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Tables of Coincidence Orientations for Ordered Tetragonal $L1_0$ Alloys for a Range of Axial Ratios

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Abstract

In this paper we develop and apply techniques for computation of CSL, DSCL and step-vector data for grain boundaries in tetragonal materials for a range of axial ratios. This has application to $L1_0$ alloys including TiAl, which is a candidate for lightweight high-temperature structural applications. Our results are compared with others and found to be more accurate and complete. We provide data for a wider range of axial ratios than those considered by previous workers. We have also derived equivalent quaternions for tetragonal crystals in tetragonal-crystal coordinates and listed conditions for selecting a unique reduced rotation in tetragonal-crystal coordinates so that a disorientation description becomes available.

Introduction

Coincidence-site lattices (CSLs) are geometrical models of grain-boundary structure that are formed by relative rotations of two congruent lattices, with a lattice site used as the origin. The ratio of the unit-cell volume of the CSL to that of the original lattice is usually denoted by Σ. Grain boundaries corresponding to relatively low Σ values have been found to exhibit special behaviors, leading Watanabe (1984) to introduce the concept of grain-boundary design as a means of improving various properties in polycrystalline materials.

In grain-bounday geometry, the displacement-shift-complete lattice (DSCL), which is a lattice of vectors representing the 'complete' displacements of one crystal with respect to the other and leaving the boundary structure shifted, is also of importance. If the relative orientation between two grains deviates by only a few degrees from a coincidence orientation with a low value of Σ, then it has often been observed that the deviation from exact coincidence is accommodated by arrays of DSC dislocations in the boundary. Knowledge of the DSCL is essential, for example, for the application of modern theories of slip transmission (Clark, Wagoner, Chen, Lee, Robertson & Birnbaum, 1992).

Knowledge of the step vector associated with a DSC dislocation is essential in determination of the height of the step in the grain boundary that is associated with the core of a grain-boundary dislocation. The step vectors for grain-boundary dislocations in cubic crystals were determined by King (1982) and in h.c.p. materials by Chen & King (1987). Quantitative confirmation of the importance of step vectors in determination of the behaviors of grain boundaries has been given by Fukutomi, Kamijo & Horiuchi (1986).

Bruggeman, Bishop & Hartt (1972) pointed out that three-dimensional CSLs can only be obtained in h.c.p. crystals when $(c/a)^2$ is a rational fraction, except for rotations about the [0001] axis. Hence it is necessary to constrain the real $(c/a)^2$ value to some proximate rational value to obtain a three-dimensional CSL, which Chen & King (1988) called a constrained CSL (CCSL), in order that a DSC lattice becomes available. The CSLs that are associated with the [0001] rotation axis are exact CSLs (ECSLs). Grain-boundary dislocations whose Burgers vectors are appropriate DSC lattice vectors will accommodate deviation from a CCSL in constraint as well as misorientation. The idea of constrained coincidence lattices extends to all non-cubic lattices. In tetragonal crystals, the CSLs that are obtained by rotations about the [001] axis are ECSLs and the CSLs that are obtained for axes other than [001] are CCSLs. Grimmer (1989) called rotations

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related with ECSLs 'common rotations' and those with CCSLs 'specific rotations'.

Interest in the grain-boundary structure in many materials with tetragonal structure is increasing. For example, TiAl, an $L1_0$ alloy, which is a candidate for lightweight high-temperature structural applications, suffers from grain-boundary embrittlement. Therefore, an understanding of the grain-boundary structure in this material is essential. In previous work (Singh, Chandrasekhar & King, 1990), we produced data appropriate to the superconducting oxide $YBa_2Cu_3O_{7-\delta}$. In this paper we improve upon the techniques and apply them to compute CSL, DSCL and step-vector data for tetragonal crystals for a range of axial ratios and give tables of coincidences for $L1_0$ alloys. Our results are compared with others and found to be more accurate and complete.

Coincidence orientations

A basis **e** of the tetragonal lattice is given by three mutually orthogonal vectors $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$ of lengths a, a and c $(=\rho a)$. The expressions for general rotation matrices for coincidence orientations of tetragonal crystals and Σ were derived by Singh, Chandrasekhar & King (1990) in terms of six integer parameters μ, ν, m, U, V and W satisfying

$$\text{g.c.d.}(m, U, V, W)=1, \quad \text{g.c.d.}(\mu, \nu)=1, \quad \frac{c^2}{a^2}=\frac{\mu}{\nu}, \tag{1}$$

where g.c.d. is an abbreviation for the greatest common divisor and μ and ν are the positive integers for rational values of c^2/a^2. (m, U, V, W) is a quaternion description of a coincidence rotation, corresponding to a rotation matrix

$$R=\frac{1}{F}\begin{bmatrix} \mu(m^2-W^2)+\nu(U^2-V^2) & 2(\nu UV-\mu mW) & 2\mu(UW+mV) \\ 2(\nu UV+\mu mW) & \mu(m^2-W^2)-\nu(U^2-V^2) & 2\mu(VW-mU) \\ 2\nu(UW-mV) & 2\nu(VW+mU) & \mu(m^2+W^2)-\nu(U^2+V^2) \end{bmatrix}. \tag{2}$$

