to Eckerlin & Kandler (1971)]*

The space group is $P6_3mc$ for graphite and $P6_3/mmc$ in the other cases.

| | $a$ | $c$ | $c/a$ |
|---|---|---|---|
| α-Be | 2·2866 | 3·5833 | 1·5671 |
| α-Ti | 2·9511 | 4·6843 | 1·5873 |
| α-Zr | 3·2321 | 5·1477 | 1·5927 |
| Mg | 3·2094 | 5·2103 | 1·6234 |
| Zn | 2·6647 | 4·9469 | 1·8565 |
| Cd | 2·9794 | 5·6186 | 1·8858 |
| Graphite | 2·4612 | 6·7079 | 2·7255 |

The common rotations satisfy

$$m = W = 0 \quad \text{or} \quad U = V = 0, \quad (12)$$

the specific rotations do not satisfy (12). A lower bound $\Sigma_{\text{l.b.}}$ for the multiplicity of specific rotations can be deduced from theorem 1 as shown in the Appendix. The result is:

*Theorem* 2

The multiplicity of specific rotations of a hexagonal lattice with axial ratio determined by $\mu$ and $\nu$ cannot be smaller than

$$\Sigma_{\text{l.b.}} = \begin{cases} \sqrt{\mu\nu}/2 & \text{if } 3|\mu, 4|\nu \\ 2\sqrt{\mu\nu} & \text{if } 3\nmid\mu, 4\nmid\nu \\ \sqrt{\mu\nu} & \text{otherwise.}^* \end{cases} \quad (13)$$

Consider as an example the specific rotations with $\Sigma \leq 21$ and $1{\cdot}52 \leq c/a \leq 1{\cdot}68$. This range of $c/a$ is relevant for Be, Ti, Zr and Mg as shown in Table 1.

The values of $\mu$ and $\nu$ that are possible according to (13) are listed in Table 2.

Theorem 1 makes it possible to determine also an upper bound for the minimum value of the multiplicity of specific rotations:

*Lemma* 1

Put $\mu' = \mu/3$ if $3|\mu$, $\mu' = \mu$ otherwise, and $\nu' = \nu/4$ if $4|\nu$, $\nu' = \nu$ otherwise. Write $P = \mu'\nu'$ as a product $P = pq$ of two integers $p$ and $q$ with $|p - q|$ as small as possible. Then $\Sigma_{\min} \leq p + q$.

Applying lemma 1 to the 19 pairs $\mu, \nu$ listed in Table 2, one easily finds that it gives an upper bound $\Sigma_{\text{u.b.}}$ for $\Sigma_{\min}$ that satisfies $\Sigma_{\text{u.b.}} = \Sigma_{\min}$ in all 19 cases.

Lemma 1 can be proved by considering the hexagonal quadruple

$$(m, U, V, W) = \begin{cases} (0, \mu/\mu_0, 0, \nu/\nu_0) & 3\nmid\mu, 4\nmid\nu \\ (0, \mu/\mu_0, 0, \nu/2\nu_0) & 3\nmid\mu, 4|\nu \\ (\nu/\nu_0, \mu/\mu_0, 0, 0) & 3|\mu, 4\nmid\nu \\ (\nu/2\nu_0, \mu/\mu_0, 0, 0) & 3|\mu, 4|\nu \end{cases} \text{if},$$

* $u|v$ $(u \nmid v)$ states that the integer $v$ is (is not) an integral multiple of the integer $u \neq 0$.

Table 2. *The values of the axial ratio in the interval* $1{\cdot}52 \le c/a \le 1{\cdot}68$ *for which specific rotations of the hexagonal lattice with* $\Sigma \le 21$ *are possible according to theorem* 2

The lower bound for the multiplicity $\Sigma_{\rm l.b.}$ has been rounded to the next-higher integer; the minimum value of the multiplicity $\Sigma_{\rm min}$ has been determined with a computer program. The values of $c/a$ are arranged in increasing order; $c^2/a^2 = \mu/\nu$.

