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A New Geometrical Method for Constructing Coincident Site Lattices for Cubic Crystals

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Abstract*—A simple independent method for geometrical construction of two-dimensional coincidence site lattices (CSL) based on vector representation of lattice sites is put forward. In this method, the construction of such CSLs is achieved by mutual rotation of a unique vector, termed a sigma generating vector, which has the magnitude of a non-prime integer and is present in an identically oriented superimposed zero-layer lattice of two identical cubic crystals. The angle of rotation of the bi-crystal is expressed in terms of some unique nonprime integers that describe the orientation of the sigma generating vector within the lattices of each constituting crystal. The method provides a better mathematical explanation of why the magnitude of the sigma generating vector referred to as Σ can be used to designate a periodic boundary in cubic crystals by a certain value of Σ. The cell parameters of the two-dimensional CSL thus formed can be described in terms of both the magnitude (termed as Σ) of the square root of the sigma generating vector as well as the lattice parameters of the constituting crystals. Addition of a third axis along the rotation axis of these two-dimensional CSLs yields related three dimensional CSLs.

***Keywords*—coincident site lattices, grain boundaries, network of two-dimensional lattice unit in cubic crystals, sigma-generating vector**

I. INTRODUCTION

Two identical infinite lattices of the same crystal can be related to each other by any set of rotation or reflection. If such a rotation about a common axis results in points in space, which are common to both lattices and form common sub-lattices, a coincidence-site lattice (CSL) is generated. CSLs, which were originally developed by Kronberg & Wilson [1] and Aust & Rutter [2] and later elaborated by Brandon, Raganathan and Wald [3] are of prime importance in the study of periodic grain boundary structure. Along a grain boundary, two adjoining interface lattices of identical cell parameters develop a dichromatic pattern of three-dimensional periodicity. The CSL describes the periodicity of the dichromatic pattern and can characterize dislocation free grain boundary. In the last three decades, the atomic structure of many grain boundaries in chemically pure metals has been investigated [4-8]. In many cases, the concept of CSL along with Displacement Shift Complete (DSC) lattice [9] and the O-lattice model [10] based on geometrical construction of adjoining crystals forming boundaries has been successfully used for boundary characterization. The construction of CSLs is mainly involved in initial achievement of coincidence points by planar rotation around an axis common to both of the participating crystals. Once a two dimensional CSL is constructed, adding a third axis along the rotation axis results in three dimensional CSLs. In this respect a simple process of construction of CSLs from a cubic crystal was given by Raganathan [11]. According to this process, calculation of Sigma (Σ) value, which designates bi-crystal, and corresponding angle of rotation, θ, about the rotation axis [uvw] of a periodic bi-crystal can be obtained from the following generating functions:

$$\Sigma = x^2 + Ny^2 \quad (1)$$

$$\tan(\theta/2) = y\sqrt{N}/x \quad (2)$$

where $N = u^2 + v^2 + w^2$, and x and y are co-prime integers.

The generating function of equation (1) owes its origin in the existence of either a primitive or a centered rectangular network of lattices that are always present for any (hkl) plane of a cubic crystal. For a bi-crystal, the x and y in equations (1) and (2) represent values that correspond to the number of axial length along two orthogonal directions of rectangular lattice unit of either composite crystal. The value of Σ must be an odd integer. If in any instance equation (1) yields an even integer value, the related value must be divided by the correct multiple of 2 to yield an odd number.

Determination of cell parameters, as well as the lattice occupancies existing within the CSL lattice of fcc crystals formed by rotation around <001> axis and by the generating function of Raganathan is not a straight forward task. However, various mathematical methods in determining cell parameters and lattice constituency of CSLs using the concept of equation (2) and (3) are available in the literature [12-14]. . However, difficulties still exist in the application of these methods, especially to calculating cell parameters of the <100> CSLs of a bi-crystal made of fcc crystals. The centered square lattice net found along <100> orientation of this crystal by definition of symmetry is not different than a primitive square net. As a result application of rotation symmetry provided by these mathematical models on the centered square lattice net for providing the desired CSL and its cell parameters requires a few mathematical manipulations. Hence, a more simple geometrical approach for constructing CSLs and its lattice parameters in cubic crystals is called for. This paper provides a simple independent geometrical process, which not only is capable of constructing CSLs for cubic crystals of any Bravais lattice but also yields the cell parameters of resulting CSLs in terms of Σ as well as the cell parameter of the constituting crystals forming bi-crystal.