The expression for Σ can be given as

$$F=\mu s=\mu(m^2+W^2)+\nu(U^2+V^2)=\alpha\Sigma. \tag{3}$$

The problem of finding coincidence orientations then becomes that of determining appropriate values of m, U, V, W, μ and ν, and finding the corresponding value of α. Singh, Chandrasekhar & King (1990) have shown that

$$\nu/\mu=\tau, \quad \text{g.c.d.}(\mu,\nu)=1; \tag{4}$$

$$4\mu m^2=F+r_{11}^{+}+r_{22}^{+}+r_{33}^{+}, \tag{5a}$$
$$4\mu mU=r_{23}^{-}-r_{23}^{+}, \tag{5b}$$
$$4\mu mV=r_{13}^{+}-r_{13}^{-}, \tag{5c}$$
$$4\mu mW=r_{12}^{-}-r_{12}^{+}, \tag{5d}$$
$$4\mu UW=r_{13}^{+}+r_{13}^{-}, \tag{5e}$$
$$4\mu VW=r_{23}^{+}+r_{23}^{-}, \tag{5f}$$
$$4\mu W^2=F-r_{11}^{+}-r_{22}^{+}+r_{33}^{+}, \tag{5g}$$
$$4\nu U^2=F+r_{11}^{+}-r_{22}^{+}-r_{33}^{+}, \tag{5h}$$
$$4\nu mU=r_{32}^{+}-r_{32}^{-}, \tag{5i}$$
$$4\nu UW=r_{31}^{+}+r_{31}^{-}, \tag{5j}$$
$$4\nu UV=r_{21}^{+}+r_{21}^{-}, \tag{5k}$$
$$4\nu mV=r_{31}^{-}-r_{31}^{+}, \tag{5l}$$
$$4\nu VW=r_{32}^{+}+r_{32}^{-}, \tag{5m}$$
$$4\nu V^2=F-r_{11}^{+}+r_{22}^{+}-r_{33}^{+}, \tag{5n}$$

where F is defined by (2) and r_{ij}^{+}/F and r_{ij}^{-}/F are the elements of the rotation matrices R and R^{-1}, respectively. The constraints given in (5) were derived by Singh, Chandrasekhar & King (1990) by use of the fact that the necessary and sufficient condition for the three-dimensional CSLs to occur is that R and R^{-1}, in lattice coordinates, are both rational.

From the set of equations (5) and the α-hex theorem given in the paper by Grimmer & Warrington (1987), it can be deduced that α is a factor of $4\mu\nu$. This is used to obtain constraints on the values of α, m, U, V and W. Thus, we obtain the values of these parameters for which coincidence rotations can exist and also the associated Σ values. These constraints ensure that the matices ΣR and ΣR^{-1} are integral and indeed yield coincidence rotations.

Equations (4) and (5) and the fact that α is a factor of all the expressions in (5) serve to derive a lower bound on Σ for constrained coincidence rotations for any given axis of rotation (Grimmer, 1992*a*). It follows from (5*b*) and (5*i*) that $\alpha|4mU$, from (5*c*) and (5*l*) that $\alpha|4mV$, from (5*e*) and (5*j*) that $\alpha|4UW$, and from (5*f*) and (5*m*) that $\alpha|4VW$, where '|' means 'is a factor of'. For constrained coincidence, $m\neq 0$, $U\neq 0$ or $m\neq 0$, $V\neq 0$ or $W\neq 0$, $U\neq 0$ or $W\neq 0$, $V\neq 0$.

In the first case, one has

$$\Sigma=F/\alpha\geq(\mu m^2+\nu U^2)/\alpha\geq 2(\mu m^2\nu U^2)^{1/2}/\alpha$$
$$\geq 2(\mu\nu)^{1/2}mU/4mU\geq(\mu\nu)^{1/2}/2, \tag{6}$$

where we have used the first result, *i.e.* $\alpha|4mU$. Similar results are obtained for the other cases.

A stronger bound given by Grimmer (1992*b*) is:

$$\text{if } \mu \text{ is odd or a multiple of 4 then } \Sigma \geq (\mu\nu)^{1/2},$$
$$\text{otherwise } \Sigma \geq (2\mu\nu)^{1/2}. \quad (7)$$

This bound makes it possible to determine all possible values of μ and ν for a given upper limit on Σ and for a given range of axial ratios c/a that may give rise to constrained coincidence.

Equivalent quaternion descriptions for tetragonal system, disorientation and choice of a representative class

Simple applications of the theory outlined above yield coincidence rotations, some of which may give physically identical structures although they derive from different rotations. Such rotations are termed 'equivalent' and it is desirable to have a systematic means of selecting only one among any set of equivalent rotations. The tables produced for $YBa_2Cu_3O_{7-\delta}$ by Singh, Chandrasekhar & King (1990) include some cases of equivalent rotations that were not correctly removed and we develop here a method to ensure that only a single representative of each set is selected. Grimmer (1980) defined the disorientation as the minimum angle among the $2N^2$ equivalent rotations in the positive sense around an axis in the standard stereographic triangle, where N is the number of symmetry rotations of the lattice.