| $\mu$ | $\nu$ | $c^2/a^2$ | $c/a$ | $\Sigma_{\rm l.b.}$ | $\Sigma_{\rm min}$ |
|---|---|---|---|---|---|
| 7 | 3 | 2·333 | 1·528 | 10 | 10 |
| 19 | 8 | 2·375 | 1·541 | 13 | 21 |
| 12 | 5 | 2·4 | 1·549 | 8 | 9 |
| 29 | 12 | 2·417 | 1·555 | 19 | 32 |
| 39 | 16 | 2·438 | 1·561 | 13 | 17 |
| 27 | 11 | 2·455 | 1·567 | 18 | 20 |
| 5 | 2 | 2·5 | 1·581 | 7 | 7 |
| 33 | 13 | 2·538 | 1·593 | 21 | 24 |
| 51 | 20 | 2·55 | 1·597 | 16 | 22 |
| 18 | 7 | 2·571 | 1·604 | 12 | 13 |
| 31 | 12 | 2·583 | 1·607 | 20 | 34 |
| 13 | 5 | 2·6 | 1·612 | 17 | 18 |
| 21 | 8 | 2·625 | 1·620 | 7 | 9 |
| 8 | 3 | 2·667 | 1·633 | 10 | 10 |
| 27 | 10 | 2·7 | 1·643 | 17 | 19 |
| 30 | 11 | 2·727 | 1·651 | 19 | 21 |
| 11 | 4 | 2·75 | 1·658 | 7 | 12 |
| 14 | 5 | 2·8 | 1·673 | 17 | 17 |
| 45 | 16 | 2·813 | 1·677 | 14 | 16 |

where $\mu_0$ is a divisor of $\mu'$, $\nu_0$ a divisor of $\nu'$. From the $\Sigma$-hex theorem it follows in all four cases that $\Sigma = \nu'\mu_0/\nu_0 + \mu'\nu_0/\mu_0$. The integers $\mu_0$ and $\nu_0$ can be chosen such that $p = \mu'\nu_0/\mu_0$ and $q = \nu'\mu_0/\nu_0$ have the properties stated in lemma 1.

In order to compute tables of the coincidence rotations for a given value of $c/a$ one has to know the possible values of $F/\Sigma$. The quantity $F/\Sigma$ is always a divisor of $12\mu\nu$. This was stated first by Bleris *et al.* (1982) and proved rigorously by Grimmer & Warrington (1987). Theorem 1 makes it possible in many cases to give a stronger result: $F/\Sigma$ is a divisor of $6\mu\nu$ if $\nu$ is even and a divisor of $3\mu\nu$ if $\nu$ is a multiple of 4.

The connection between rotations that describe the same relative orientation of two hexagonal lattices has been discussed before, *e.g.* by Grimmer & Warrington (1987). A unique representative is chosen in each class of equivalent rotations if one requires the four parameters $m$, $U$, $V$, $W$ to satisfy

$$U \ge 2V \ge 0, \qquad W \ge 0 \tag{14}$$

$$m \ge (\nu/4\mu)^{1/2} U, \qquad m \ge (\nu/12\mu)^{1/2}(2U - V),$$

$$m \ge (2/3^{1/2} + 1)\, W \tag{15}$$

$$W \le (\nu/4\mu)^{1/2}(U - 2V) \quad \text{if } m = (\nu/4\mu)^{1/2} U \tag{16}$$

$$W \le (3\nu/4\mu)^{1/2} V \quad \text{if } m = (\nu/12\mu)^{1/2}(2U - V) \tag{17}$$

$$U \ge (2 + 3^{1/2}) V \quad \text{if } m = (2/3^{1/2} + 1)\, W. \tag{18}$$

The representative is a rotation with minimum angle and axis in a standard stereographic triangle (SST) defined by (14). Table 3 gives the equivalence classes of specific rotations with $\Sigma \le 21$ and $1{\cdot}52 \le c/a \le 1{\cdot}68$. The number of different rotations in the class is $12\omega$. The axes of 180° rotations are given by their Weber indices $[uv.w]$ (*cf.* Frank, 1965), not by their hexagonal components $[U'V'W'] \sim [2u + v\, u - v\, w]$; $u \ge v \ge 0$, $w \ge 0$ for axes in the SST. The planes perpendicular to these axes, called symmetry planes, are given by their Miller-Bravais indices $(hk.l) \sim (3\nu u\, 3\nu v.\, 2\mu w)$.