II. SIGMA; AN ODD INTEGER MAGNITUDE OF A SPECIAL POSITION VECTOR OF TWO-DIMENSIONAL LATTICES IN CUBIC CRYSTAL

One of the conventions of the designation of periodic grain boundaries is to refer the boundary by an odd integer known as Sigma (Σ), which is derived from Raganathan's generating function [11]. This convention of grain boundary designation can have its origin in a special position vector within two dimensional lattices. This special vector can be obtained from a mathematical theorem known as Fermat's last theorem [15], which states that no three positive integers (*a, b, c*) can satisfy the equation $a^n + b^n = c^n$ for any integer value of *n* greater than two. This theorem was not proven until 1995 despite the efforts of many mathematicians. A special case of Fermat's theorem ($n = 2$) is the Pythagorean triples [16], which are a set of three co-prime integers, referred in this text as G, S and T, related to each other by the following equation:

$$G^2 = S^2 + T^2 \quad (3)$$

Simple calculation involving Pythagorean triples reveals that Fermat's theorem in this form, i.e. equation (3), is not generally valid for most even values of G except a few for which division by a certain multiple of 2 yields an odd number. For example, the square of G=10 can be obtained by the summation of the square of S= 8 and T=6. However, each of the integers 10, 8 and 6 can be divided by 2, and therefore, they are not prime integers. Each integer upon division becomes a prime integer. G= 5 is an odd integer whose square is the summation of the square of the remaining two prime integers, 3 and 4.

Similar calculations also reveal that the square of many unique odd integers for G of equation (3) become equal to the summation of squares of certain unique integer for S and T. For example, odd integers such as 5, 13, 17 and 25 for G in equation (3) become equal to the summation of squares of certain unique integers for S and T. However, the same cannot be true for integers such as 3, 7 and 9. The reason for this is that S and T are equally weighted in terms of magnitude and therefore each S and T upon squaring as a prime integer cannot always yield an integer that is the square of an odd integer. Geometrically, this situation occurs only for the vector algebra representing two-dimensional periodicity of a square unit.

A simple cube along its axial projection exhibits a square unit with equal magnitude cell edges. A position vector **G** within such a two dimensional periodic network of axially projected squares can be represented by unit axial vectors **S** and **T** as given in equation (3). However, a simple cube also exhibits a primitive as well as a centered rectangular unit along all non-axial directions [11]. Simple geometrical analysis shows that the cell lengths of any of such two -dimensional projection units of the cube are not independent, but assume a definite ratio with each other. For example, along a face diagonal direction, the projected rectangular unit of the cube possesses $1:\sqrt{2}$ proportionality with the axial lengths, a and b of its rectangular unit. The ratio of the lengths of cell edges of such a rectangular unit obtained for various orientations of a cube is different. The presence of a definite ratio in the magnitude of the axial length of such projected rectangular units of a cube is interesting from view point of the satisfaction of equation (3). It can be found that inclusion of a relevant magnitude (*m*) of the cell edges of a projected rectangular unit of a cube in association with certain unique values of S and T allows equation (3) to yield an odd integer or an even multiple of an odd integer for G. For example, an odd value of 13 for G can be obtained by equation (3) by inserting *m*=1 into either of the co-prime unique integers, S = 12 and T = 5. The same G=13 can be obtained by co-prime unique integers S=11 and T=4, if $m= \sqrt{3}$. Hence, the inclusion of relevant ratio, *m*, in equation (3) yields the vector algebra of any two dimensional orthogonal primitive unit of any axially projected cubic crystal. With this inclusion equation (3) assumes the following form:

$$G_1^2 = S^2 + (mT)^2 \quad (4)$$

where G_1 is either an odd integer or an even multiple of an odd integer. As discussed earlier, a cubic crystal yields two-dimensional arrays of orthogonal units for an arbitrary projection. This implies that equation (4) can be used to represent the vector algebra for two-dimensionally periodic orthogonal units of a cubic crystal. Hence, a position vector within the assembly of such primitive rectangular units can be expressed in dimensionless form as:

$$\mathbf{G}_1 = \begin{bmatrix} S & mT \end{bmatrix} \begin{bmatrix} \mathbf{i} \\ \mathbf{j} \end{bmatrix} \quad (5)$$

where **i** and **j** are the axial unit vectors, and the angle between $\mathbf{G_1}$ and the normalized axial unit of the rectangular lattice network is:

$$\tan\theta = m\,T/S \quad (6)$$

Equation (5) also yields position vectors for the network of centered orthogonal lattice units as found in various projections of a cubic crystal. In this respect, crystal symmetry indicates that a centered square unit of lattices is by itself not a new lattice unit and can regarded as a primitive square unit with a cell parameter that is $1/\sqrt{2}$ times the lattice parameter of an otherwise primitive square unit in which a lattice lied at the center. Hence, a position vector in the lattice network of centered square units has to be referred to on the basis of such a primitive square unit. On the other hand, the same crystal symmetry also indicates that a centered rectangular lattice unit is different than that of the primitive rectangular lattice unit. For lattices of this variety of unit the determination of $\mathbf{G_1}$ by equation (5) can be made on the basis that the magnitude of each participating cell edge is one half of that for the unit. This consideration of cell edge division brings additional extinction conditions for the presence of a position vector for $\mathbf{G_1}$. The additional condition of extinction of a position vector is S ± T is an odd integer. Thus, the $\mathbf{G_1}$ (determined by the basis cell division discussed above) within a network of centered rectangular lattice unit formed by S and T with the condition that S ± T is odd integer cannot represent a position vector. Under this circumstance, the magnitude of the position vector for $\mathbf{G_1}$ has to be obtained by equation (5) after multiplying both S and *T* by 2. This makes the magnitude an even integer in terms of the reduced cell edges but results in an odd integer in terms of actual cell edges. An example of such a network of centered orthogonal lattice units can be found along the [111] of a face centered cubic crystal. A typical $\mathbf{G_1}$ with a magnitude (Σ) of 7 for this lattice network that has $m=\sqrt{3}$ can be achieved by equation (5) with the values of S and T of 2 and 1 respectively. These values of S and T allow S ± T to yield an odd integer. Hence, the $\mathbf{G_1}$ determined on the basis of the magnitude of each participating cell as half of the actual cell

length of the square cannot yield a position vector. Under this consideration of the participating cell unit, obtaining a position vector for the $\mathbf{G_1}$ **r**equires each of related S and *T* values to be multiplied by 2 to yield the values of 4 and 2, respectively. This results in the $\mathbf{G_1}$ vector having of magnitude 14, which is even in terms of divided cell edges. The same vector if calculated on the basis of the actual cell edges yields a magnitude of 7, which is an odd integer.

Discussion so far reveals that in an arbitrary orientation of a cubic crystal, the position vector $\mathbf{G_1}$ in equation (5) can only generate either an odd magnitude or an integer multiple of an odd magnitude. This unique property of the vector $\mathbf{G_1}$ is in line with the Raganathan's designation of Σ for his generating function, and therefore, can allow the resulting magnitude of the vector $\mathbf{G_1}$ to be termed as Σ. Such a designation of the odd magnitude enables the vector $\mathbf{G_1}$ to be termed as sigma generating vector (SGV). In a recently developed method [17] for constructing coincident site lattices of cubic crystals, the calculation of the Σ value of a symmetrical bi-crystal has also been obtained from the magnitude of the same two-dimensional lattice vector (**G**), the sigma generating vector (SGV). Table 1 lists the value of m, S and T for various values of the magnitude of $\mathbf{G_1}$.