Two rotation matrices, R and R' are equivalent if $R' = SRT$ or $R' = SR^{-1}T$, where S and T describe symmetry rotations for a particular crystal structure. It was shown by Grimmer (1974, 1980) that the number, n, of equivalent rotations is given by $n = 2N^2/m$, where m is a factor of $2N$. Similarly, two quaternions Q and Q' are equivalent if $Q' = Q_sQQ_t$ or $Q' = Q_sQ^{-1}Q_t$, where Q_s and Q_t describe symmetry quaternions for a particular crystal structure. In the case of tetragonal crystals there are eight symmetry matrices and therefore 2×8^2 equivalent rotations and 4×8^2 quaternions since there are two quaternions $\pm Q$ associated with every rotation (Du Val, 1964; Grimmer, 1974). The equivalent quaternions were obtained by Grimmer (1980) for arbitrary crystal structures. He listed the equivalent quaternions in orthogonal coordinates. Gertsman (1990) in his paper on vector–quaternion description of misorientation, however, gave the values in tetragonal coordinates. We list the equivalent quaternions in tetragonal coordinates obtained from those given by Grimmer (1980). To avoid any confusion in the comparison of our results with Gertsman's, it should be noted that the terms K, L, M, N for quaternions in the paper by Gertsman are U, V, W, m, respectively, in ours.

Table 1. *Axial ratios of 19 alloys based on* $L1_0$ *structure*

The first column gives the value of (c/a) for the pseudo-face-centered tetragonal unit cells of the alloys. The values of $(c/a)^2$, $2^{1/2}c/a$ and $(2^{1/2}c/a)^2$ have been calculated from the values of c/a given in the first column.

Alloy	c/a	$(c/a)^2$	$2^{1/2}c/a$	$(2^{1/2}c/a)^2$
δ-CuTi	0.643	0.413	0.909	0.827
θ-PdZn	0.186	0.666	1.154	1.332
θ-CdPd	0.845	0.714	1.195	1.428
PtZn	0.860	0.740	1.216	1.479
HgPd	0.862	0.743	1.219	1.486
α-BiLi	0.894	0.799	1.264	1.598
δ-HgPt	0.910	0.828	1.287	1.656
θ-CdPt	0.914	0.835	1.293	1.671
CuAu	0.926	0.857	1.310	1.715
NiPt	0.939	0.882	1.328	1.763
β''-InMg	0.960	0.922	1.358	1.843
FePd	0.966	0.933	1.366	1.866
FePt	0.968	0.937	1.369	1.874
CoPt	0.973	0.947	1.376	1.893
BiNa	0.980	0.960	1.386	1.921
AgTi	0.993	0.986	1.040	1.972
TiAl	1.020	1.040	1.442	2.081
HgZr	1.320	1.742	1.867	3.485
HgTi	1.343	1.804	1.899	3.607

The equivalent quarternions are obtained by multiplication of the symmetry quaternions with the coincidence quaternions $[A, B, C, D]$. The symmetry quaternions for tetragonal systems in crystal coordinates can be obtained by use of (Singh, Chandrasekhar & King, 1990)

$$[A, B, C, D] = \pm[\cos(\theta/2), n_1\rho\sin(\theta/2), n_2\rho\sin(\theta/2), n_3\rho\sin(\theta/2)], \quad (8)$$

where $0 \leq \theta \leq \pi$ describes a right-handed rotation about an axis with tetragonal-crystal components n_1, n_2, n_3 satisfying $n_1^2 + n_2^2 + \rho^2 n_3^2 = 1$. Therefore, the symmetry quaternions for tetragonal crystals in tetragonal-crystal coordinates are

$$[1,0,0,0],\ 2^{-1/2}[1,0,0,1],\ [0,0,0,1],\ 2^{-1/2}[-1,0,0,1],$$
$$[0,\rho,0,0],\ [0,0,\rho,0],\ 2^{-1/2}[0,\rho,\rho,0],\ 2^{-1/2}[0,\rho,-\rho,0].$$

The multiplication law for unit quaternions is

$$[\alpha,\beta,\gamma,\delta].[\alpha',\beta',\gamma',\delta'] = [\alpha.\alpha' - \delta.\delta' - (\beta.\beta' + \gamma.\gamma'),$$
$$\alpha.\beta' + \beta.\alpha' + \gamma.\delta' - \delta.\gamma',$$
$$\alpha.\gamma' - \beta.\delta' + \gamma.\alpha' + \delta.\beta',$$
$$\alpha.\delta' + \delta.\alpha' + (\beta.\gamma' - \gamma.\beta')].$$