The equivalence classes of common rotations with $\Sigma \le 60$ are listed in Table 4. The number of different rotations in each of these classes is 24, *i.e.* $\omega = 2$. The Miller-Bravais indices of the symmetry plane coincide with the Weber indices of the axis of the corresponding 180° rotation.

The common rotations of hexagonal lattices have been known for several years (Warrington, 1975; Bonnet *et al.*, 1981; Bleris *et al.*, 1982). The present author has computed the specific rotations for

$$1{\cdot}50 \le c/a \le 1{\cdot}70 \quad \text{and} \quad \Sigma \le 25$$

$$1{\cdot}82 \le c/a \le 1{\cdot}92 \quad \text{and} \quad \Sigma \le 35$$

$$2{\cdot}65 \le c/a \le 2{\cdot}82 \quad \text{and} \quad \Sigma \le 35.$$

A comparison with published tables showed that Table 1 in Bleris *et al.* (1982) gives all solutions with $1{\cdot}545 < c/a < 1{\cdot}675$ and $\Sigma \le 20$. One value of $c/a$ is lacking in Delavignette (1982) and three in Delavignette (1983) as shown in Tables 5 and 6. The reason some solutions were missed becomes apparent from Table 2 in Delavignette (1982), where a rule for the value of $\Sigma_{\rm min}$ expressed in terms of $\mu$ and $\nu$ is given. The value $\Sigma_D$ obtained from that rule is either equal to or higher than the upper bound $\Sigma_{\rm u.b.}$ obtained from lemma 1, *i.e.*

$$\Sigma_{\rm l.b.} \le \Sigma_{\rm min} \le \Sigma_{\rm u.b.} \le \Sigma_D. \tag{19}$$

Consider as an example $c/a = 1{\cdot}880$; *i.e.* $\mu = 99$, $\nu = 28$, where $\Sigma_D = 99/3 + 28/4 = 40$ whereas $\Sigma_{\rm min} = \Sigma_{\rm u.b.} = 33/3 + 7 \times 3 = 32$.

The article by Bonnet *et al.* (1981) contains all solutions with $\Sigma \le 25$ and $1{\cdot}57 < c/a < 1{\cdot}64$, $1{\cdot}83 < c/a < 1{\cdot}91$ and $2{\cdot}69 < c/a < 2{\cdot}77$ with the exceptions of $c/a = 1{\cdot}620$, $\Sigma = 21a$ (see Table 3), $c/a = 1{\cdot}852$, $\Sigma = 18$ and $c/a = 1{\cdot}871$, $\Sigma = 21b$ (see Table 3 in Delavignette, 1982). The present author expects that the first solution should appear for Mg, the second for Zn and the third for Zn and Cd according to the criteria used by Bonnet *et al.* (1981).

### 3. Concluding remarks

The $\Sigma$-hex theorem makes it possible to determine a lower and an upper bound for $\Sigma_{\rm min}$, the minimum

Table 3. *The equivalence classes of specific rotations with $\Sigma \leq 21$ and $1{\cdot}52 \leq c/a \leq 1{\cdot}68$*