Periodicity of the lattice network within the two-dimensional lattices also allows the vector $\mathbf{G_1}$ to possess a co-planar normal vector $\mathbf{G_2}$ in dimensionless form by the following equation:

$$\mathbf{G}_2 = \begin{bmatrix} m^2T & -mS \end{bmatrix} \begin{bmatrix} \mathbf{i} \\ \mathbf{j} \end{bmatrix} \qquad (7)$$

This vector $\mathbf{G}_2$ with its counterpart $\mathbf{G_1}$ in association with the translation symmetry of the lattices can define a sub-lattice unit within the lattice network. The situation is depicted in Figure 1a for the [001] projected square lattice network of a primitive cubic crystal. For the lattice network the Σ value for the SGV ($\mathbf{G_1}$) resulting from axial ratio, *m*=1, and unique values of *S*=3, *T*=4 is 5. The SGV ($\mathbf{G_1}$) and it normal $\mathbf{G}_2$ are also shown in the figure as **OA**, **OC** respectively. The resulting sub-lattice from the pair of vectors is outlined in the figure as OABC.

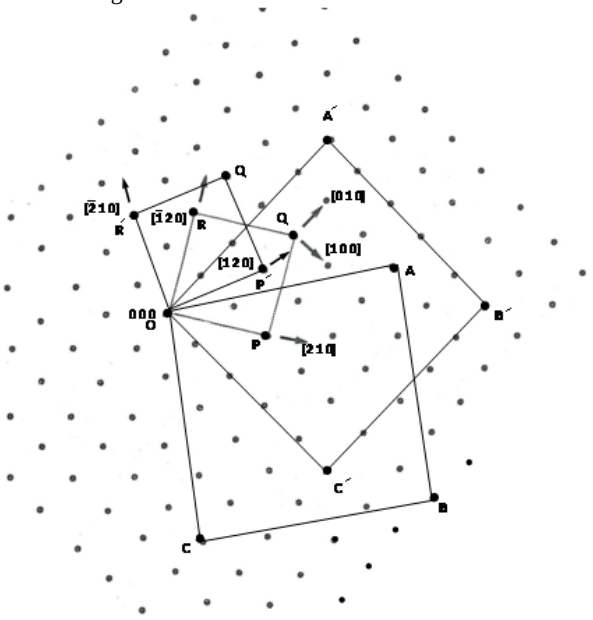

Figure 1a: A schematic representation of SGV and its related vectors and sub-lattices in a two-dimensional lattice network of a primitive cubic crystal viewed along [001].

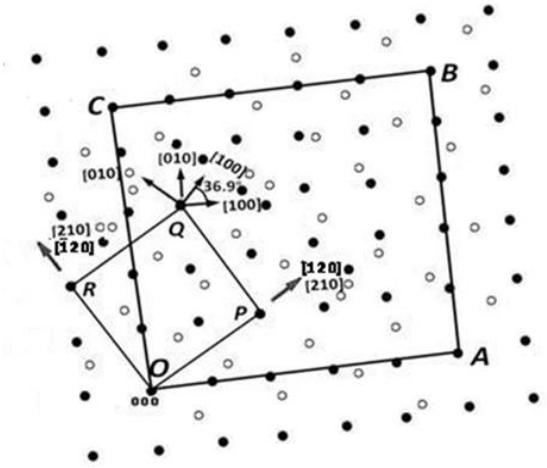

Figure 1b: The Schematic of a Σ= 5 CSL formation due to a mutual rotation around common [001] rotation of two primitive cubic crystals of the same species. The lattices of the constituting crystals are shown as filled and unfilled circles

III. THE AREA OF SUB-LATTICES UNIT FORMED BY SGV AND THE SQUARE ROOT OF SGV ASSUMES A RATIO THAT REPRESENTS □ OF CORRESPONDING SGV

Another consideration of adopting Σ as the designation of periodic boundary is that the Σ assumes the same odd integer (each is obtained by the generating function) in representing the ratio of the area of the primitive cell of the CSL and the constituting crystals. This characteristic of Σ for periodic bi-crystal can also be related to the SGV.