Singh, Chandrasekhar & King (1990) give the relation between the quaternions in cubic coordinates $[\alpha, \beta, \gamma, \delta]$ and the quaternions in tetragonal-crystal coordinates $[A, B, C, D]$, which can be written as

$$[\alpha, \beta, \gamma, \delta] = \pm[A, B/\rho, C/\rho, D]. \quad (9)$$

The multiplication law for tetragonal crystals in crystal coordinates can be obtained if the tetragonal quadruples $[A, B, C, D]$ and $[A', B', C', D']$ are

replaced by quarternions in accordance with (9), with use made of the usual multiplication law given above and a change back to tetragonal quadruples. This results in

$$[A, B, C, D].[A', B', C', D'] =$$
$$[A.A' - D.D' - \rho^{-2}(B.B' + C.C'),$$
$$A.B' + B.A' + C.D' - D.C',$$
$$A.C' - B.D' + C.A' + D.B',$$
$$A.D' + D.A' + \rho^{-2}(B.C' - C.B')], \quad (10)$$

where $\rho = c/a$.

Therefore, the equivalent quaternions for the tetragonal system, in crystal coordinates, can be given by the permutations and arbitrary sign changes of the four components [(1), (14)(23), (23) and (14)] in the quarternions

$$[A, B, C, D],$$
$$[B/\rho, A\rho, D\rho, C/\rho],$$
$$2^{-1/2}[A + D, B + C, B - C, A - D],$$
$$2^{-1/2}[(B + C)/\rho, (A + D)\rho, (A - D)\rho, (B - C)/\rho], \quad (11)$$

where $A^2 + D^2 + \rho^{-2}(B^2 + C^2) = 1$. These quaternions can be written in terms of m, U, V, W, μ and ν by use of the definitions

$$\tau = \rho^{-2}, \quad (12)$$
$$s = m^2 + W^2 + \tau(U^2 + V^2), \quad (13)$$
$$A = ms^{-1/2}, \quad B = Us^{-1/2}, \quad C = Vs^{-1/2}, \quad D = Ws^{-1/2}, \quad (14)$$

This results in

$$s^{-1/2}[m, U, V, W], \quad (15a)$$
$$s^{-1/2}(\nu/\mu)^{1/2}(1/\nu)[\nu U, \mu m, \mu W, \nu V], \quad (15b)$$
$$2^{-1/2}s^{-1/2}[m + W, U + V, U - V, m - W], \quad (15c)$$
$$s^{-1/2}(\nu/\mu)^{1/2}(1/\nu)[\nu(U + V), \mu(m - W), \mu(m + W), \nu(U - V)]. \quad (15d)$$

The conditions for disorientations were given by Grimmer (1980) and can now be written in tetragonal coordinates as

$$U \geq V \geq 0, \quad W \geq 0, \quad (16a)$$
$$m \geq (\nu/\mu)^{1/2}U, \quad (16b)$$
$$m \geq 2^{-1/2}(\nu/\mu)^{1/2}(U + V), \quad (16c)$$
$$m \geq (2^{1/2} + 1)W, \quad (16d)$$
$$\text{if } m = (\nu/\mu)^{1/2}U \text{ then } W \leq (\nu/\mu)^{1/2}V, \quad (16e)$$
$$\text{if } 2^{1/2}m = (\nu/\mu)^{1/2}(U + V) \text{ then } 2^{1/2}W \leq (\nu/\mu)^{1/2}(U - V), \quad (16f)$$
$$\text{if } m = (2^{1/2} + 1)W \text{ then } U \geq (2^{1/2} + 1)V. \quad (16g)$$

These conditions give a unique representative in each class of equivalent rotations. The representative is the rotation with minimum angle and axis in a standard stereographic triangle defined by $U \geq V \geq 0$, $W \geq 0$.

Coincidence systems for $L1_0$ alloys

The unit cell of $L1_0$-type alloys is face-centred tetragonal (f.c.t.) with axial ratio c/a varying from 0.643 to 1.343. Table 1 lists the values of c/a for 19 alloys with the $L1_0$ structure. To determine all possible coincidence systems for the $L1_0$ alloys, there are two possible choices for primitive tetragonal-crystal lattices, one with an axial ratio c/a corresponding to pseudo-face-centered tetragonal structure (pseudo-f.c.t.) and the other with an axial ratio of $2^{1/2}(c/a)$ corresponding to a pseudo-body-centered tetragonal (pseudo-b.c.t.) unit cell. These descriptions are shown in Fig. 1 for the $L1_0$ CuAu cell. The structures in Figs. 1(*a*) and 1(*c*) are termed pseudo-f.c.t. and pseudo-b.c.t. since the four face-centred atoms in Fig. 1(*a*) and the body-centred atom in Fig. 1(*c*) are of different kinds (Au atoms in these figures). Since Cu and Au sites are not equivalent, the cell is always correctly described as primitive tetragonal. The pseudo-f.c.t. description is used frequently in the