| Axial ratio | $\Sigma$ | $\omega$ | $\Theta$ (°) | Representative $m$ | $U$ | $V$ | $W$ | Axes in the SST of 180° rotations | | Symmetry planes in the SST | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1·528 | 10 | 6 | 66·42 | 1 | 2 | 1 | 0 | 1 1.3 | 7 7.9 | 3 3.14 | 1 1.2 |
| | 16 | 6 | 82·82 | 3 | 7 | 0 | 0 | 7 0.9 | 1 0.1 | 1 0.2 | 9 0.14 |
| | 19 | 6 | 74·74 | 6 | 14 | 7 | 0 | 7 7.18 | 2 2.3 | 1 1.4 | 3 3.7 |
| 1·541 | 21 | 6 | 35·95 | 2 | 2 | 1 | 0 | 1 1.6 | 19 19.12 | 2 2.19 | 1 1.1 |
| 1·549 | 9 | 6 | 83·62 | 5 | 12 | 0 | 0 | 4 0.5 | 1 0.1 | 1 0.2 | 5 0.8 |
| | 12 | 6 | 48·19 | 5 | 6 | 0 | 0 | 2 0.5 | 2 0.1 | 1 0.4 | 5 0.4 |
| | 16 | 6 | 75·52 | 5 | 12 | 6 | 0 | 2 2.5 | 2 2.3 | 1 1.4 | 5 5.12 |
| | 17 | 6 | 65·68 | 1 | 2 | 1 | 0 | 1 1.3 | 4 4.5 | 5 5.24 | 1 1.2 |
| | 19 | 6 | 54·62 | 5 | 8 | 4 | 0 | 4 4.15 | 1 1.1 | 1 1.6 | 5 5.8 |
| | 21*a* | 6 | 25·21 | 5 | 3 | 0 | 0 | 1 0.5 | 4 0.1 | 1 0.8 | 5 0.2 |
| | 21*b* | 6 | 58·41 | 2 | 3 | 0 | 0 | 1 0.2 | 8 0.5 | 5 0.16 | 1 0.1 |
| 1·561 | 17 | 6 | 58·03 | 2 | 3 | 0 | 0 | 1 0.2 | 13 0.8 | 4 0.13 | 1 0.1 |
| 1·567 | 20 | 6 | 84·26 | 11 | 27 | 0 | 0 | 9 0.11 | 1 0.1 | 1 0.2 | 11 0.18 |
| 1·581 | 7 | 6 | 64·62 | 1 | 2 | 1 | 0 | 1 1.3 | 5 5.6 | 1 1.5 | 1 1.2 |
| | 11*a* | 6 | 35·10 | 2 | 2 | 1 | 0 | 1 1.6 | 5 5.3 | 1 1.10 | 1 1.1 |
| | 11*b* | 6 | 84·78 | 2 | 5 | 0 | 0 | 5 0.6 | 1 0.1 | 1 0.2 | 3 0.5 |
| | 13*a* | 6 | 57·42 | 2 | 3 | 0 | 0 | 1 0.2 | 5 0.3 | 3 0.10 | 1 0.1 |
| | 13*b* | 6 | 76·66 | 4 | 10 | 5 | 0 | 5 5.12 | 2 2.3 | 1 1.4 | 2 2.5 |
| | 17*a* | 6 | 40·12 | 1 | 1 | 0 | 0 | 1 0.3 | 5 0.2 | 1 0.5 | 3 0.2 |
| | 17*b* | 12 | 79·84 | 2 | 5 | 1 | 0 | 4 1.6 | | 4 1.10 | |
| | 19*a* | 12 | 65·10 | 3 | 5 | 0 | 1 | | 4 1.3 | | 4 1.5 |
| | 19*b* | 6 | 86·98 | 2 | 6 | 3 | 0 | 1 1.2 | 5 5.9 | 3 3.10 | 1 1.3 |
| 1·604 | 13 | 6 | 85·59 | 7 | 18 | 0 | 0 | 6 0.7 | 1 0.1 | 1 0.2 | 7 0.12 |