Simple analysis of the orthogonal network of the lattice in the cubic crystal reveals that the square root value of the odd nonprime magnitude of SGV ($\mathbf{G_1}$) is the summation of the square of two different or identical unique non-prime integers. Analogous to equation (4), the finding just described can be expressed by the following equation:

$$[\sqrt{G_1}]^2 = S'^2 + (m\,T')^2 \qquad (8)$$

where S' and T' are co-prime integers that may or not be equal. In vector form equation (6) can be written in dimensionless form is:

$$\sqrt{\mathbf{G}_1} = \begin{bmatrix} S' & mT' \end{bmatrix} \begin{bmatrix} \mathbf{i} \\ \mathbf{j} \end{bmatrix} \qquad (9)$$

where the angle θ' between $\sqrt{\mathbf{G}_1}$ and the normalized axial unit of the rectangular lattice network is:

$$\tan\theta' = m\,T'/\,S' \qquad (10)$$

Equation (9) is also valid for the network of centered orthogonal lattice units. For a network of centered rectangular lattice units the condition of extinction for the presence of a position vector for $\sqrt{\mathbf{G}_1}$ by equation (9) is identical to that present for $\mathbf{G}_1$ by equation (5).This indicates that for a position vector for $\sqrt{\mathbf{G}_1}$ by equation (9) requires S '± T' be even. In the case where S '± T' is odd the value of $\sqrt{\mathbf{G}_1}$ by equation (9) then has to be obtained after multiplying both S' and T' by 2. The unique relationship in equation (9) indicates that for each Σ generating position vector ($\mathbf{G}_1$) present in any orthogonal lattice network of a cubic crystal, another position vector exists for $\sqrt{\mathbf{G}_1}$. Table 1 also lists S ' and T' values associated with various values of the magnitude of $\mathbf{G}_1$.

Analogous to the odd integer generating vector $\mathbf{G}_1$, this $\sqrt{\mathbf{G}_1}$ vector also has a co-planar normal vector that can be expressed in dimensionless form as:

Table 1. Data in relation to the construction of CSLs

Σ	Rotation axis	Type[1]	m	S	T	S'	T'	θ'(°)	Parameters[2]	Cell-axes[3]
1	001	Primitive square (in BCC) a, a	1	2	0	1	1	0	No CSL	
		Centered square (in FCC) $a/\sqrt{2}, a/\sqrt{2}$	1	2	0	1	1			
3	110	Primitive rectangle (in FCC) $a, a/\sqrt{2}$	√2	1	2	1	1	70.5	$a\sqrt{\Sigma}, (a/\sqrt{2})\sqrt{\Sigma}$	<111>, <112>
		Centered rectangle (in BCC) $a, a\sqrt{2}$	√2	1	2	1	1	70.5	$a/2\sqrt{\Sigma}, (a\sqrt{2}))\sqrt{\Sigma}$	<112>, <111>
5	001	Primitive square (in BCC) a, a	1	3	4	2	1	36.9	$a\sqrt{\Sigma}, a\sqrt{\Sigma}$	<210>, <210>
		Centered square (in FCC) $a/\sqrt{2},\ a/\sqrt{2}$	1	3	4	2	1	36.9	$\left(\frac{a}{\sqrt{2}}\right)\sqrt{\Sigma}, \left(\frac{a}{\sqrt{2}}\right)\sqrt{\Sigma}$	<310>, <310>
7	111	Centered rectangle (in BCC) $a\sqrt{2}, a\sqrt{6}$	√3	1	4	2	1	81.8	$(a\sqrt{2})\sqrt{\Sigma}, (a\sqrt{6})\sqrt{\Sigma}$	<123>, <145>
		(in FCC) $a/\sqrt{2}$, $a\sqrt{6}/2$	√3	1	4	2	1	81.8	$\left(\frac{a}{\sqrt{2}}\right)\sqrt{\Sigma}, \left(\frac{a\sqrt{6}}{2}\right)\sqrt{\Sigma}$	<123>, <145>
9*	110	Primitive rectangle (in FCC) $a, a/\sqrt{2}$	√2	3	6	1	2	141	$a\sqrt{\Sigma}, (a/\sqrt{2})\sqrt{\Sigma}$	<122>, <114>
		Centered rectangle (in BCC) a, a □2	√2	3	6	1	2	141	$a\sqrt{\Sigma}, a\sqrt{2}\sqrt{\Sigma}$	<114>, <122>
11	110	Primitive rectangle (in FCC) $a, a\sqrt{2}$	√2	7	6	3	1	50.5	$a\sqrt{\Sigma}, a\sqrt{2}\sqrt{\Sigma}$	<113>, <233>
		Centered rectangle (in BCC) $a, a\sqrt{2}$	√2	7	6	3	1	50.5	$a\sqrt{\Sigma}, a/\sqrt{2}\sqrt{\Sigma}$	<233>, <113>
13	100	Primitive square (in BCC) a, a	1	1 2	5	2	3	*22.6*	$a\sqrt{\Sigma}, a\sqrt{\Sigma}$	<230>, <230>
		Centered square (in FCC) $a\sqrt{2}, a\sqrt{2}$	1	1 2	5	2	3	22.6	$\left(\frac{a}{\sqrt{2}}\right)\sqrt{\Sigma}, \left(\frac{a}{\sqrt{2}}\right)\sqrt{\Sigma}$	<150>, <150>