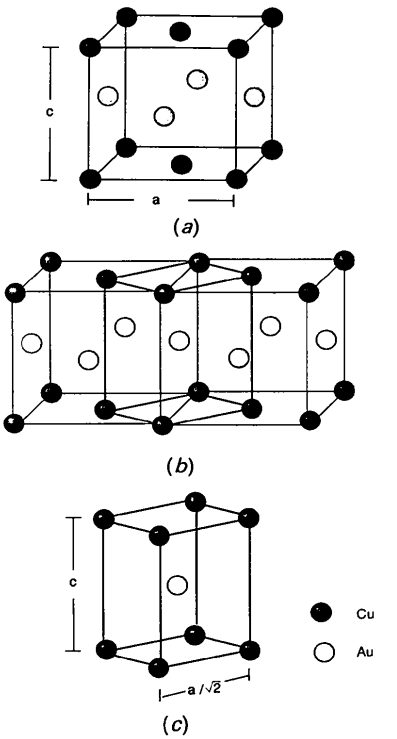

Fig. 1. Unit cell of CuAu(1), an $L1_0$ alloy. (*a*) Pseudo-face-centered tetragonal cell. (*b*) Relation between pseudo-face- and pseudo-body-centered unit cells. (*c*) Pseudo-body-centered tetragonal cell.

metallurgical literature as a result of a tradition of regarding the $L1_0$ structure as 'ordered f.c.c.'. In the present study we have determined the coincidence systems for the primitive tetragonal cell based on the pseudo-b.c.t. description, making use of the methods given by Singh, Chandrasekhar & King (1990) and (7) and (16). The CSL and DSC vectors were determined by use of the method of Grimmer & Warrington (1987) and the step vectors were determined by the method given by Chen & King (1987).

Gertsman (1990) determined all possible coincidence systems up to $\Sigma \leq 49$ for $L1_0$ alloys based on the body-centered description of the unit cell. However, he used only the axial ratio of $2^{1/2}$. His justification for the choice of axial ratio of $2^{1/2}$ is based on the data of $(2^{1/2}c/a)^2$ of seven alloys varying from 1.84 to 2.04. It is evident from Table 1 that the axial ratio $(2^{1/2}c/a)^2$ for the b.c.t. structure varies from 0.827 to 3.607. Therefore, the restrictions imposed by Gertsman do not provide sufficient data for all $L1_0$ alloys. Furthermore, Shin & King (1991) have demonstrated that there can be a compensation effect between the misorientation accommodation and the axial-ratio accommodation that can lead to large dislocation spacings in equilibrated grain boundaries even at extreme deviations from the ideal coincidence misorientations and axial ratios. In the light of this result and the broader range of axial ratios shown in Table 1, it is important to determine coincidence orientations for large ranges of axial ratio. We present our results for all possible coincidence systems for primitive tetragonal lattices based on the body-centered cell with $0.800 \leq 2^{1/2}c/a \leq 1.900$. We have used (7) to get all possible values of μ and ν for an upper limit of Σ and for the above range of axial ratios.

The rotations about [001] are exact rotations and are the same as rotations about ⟨100⟩ axes in cubic crystals. Table 2 gives a comprehensive list of Σ values, rotation axes, rotation angles, CSLs, DSCs and step vectors for rotations other than the [001] axis with $\Sigma \leq 7$ and $0.800 \leq 2^{1/2}c/a \leq 1.900$ for primitive tetragonal lattices based on a pseudo-b.c.t. unit cell. The values are also included for $c/a = 1.000$ since this would give constrained coincidence systems in the case of $L1_0$ alloys. All the vectors in Table 2 are listed columnwise, with the three columns of step vectors corresponding respectively to the columns of the DSC vectors. All of the coincidence systems are characterized by the unique disorientation description given in (16*a*). Note the large number of high-coincidence systems: there are 45 distinct CCSLs with $\Sigma \leq 7$.

Gertsman (1990), discussing vector–quaternion descriptions of misorientations, gave a set of rules for the calculation of Σ for cubic, tetragonal and hexagonal packed crystal lattices. We generated a table of coincidences for $\Sigma \leq 50$ and the axial ratios ranging from 0.800 to 1.900 using his rules to compare our results with the tables produced by us using his algorithm. We found there are certain discrepancies in the results. It is interesting to note that all of the values of Σ for the axial ratio of $2^{1/2}$ given in his paper match with ours and that these were the only data that he presented. Given below is an example to illustrate the discrepancies in our results and those obtained by use of Gertsman's method for the calculation of Σ.

Since the quaternions (K, L, M, N) in Gertsman (1990) are equivalent to (U, V, W, m) in the present study, the rules for the calculation of Σ given by Gertsman rewritten in terms of quadruples (m, U, V, W) are: if $\Sigma = \xi[\nu(U^2 + V^2) + \mu(m^2 + W^2)]$ and $\xi = 1/\alpha\beta\gamma$, then $\alpha = 2$ when $U^2 + V^2$ and $m^2 + W^2$ are even integers, otherwise $\alpha = 1$ and

$$\beta = \text{g.c.d.}[\mu, 2U, 2V, (U^2 + V^2)/\alpha],$$

$$\gamma = \text{g.c.d.}[\nu, 2W, 2m, (m^2 + W^2)/\alpha].$$

Example. $m = 3$, $U = 5$, $V = 0$, $W = 0$, $\mu = 25$, $\nu = 9$. This gives $\Sigma = 15$. If we apply Gertsman's rules given below, we get