| | 17 | 6 | 49·68 | 7 | 9 | 0 | 0 | 3 0.7 | 2 0.1 | 1 0.4 | 7 0.6 |
| 1·612 | 18 | 6 | 63·61 | 1 | 2 | 1 | 0 | 1 1.3 | 13 13.15 | 5 5.26 | 1 1.2 |
| 1·620 | 9 | 6 | 56·25 | 2 | 3 | 0 | 0 | 1 0.2 | 7 0.4 | 2 0.7 | 1 0.1 |
| | 13 | 6 | 85·59 | 2 | 6 | 3 | 0 | 1 1.2 | 7 7.12 | 2 2.7 | 1 1.3 |
| | 15*a* | 6 | 29·93 | 4 | 3 | 0 | 0 | 1 0.4 | 7 0.2 | 1 0.7 | 2 0.1 |
| | 15*b* | 6 | 86·18 | 8 | 21 | 0 | 0 | 7 0.8 | 1 0.1 | 1 0.2 | 4 0.7 |
| | 17 | 6 | 49·68 | 4 | 6 | 3 | 0 | 1 1.4 | 7 7.6 | 1 1.7 | 2 2.3 |
| | 21*a* | 12 | 70·53 | 4 | 9 | 3 | 0 | 2 1.4 | | 2 1.7 | |
| | 21*b* | 12 | 73·40 | 6 | 14 | 7 | 2 | | 2 1.2 | | 4 2.7 |
| 1·633 | 10 | 6 | 78·46 | 3 | 8 | 4 | 0 | 4 4.9 | 2 2.3 | 1 1.4 | 3 3.8 |
| | 11 | 6 | 62·96 | 1 | 2 | 1 | 0 | 1 1.3 | 8 8.9 | 3 3.16 | 1 1.2 |
| | 14 | 6 | 44·42 | 3 | 4 | 2 | 0 | 2 2.9 | 4 4.3 | 1 1.8 | 3 3.4 |
| | 17 | 6 | 86·63 | 3 | 8 | 0 | 0 | 8 0.9 | 1 0.1 | 1 0.2 | 9 0.16 |
| | 18 | 6 | 70·53 | 1 | 2 | 0 | 0 | 2 0.3 | 4 0.3 | 3 0.8 | 3 0.4 |
| 1·643 | 19 | 6 | 86·98 | 10 | 27 | 0 | 0 | 9 0.10 | 1 0.1 | 1 0.2 | 5 0.9 |
| | 21 | 6 | 64·62 | 5 | 9 | 0 | 0 | 3 0.5 | 3 0.2 | 1 0.3 | 5 0.6 |
| 1·651 | 21 | 6 | 87·27 | 11 | 30 | 0 | 0 | 10 0.11 | 1 0.1 | 1 0.2 | 11 0.20 |
| 1·658 | 12 | 6 | 33·56 | 2 | 2 | 1 | 0 | 1 1.6 | 11 11.6 | 1 1.11 | 1 1.1 |
| | 14 | 6 | 55·15 | 2 | 3 | 0 | 0 | 1 0.2 | 11 0.6 | 3 0.11 | 1 0.1 |
| | 15 | 6 | 62·18 | 1 | 2 | 1 | 0 | 1 1.3 | 11 11.12 | 2 2.11 | 1 1.2 |
| | 18 | 12 | 77·16 | 2 | 5 | 1 | 0 | 4 1.6 | | 4 1.11 | |
| | 20 | 6 | 84·26 | 2 | 6 | 3 | 0 | 1 1.2 | 11 11.18 | 3 3.11 | 1 1.3 |
| 1·673 | 17 | 6 | 79·84 | 5 | 14 | 7 | 0 | 7 7.15 | 2 2.3 | 1 1.4 | 5 5.14 |
| | 19 | 6 | 61·73 | 1 | 2 | 1 | 0 | 1 1.3 | 14 14.15 | 5 5.28 | 1 1.2 |
| 1·677 | 16 | 6 | 75·52 | 4 | 9 | 0 | 0 | 3 0.4 | 5 0.4 | 2 0.5 | 2 0.3 |
| | 17 | 6 | 65·68 | 8 | 15 | 0 | 0 | 5 0.8 | 3 0.2 | 1 0.3 | 4 0.5 |
| | 19 | 6 | 54·62 | 2 | 3 | 0 | 0 | 1 0.2 | 15 0.8 | 4 0.15 | 1 0.1 |