*. The θ is due to the construction of a second order CSL of Σ=1.. [1]Type of two-dimensional lattice network unit with the magnitude of the two cell edges expressed in terms lattice parameter, a of cubic crystal.

2. Lattice parameters of two-dimensional CSL expressed in terms of Σ and lattice parameter, a of the constituting crystal

3. Cell axes of the CSL are expressed in terms of the direction <uvw> of the constituting crystal

$$\sqrt{\mathbf{G}_2} = \begin{bmatrix} m^2T' & -mS' \end{bmatrix} \begin{bmatrix} \mathbf{i} \\ \mathbf{j} \end{bmatrix} \tag{11}$$

Translational symmetry of the lattices also allows the pair of vectors $\sqrt{\mathbf{G}_1}$ and $\sqrt{\mathbf{G}_2}$ to form a sub-lattice unit within the lattice network. In Figure 1a, the magnitude of position vector $\sqrt{\mathbf{G}_1}$ is $\sqrt{5}$, which was obtained using unique non-prime integers S' = 2 and T' = 1 in equation (9). The vector $\sqrt{\mathbf{G}_1}$ and its co-planar normal $\sqrt{\mathbf{G}_2}$ are designated as **OP** and **OR** respectively in the figure. The sub -lattice unit associated with these vectors is designated in the figure as OPQR. The $\square\mathbf{G}_1$ for this lattice network results from axial ratio *m*=1 and unique values of S' = 2, T' = 1 and assumes the value of $\sqrt{5}$. The axial ratio of the sub-lattice formed by position vectors $\square\mathbf{G}_1$ and $\square\mathbf{G}_2$ also assumes the value of m. This indicates that the like the sub-lattices belonging to $\mathbf{G}_1$ and $\mathbf{G}_2$ the sub-lattice defined by $\sqrt{\mathbf{G}_1}$ and $\square\mathbf{G}_2$ also assume the shape of the network of lattices. It is interesting to note that the ratio between the area of sub-lattices unit formed by SGV and by the square root of SGV is the odd number that represents the Σ of the SGV. This ratio implies that the area of the sub-lattice unit formed by a specific SGV must be Σ times larger than that formed by the square root of that particular SGV. This characteristic of sub-lattice occupancy is also valid between the basic network unit of lattices and the sub-lattice unit formed by the square root of SGV just discussed. The geometrical condition of the SGV allows the cell edge of the basic network unit to become $1/\Sigma$ .This yields the area of the basic network unit as $1/\Sigma^2$, which is Σ time smaller than the area of the sub-lattice unit formed by $\sqrt{\Sigma}$ (the square root of SGV). Such characteristics of SGV imply that within the two-dimensional network of lattices of cubic crystal, there exists a sub-lattice unit that has one cell axis equal to the magnitude of the square root of SGV. The area of this sub-lattice unit is Σ times larger than the area of the basic lattice unit. In bi-crystal, each constituting crystal must retain this property of Σ irrespective of its orientation. This lattice occupancy property of various sub-lattices generated by SGV is preliminary to what is expected to be present in the CSL of the periodic bi-crystal. The CSL of cubic crystals constructed by other geometrical methods reveal the same lattice occupancy properties just mentioned.[18]