$$\Sigma = \xi[9(25) + 25(9)] = 450\xi,$$

$$U^2 + V^2 = 25 \text{ (odd) and } m^2 + W^2 = 9 \text{ (odd)},$$

$$\text{hence } \alpha = 1,$$

$$\beta = \text{g.c.d.}(25,10,0,25/1) = 5,$$

$$\gamma = \text{g.c.d.}(9,0,6,9/1) = 3.$$

Hence,

$$\xi = 1/\alpha\beta\gamma = 1/15$$

and therefore

$$\Sigma = 450/15 = 30.$$

Gertsman's algorithm for the calculation of Σ for tetragonal crystals gives the value of Σ to be 30, while our calculations yield $\Sigma = 15$. Fig. 2 gives the geometrical construction of this coincidence system

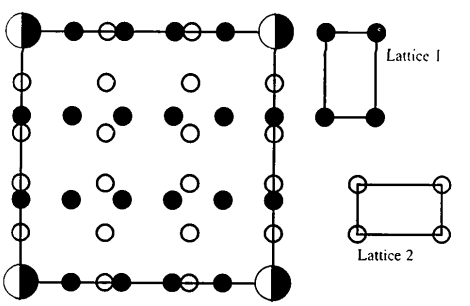

Fig. 2. Schematic diagram of the coincidence site lattice for the $\Sigma = 15/90°/[100]$ system, with the axial ratio of 1.667.

Table 2. *CSL, DSC and step vectors with* $\Sigma \leq 7$, $0.800 \leq 2^{1/2}c/a \leq 1.900$ *for the primitive tetragonal lattices based on pseudo-b.c.t. description of the unit cell*

The 'System' column gives the value of Σ, the rotation axis and the rotation angle (°). The elements of the rotation matrix and DSC lattice have been multiplied by Σ. All vectors are to be read columnwise. The first given step vector corresponds to the first given DSC vector *etc.*