value of the multiplicity of specific rotations for a given axial ratio $c^2/a^2 = \mu/\nu$. Complete tables of specific rotations with $c/a$ in a given interval and $\Sigma$ not larger than some given value $\Sigma_c$ can be obtained by considering all pairs $\mu$, $\nu$ for which $\Sigma_{\text{l.b.}} \leq \Sigma_c$. This result has been used to complete published tables of specific rotations. No cases are known to the author where $\Sigma_{\text{u.b.}} = \Sigma_{\text{min}}$ does not hold, a general proof of this relation is lacking, however. It would simplify the computation of specific rotations with $\Sigma \leq \Sigma_c$ and $c/a$ in a given interval by eliminating straightaway the pairs $\mu$, $\nu$ with $\Sigma_{\text{l.b.}} \leq \Sigma_c < \Sigma_{\text{u.b.}}$.

Stimulating discussions with Drs R. Bonnet and S. Lartigue and Professor L. Priester are gratefully acknowledged.

Table 4. *The equivalence classes of common rotations with $\Sigma \le 60$*

The hexagonal quadruples of the representatives have the form $(m\,0\,0\,W)$

| $\Sigma$ | Representative $\Theta$ (°) | $m$ | $W$ | Axes in the SST of 180° rotations | |
|---|---|---|---|---|---|
| 7 | 21·79 | 3 | 1 | 2 1.0 | 4 1.0 |
| 13 | 27·80 | 7 | 3 | 5 2.0 | 3 1.0 |
| 19 | 13·17 | 5 | 1 | 3 2.0 | 7 1.0 |
| 31 | 17·90 | 11 | 3 | 7 4.0 | 5 1.0 |
| 37 | 9·43 | 7 | 1 | 4 3.0 | 10 1.0 |
| 43 | 15·18 | 13 | 3 | 8 5.0 | 6 1.0 |
| 49 | 16·43 | 4 | 1 | 5 3.0 | 11 2.0 |

Table 5. *Additional values of the axial ratio in the intervals considered by Delavignette* (1982, 1983) *for which specific rotations of the hexagonal lattice exist with $\Sigma \le 35$*

The lower bound for the multiplicity $\Sigma_{\text{l.b.}}$ has been rounded to the next-higher integer.

| $\mu$ | $\nu$ | $c^2/a^2$ | $c/a$ | $\Sigma_{\text{l.b.}}$ | $\Sigma_{\min} = \Sigma_{\text{u.b.}}$ |
|---|---|---|---|---|---|
| 99 | 28 | 3·536 | 1·880 | 27 | 32 |
| 117 | 16 | 7·313 | 2·704 | 22 | 25 |
| 91 | 12 | 7·583 | 2·754 | 34 | 34 |
| 153 | 20 | 7·65 | 2·766 | 28 | 32 |

Table 6. *Additional equivalence classes of specific coincidence rotations with $\Sigma \le 35$ and axial ratios in the ranges considered by Delavignette* (1982, 1983)

Each of these five classes contains 72 rotations (*i.e.* $\omega = 6$).

| Axial ratio | $\Sigma$ | Representative $\Theta$ (°) | $m$ | $U$ | $V$ | $W$ | Axes in the SST of 180° rotations | | Symmetry planes in the SST | |
|---|---|---|---|---|---|---|---|---|---|---|
| 1·880 | 32 | 71·79 | 14 | 33 | 0 | 0 | 11 0.14 | 3 0. 2 | 1 0. 3 | 7 0.11 |
| 2·704 | 25 | 87·71 | 2 | 9 | 0 | 0 | 3 0. 2 | 13 0. 8 | 4 0.13 | 1 0. 3 |
| | 32 | 51·32 | 4 | 9 | 0 | 0 | 3 0. 4 | 13 0. 4 | 2 0.13 | 2 0. 3 |
| 2·754 | 34 | 76·39 | 6 | 26 | 13 | 0 | 13 13.18 | 7 7. 6 | 1 1. 7 | 3 3.13 |
| 2·766 | 32 | 86·42 | 2 | 9 | 0 | 0 | 3 0. 2 | 17 0.10 | 5 0.17 | 1 0. 3 |

## APPENDIX

### A lower bound for the multiplicity of specific rotations

#### A.1. *Introduction*

Equivalent rotations create CSL's with the same multiplicity. Equations (14), (15) show therefore that it suffices to give a lower bound for the multiplicity of rotations that satisfy

$$U \ge 2V \ge 0, \quad W \ge 0, \quad m \ge (2/3^{1/2}+1)W. \quad (20)$$

Such rotations are specific if

$$m > 0 \quad \text{and} \quad U > 0. \quad (21)$$

It follows from the $\Sigma$-hex theorem that

$$F \ge F_0 = 3\mu m^2 + (3/4)\nu U^2 \quad \text{if } W = 0, \quad (22)$$

$$F \ge F_W = 4(2+3^{1/2})\mu W^2 + (3/4)\nu U^2 \quad \text{if } W > 0. \quad (23)$$

Define

$$\Sigma_0 = F_0/mU \quad \text{and} \quad \Sigma_W = F_W/WU. \quad (24)$$

It follows that

$$\Sigma_0 = 3\mu(m/U) + \tfrac{3}{4}\nu(U/m) = f(m/U).$$

The value of $x = m/U$ for which $f(x)$ becomes a minimum is obtained by setting

$$\frac{\mathrm{d}f}{\mathrm{d}x} = 0,$$

*i.e.*

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(3\mu x + \frac{3\nu}{4x}\right) = 3\mu - \frac{3\nu}{4x^2} = 0 \Rightarrow x = \frac{1}{2}\left(\frac{\nu}{\mu}\right)^{1/2}.$$

This gives

$$\Sigma_0 \ge 3(\mu\nu)^{1/2}. \quad (25)$$

Similarly it is found that

$$\Sigma_W \ge 2[3\mu\nu(2+3^{1/2})]^{1/2} > 6(\mu\nu)^{1/2}. \quad (26)$$

#### A.2. *Derivation of the bound*

The $\alpha$-hex theorem shows that $G = F/\Sigma$ has the form

$$G = F_1^2 F_2 F_3 F_4 F_5. \quad (27)$$

The notation $p\,|\,q$ will be used to state that the integer $q$ is an integral multiple of the integer $p \ne 0$; $p \nmid q$ states that $q$ is not an integral multiple of $p$.

*Case (a)*

$F_1 = 2 \Rightarrow F_3 = 1$, $m$ and $W$ odd.

(1) $F_2 = 3 \Rightarrow F_4 = \gcd(\nu, W/3, m+W) \le W/3$, $F_5 = \gcd(\mu, U/2, V/2) \le U/2 \Rightarrow G \le 2WU \Rightarrow \Sigma \ge \Sigma_W/2 > 3(\mu\nu)^{1/2}$.

(2) $F_2 = 1 \Rightarrow F_4 = \gcd(\nu, W, m) \le W$, $F_5 = \gcd(\mu, 3U/2, (U+V)/2) \le 3U/4 \Rightarrow G \le 3WU \Rightarrow \Sigma \ge \Sigma_W/3 > 2(\mu\nu)^{1/2}$.

*Case (b)*

$F_1 = 1$, $F_2 = 3 \Rightarrow F_5 = \gcd(\mu, U, V) \le U$.

If $3 \nmid \mu$ then $F_5 \le U/2$. *Proof*: $3 | U+V$ because $F_2=3$. If $V=0$ then $3|U$ and $F_5 \le U/3$; if $V \ne 0$ then $F_5 \le U/2$ because of (14). All the following lower limits on $\Sigma$ can therefore be multiplied by 2 if $3 \nmid \mu$.

(1) $F_3=1 \Rightarrow 2 \nmid \nu$ or $2 \nmid m+W$ $\Rightarrow F_4 = \gcd(\nu, W/3, m+W)$.

(1.1) $W=0 \Rightarrow F_4 \le m \Rightarrow G \le 3mU \Rightarrow \Sigma \ge \Sigma_0/3 = (\mu\nu)^{1/2}$.

(1.2) $W \ne 0 \Rightarrow F_4 \le W/3 \Rightarrow G \le WU \Rightarrow \Sigma \ge \Sigma_W > 6(\mu\nu)^{1/2}$.

(2) $F_3=2 \Rightarrow F_4 = \gcd(\nu/2, 2W/3, m+W)$.

(2.1) $W=0, 4|\nu \Rightarrow F_4 \le m \Rightarrow G \le 6mU \Rightarrow \Sigma \ge (\mu\nu)^{1/2}/2$.

(2.2) $W=0, 4 \nmid \nu \Rightarrow F_4 \le m/2 \Rightarrow G \le 3mU \Rightarrow \Sigma \ge (\mu\nu)^{1/2}$.

(2.3) $W \ne 0 \Rightarrow F_4 \le 2W/3 \Rightarrow G \le 4WU \Rightarrow \Sigma > 3(\mu\nu)^{1/2}/2$.

*Case* (*c*)

$F_1 = F_2 = 1 \Rightarrow F_5 = \gcd(\mu, 3U, U+V) \le 3U/2$.

(1) $F_3=1 \Rightarrow F_4 = \gcd(\nu, 2W, m+W)$.

(1.1) $W=0 \Rightarrow F_4 \le m \Rightarrow G \le 3mU/2 \Rightarrow \Sigma \ge 2(\mu\nu)^{1/2}$.