$2^{1/2}c/a$	System	$\Sigma \times R$	CSL	$\Sigma \times$ DSC	Step vector
0.816	$\Sigma=4$	3 1 2	0 1 1	1−1 2	1 1 1
	[110]	1 3−2	0 1−1	−1 1 2	0 0 0
	60.000	−3 3 2	−2 0 1	−1−3 2	0 0 0
0.816	$\Sigma=5$	5 0 0	1 0 0	5 0 0	0 0 0
	[100]	0 1−4	0 1−2	0 2 1	0−1 0
	78.463	0 6 1	0 1 3	0−3 1	0 1 1
0.816	$\Sigma=7$	7 0 0	1 0 0	7 0 0	0 0 0
	[100]	0 5−4	0 2−1	0 1 2	0 0 1
	44.415	0 6 5	0 1 3	0−3 1	0 2 1
0.816	$\Sigma=7$	4 3 4	−1 0 2	−1−2 4	0 1 0
	[110]	3 4−4	0 1−2	1 2 3	0−1 0
	81.787	−6 6 1	−1−1−3	−2 3 1	−2−2−1
0.845	$\Sigma=6$	6 0 0	1 0 0	6 0 0	0 0 0
	[100]	0 1−5	0 1−2	0 2 1	0−1 0
	80.406	0 7 1	0 1 4	0−4 1	0 2 1
0.866	$\Sigma=4$	4 0 0	1 0 0	4 0 0	0 0 0
	[100]	0 2−3	0 1−1	0 3 1	0 0 0
	60.000	0 4 2	0 2 2	0−2 2	0 0 2
0.866	$\Sigma=5$	3 2 3	−1 0 2	−1−1 3	1 0 0
	[110]	2 3−3	0 1−1	1 1 2	0 0 0
	78.463	−4 4 1	−1−1−2	−2 3 1	−1−1−1
0.866	$\Sigma=7$	6 1 3	−1 1 1	1−2 4	0 1 0
	[110]	1 6−3	0 1−2	−1 2 3	−1 0 0
	44.415	−4 4 5	−2 0−1	−3−1 2	−1−1−1
0.866	$\Sigma=7$	7 0 0	1 0 0	7 0 0	0 0 0
	[100]	0 1−6	0 1 3	0 3 1	0−1 0
	81.787	0 8 1	0 1 4	0−4 1	0 2 1
0.894	$\Sigma=6$	6 0 0	1 0 0	6 0 0	0 0 0
	[100]	0 4−4	0 2 0	0 0 2	0 0 1
	48.190	0 5 4	0 1 3	0−3 1	0 1 1
0.894	$\Sigma=7$	5 2 4	−1 1 1	1−2 4	0 1 1
	[110]	2 5−4	0 1−1	−1 2 3	0 0 0
	64.623	−5 5 3	−3 0−1	−1−5 3	−2−1−1
1.000	$\Sigma=3$	2−1 2	1−1 1	2−1 1	0 0 0
	[111]	2 2−1	0 1 1	−1 2 1	1 1 1
	60.000	−1 2 2	−1 0 1	−1−1 1	0 0 0
1.000	$\Sigma=5$	5 0 0	1 0 0	5 0 0	0 0 0
	[100]	0 4−3	0 2 1	0−1 2	0 1 1
	36.870	0 3 4	0−1 2	0−2−1	0 1 0
1.000	$\Sigma=7$	6−2 3	−1−1 2	3−1 2	0 0 0
	[111]	3 6−2	−1 2 0	−2 3 1	0 0 0
	38.213	−2 3 6	−1 0−1	−1−2 4	−1−1−1
1.118	$\Sigma=6$	6 0 0	1 0 0	6 0 0	0 0 0
	[100]	0 4−5	0 2−1	0 1 2	0 0 1
	48.190	0 4 4	0 2 2	0−2 2	0 1 1
1.118	$\Sigma=7$	5 2 5	−1 1 2	−1−2 4	1 0 0
	[110]	2 5−5	0 1−3	1 2 3	−1−1−1
	64.623	−4 4 3	−1 0−2	−2 3 1	−1−1−1
1.155	$\Sigma=4$	4 0 0	1 0 0	4 0 0	0 0 0
	(100)	0 2−4	0 2 2	0 2 2	0 2 1
	60.000	0 3 2	0−1 1	0−1 1	0 0 0
1.155	$\Sigma=5$	3 2 4	−2 1 1	1 1 4	0 0 0
	[110]	2 3−4	1 1−1	−1 4 1	0 0 0
	78.463	−3 3 1	−1 0−1	−1−1 1	−1 0 0
1.155	$\Sigma=7$	6 1 4	−2 1 0	2−1 2	−1 0 0
	[110]	1 6−4	1 1−1	−2 1 5	0 1 0
	44.415	−3 3 5	−1 0−2	−1−3−1	−1−1−1
1.155	$\Sigma=7$	7 0 0	1 0 0	7 0 0	0 0 0
	[100]	0 1−8	0 4−1	0 1 4	0 0 1
	81.787	0 6 1	0 3 1	0−1 3	0 1 2
1.183	$\Sigma=6$	6 0 0	1 0 0	6 0 0	0 0 0
	[100]	0 1−7	0 3−1	0 1 3	0 0 1
	80.406	0 5 1	0 3 1	0−1 3	0 1 1
1.225	$\Sigma=4$	3 1 3	−1 1 1	2 2−1	1 0 0
	[110]	1 3−3	0 1−2	−2 2 1	0−1−1
	60.000	−2 2 2	−1 0−1	0 0 2	−1−1−1
1.225	$\Sigma=5$	5 0 0	1 0 0	5 0 0	0 0 0
	[100]	0 1−6	0 3−1	0 1 3	0 0 1
	78.463	0 4 1	0 2 1	0−1 2	0 1 1
1.225	$\Sigma=7$	7 0 0	1 0 0	7 0 0	0 0 0
	[100]	0 5−6	0 1 3	0 1 3	0 1 2
	44.415	0 4 5	0−2 1	0−2 1	0−1 0
1.225	$\Sigma=7$	4 3 6	−2 1 1	1 2 5	0 0 0
	[110]	3 4−6	1 1−1	−1 5 2	0 1 1
	81.787	−4 4 1	−2 0−1	−1−2 2	−1−1−1
1.265	$\Sigma=7$	7 0 0	1 0 0	7 0 0	0 0 0
	[100]	0 3−8	0 2−3	0 3 2	0 0−1
	64.623	0 5 3	0 1 2	0−2 1	0 1 1
1.291	$\Sigma=4$	4 0 0	1 0 0	4 0 0	0 0 0
	[100]	0 1−5	0 3−1	0 1 3	0 1 1
	75.522	0 3 1	0 1 1	0−1 1	0 1 1
1.342	$\Sigma=7$	7 0 0	1 0 0	7 0 0	0 0 0
	[100]	0 2−9	0 5−1	0 1 5	0 2 1
	73.398	0 5 2	0 2 1	0−1 2	0 1 1
1.414	$\Sigma=2$	1 1 2	0 1 1	1−1 1	1 1 0
	[110]	1 1−2	0 1−1	−1 1 1	0 0 0
	90.000	−1 1 0	−1 0 0	−1−1 1	0 0 0
1.414	$\Sigma=3$	3 0 0	1 0 0	3 0 0	0 0 0
	[100]	0 1−4	0 2−1	0 1 2	0 0 0
	70.529	0 2 1	0 1 1	0−1 1	0 1 1
1.414	$\Sigma=5$	4 1 4	−1 1 2	−1−2 3	1 1 1
	[110]	1 4−4	0 1−2	1 2 2	0−1−1
	53.130	−2 2 3	−1 0−1	−2 1 1	0−1−1
1.414	$\Sigma=6$	5−3 2	1 1 2	−1 2 4	1 1 1
	[201]	3 3−6	−1 1 0	−3 0 0	0 0 0
	60.000	1 3 4	−1−1 1	1−2 2	0 0 0
1.414	$\Sigma=7$	4−1 8	−1 1 2	2−1 3	1 0 1
	[221]	5 4−4	0 2−1	−1 4 2	0 0 1
	73.398	−2 4 3	−1 0−1	−1−3 2	−1−1 0
1.500	$\Sigma=6$	6 0 0	1 0 0	6 0 0	0 0 0
	[100]	0 0−9	0 0−3	0 3 0	0−1 0
	90.000	0 4 0	0 2 0	0 0 2	0 0 1
1.528	$\Sigma=5$	5 0 0	1 0 0	5 0 0	0 0 0
	[100]	0 2−7	0 4−1	0 1 4	0 1 1
	66.422	0 3 2	0 1 1	0−1 1	0 1 0
1.581	$\Sigma=6$	5 1 5	−1 1 2	2−1 3	1 1 1
	[110]	1 5−5	0 1−3	−2 1 3	−1 0−1
	48.190	−2 2 4	−1 0−1	−2−2 0	−1 0−1
1.581	$\Sigma=7$	7 0 0	1 0 0	7 0 0	0 0 0
	[100]	0 3−10	0 5−1	0 1 5	0 1 2
	64.623	0 4 3	0 2 1	0−1 2	0 1 1
1.633	$\Sigma=5$	5 0 0	1 0 0	5 0 0	0 0 0
	[100]	0 1−8	0 2−3	0 3 2	0 0 0
	78.463	0 3 1	0 1 1	0−1 1	0 0 1
1.633	$\Sigma=7$	7 0 0	1 0 0	7 0 0	0 0 0
	[100]	0 5−8	0 3 1	0 3 1	0 1 2
	44.415	0 3 5	0−1 2	0−1 2	0 1 0
1.633	$\Sigma=7$	4 3 8	−1 1 2	6−1 1	1 0 1
	[110]	3 4−8	1 1−3	1 1 6	−1 0−1
	81.787	−3 3 1	−1 0−1	−1−1 1	−1−1−1
1.732	$\Sigma=2$	2 0 0	1 0 0	2 0 0	0 0 0
	[100]	0 1−3	0 1−1	0 1 1	0 0 0
	60.000	0 1 1	0 1 1	0−1 1	0 1 0
1.732	$\Sigma=4$	2 0 6	0−1 2	2 0 2	0 0 0
	[331]	3 2−3	−1 1 0	−1 2 1	0 0 0
	82.819	−1 2 1	−1−1 0	−1−2 1	−1−1−1
1.732	$\Sigma=5$	3 2 6	−1 1 1	4−1 1	0 0 0
	[110]	2 3−6	1 1−2	1 1 4	0 0 0
	78.463	−2 2 1	−1 0−1	−1−1 1	−1−1−1
1.732	$\Sigma=7$	6 1 6	−1 1 3	−1−3 4	1 1 1
	[110]	1 6−6	0 1−3	1 3 3	0−1−1
	44.415	−2 2 5	−1 0−1	−2 1 1	0−1−1
1.732	$\Sigma=7$	7 0 0	1 0 0	7 0 0	0 0 0
	[100]	0 1−12	0 2−3	0 3 2	0−1 0
	81.787	0 4 1	0 1 2	0−2 1	0 1 1