(1.2) $W \ne 0 \Rightarrow F_4 \le 2W \Rightarrow G \le 3WU \Rightarrow \Sigma > 2(\mu\nu)^{1/2}$.

(2) $F_3=2 \Rightarrow F_4 = \gcd(\nu/2, 2W, m+W)$.

(2.1) $W=0, 4|\nu \Rightarrow F_4 \le m \Rightarrow G \le 3mU \Rightarrow \Sigma \ge (\mu\nu)^{1/2}$.

(2.2) $W=0, 4 \nmid \nu \Rightarrow F_4 \le m/2 \Rightarrow G \le 3mU/2 \Rightarrow \Sigma \ge 2(\mu\nu)^{1/2}$.

(2.3) $W \ne 0, 4|\nu \Rightarrow F_4 \le 2W \Rightarrow G \le 6WU \Rightarrow \Sigma > (\mu\nu)^{1/2}$.

(2.4) $W \ne 0, 4 \nmid \nu \Rightarrow F_4 \le W \Rightarrow G \le 3WU \Rightarrow \Sigma > 2(\mu\nu)^{1/2}$.

*Summary*

It follows from cases (*a*)-(*c*) that

$$\Sigma \ge \begin{cases} (\mu\nu)^{1/2}/2 & \text{if } 3|\mu, 4|\nu \\ 2(\mu\nu)^{1/2} & \text{if } 3\nmid\mu, 4\nmid\nu \\ (\mu\nu)^{1/2} & \text{otherwise.} \end{cases}$$


### References

Bleris, G. L., Nouet, G., Hagège, S. & Delavignette, P. (1982). *Acta Cryst.* A38, 550-557.

Bonnet, R., Cousineau, E. & Warrington, D. H. (1981). *Acta Cryst.* A37, 184-189.

Delavignette, P. (1982). *J. Phys.* (*Paris*) *Colloq.* **43**, C6, 1-13.

Delavignette, P. (1983). *J. Microsc. Spectrosc. Electron.* **8**, 111-124.

Eckerlin, P. & Kandler, H. (1971). *Landolt-Börnstein, New Series, Group III*, Vol. 6. Berlin: Springer.

Frank, F. C. (1965). *Acta Cryst.* **18**, 862-866.

Grimmer, H. (1976). *Acta Cryst.* A32, 783-785.

Grimmer, H. & Warrington, D. H. (1983). *Z. Kristallogr.* **162**, 88-90.

Grimmer, H. & Warrington, D. H. (1985). *J. Phys.* (*Paris*) *Colloq.* **46**, C4, 231-236.

Grimmer, H. & Warrington, D. H. (1987). *Acta Cryst.* A43, 232-243.

Hagège, S. & Nouet, G. (1985). *Scr. Metall.* **19**, 11-16.

Warrington, D. H. (1975). *J. Phys.* (*Paris*) *Colloq.* **36**, C4, 87-95.


*Acta Cryst.* (1989). A45, 325-333

# Electron Inelastic Plasmon Scattering and its Resonance Propagation at Crystal Surfaces in RHEED

By Z. L. Wang,*† J. Liu and J. M. Cowley

*Department of Physics, Arizona State University, Tempe, AZ* 85287-1504, *USA*

(*Received* 26 *September* 1988; *accepted* 9 *December* 1988)


## Abstract

The modified multislice theory [Wang (1989). *Acta Cryst.* A45, 193-199] has been employed to calculate the electron reflection intensity with and without considering the plasmon diffuse scattering in the geometry of reflection high-energy electron diffraction (RHEED). It has been shown that the inelastic scattering can greatly enhance the reflectance of a surface, depending critically on the incident conditions of the electrons. At some incidences, the inelastic resonance reflection is enhanced, which is considered as the 'true' surface resonance state. This happens within a very narrow angular range (<1 mrad). For 'true' resonance states, the inelastic intensity is much stronger than for other conditions as shown both theoretically and experimentally. The enhancement of the reflection intensity may not be the proper criterion for identifying the 'true' surface resonance. Besides the surface plasmon peaks, an 'extra' peak, located at 4·5 eV, is observed in the


* Present address: Cavendish Laboratory, University of Cambridge, Madingley Road, Cambridge CB3 0HE, England.

† To whom correspondence should be addressed.

0108-7673/89/050325-09$03.00 