and it can be clearly seen that the value of Σ is indeed 15 and in agreement with our calculations. Approximately 20% of the results obtained by use of Gertsman's algorithm contain an error of a factor of either 2 or $\frac{1}{2}$ in the value of Σ. This appears to be related to the determination of ξ, the components of which are given without derivation in his paper. We are therefore unable to identify the exact nature of the error.

Concluding remarks

We have generated tables of coincidence orientations, CSL, DSC and step vectors for the ordered tetragonal $L1_0$ alloys for the primitive tetragonal cell based on the pseudo-b.c.t. description with $\Sigma \leq 50$ and $0.800 \leq 2^{1/2}c/a \leq 1.900$. We have made use of the conditions given in (7) and (16) to ensure the completeness of our results. We have also shown that the rules for the determination of Σ for tetragonal crystals given in Gertsman (1990) do not always give the correct value. The data to be deposited comprise a comprehensive list of Σ values, axes, angles, CSLs, DSCs and step vectors for $L1_0$ alloys for $\Sigma \leq 50$ and $0.800 \leq 2^{1/2}c/a \leq 1.900$.*

* Lists of Σ values, axes, angles, CSLs, DSCs and step vectors for $L1_0$ alloys for $\Sigma \leq 50$ with $0.800 \leq 2^{1/2}c/a \leq 1.900$ have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55719 (258 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Crystalline-State Racemization of a Chiral Cyanoethyl Group Connected by a Hydrogen Bond

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Abstract

The crystal of [(*R*)-1-cyanoethyl]bis(dimethylglyoximato)(pyrrolidine)cobalt(III) (dimethylglyoximato = 2,3-butanedione dioximato) revealed a gradual change of cell parameters keeping the single-crystal form when it was irradiated by X-rays. It contains one water molecule as solvent in the asymmetric unit. The reactive cyanoethyl group is hydrogen bonded to the water molecule. In spite of the

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