IV. THE AXIAL POSITION VECTOR RELATED TO SGV OF THE LATTICE NETWORK AND ITS SQUARE ROOT FORM ANOTHER PAIR OF SUB-LATTICE UNIT

In the orthogonal lattice network of two dimensional lattices of cubic crystal, each axial position vector assumes a magnitude that is an integer multiple of the magnitude of the axial unit vector. The existence of only integer Σ values for the magnitude (due to unique value of S and T) of the SGV within the same lattice network suggests that each SGV finds a position vector of equal magnitude along the axial direction of the lattice network unit. In view of $\mathbf{G}_1$ not being able to assume either an even or a prime integer it is also true that no other position vector except the SGV can find a position vector of equal magnitude along the axial direction of the lattice network unit. This position vector ($\mathbf{G}_1'$) can be expressed in dimensionless form as:

$$\mathbf{G}_1' = \begin{bmatrix} 0 & |G_1| \end{bmatrix} \begin{bmatrix} \mathbf{i} \\ \mathbf{j} \end{bmatrix} = \begin{bmatrix} 0 & \Sigma \end{bmatrix} \begin{bmatrix} \mathbf{i} \\ \mathbf{j} \end{bmatrix} \tag{12}$$

where Σ is the magnitude of $\mathbf{G}_1$. This vector also has a normal vector $\mathbf{G}_2'$ that lies along the other axis of the lattice network unit and can be obtained in dimensionless form by the following relation:

$$\mathbf{G}_2' = \begin{bmatrix} |\mathbf{G}_2| & 0 \end{bmatrix} \begin{bmatrix} \mathbf{i} \\ \mathbf{j} \end{bmatrix} = \begin{bmatrix} m\Sigma & 0 \end{bmatrix} \begin{bmatrix} \mathbf{i} \\ \mathbf{j} \end{bmatrix} \tag{13}$$

In Figure 1a, the vectors $\mathbf{G}_1'$ and $\mathbf{G}_2'$ are designated as **OP'** and **OR'** respectively. The resulting sub-lattice from these two position vectors is also outlined in the figure as OP'Q'R'. The preceding discussion implies that the SGV present within the lattices has its counterpart aligned along their respective axial position vectors. These two vectors are related by a simple rotation of either vector around an axis to which the lattice network is normal. Simple geometrical analysis reveals that the angle of rotation, θ, is the angle between $\mathbf{G}_1$ and the normalized axial unit of the rectangular lattice network, as given in equation (6).

Furthermore, translation symmetry of the lattices reveals that the pair of vectors $\mathbf{G}_1'$, $\mathbf{G}_2'$ can define a sub lattice unit within the lattice network. In Figure 1a the sub-lattice unit related to this pair of vectors is outlined as OA'B'C'. **S**imple rearrangement of equation (5) also reveals that $\mathbf{G}_1$ and $\sqrt{\mathbf{G}_1}$ are related by the following relationship:

$$\left|\mathbf{G}_1'\right| = \sqrt{\left(S'\left|\sqrt{G_1}\right|\right)^2 + \left(mT'\left|\sqrt{G_1}\right|\right)^2} = \left|\mathbf{G}_1\right| \tag{14}$$

For the sub-lattice unit of $\mathbf{G}_1$, $\mathbf{G}_2$ the unit vectors **i** and **j** lie along $\mathbf{G}_1'$ and $\mathbf{G}_2'$ and indicate that the $\mathbf{G}_1'$, $\sqrt{\mathbf{G}_1'}$ generated by equation (9) from this sub-lattice unit is identical to that generated from the lattice network unit. Owing to the identical magnitude of $\mathbf{G}_1'$ and $\mathbf{G}_1$, the vector $\mathbf{G}_1'$ assumes a relationship with its $\sqrt{\mathbf{G}}'$ that is identical to that given for $\mathbf{G}_1$ and $\sqrt{\mathbf{G}_1}$ in equation (14). This identical relationship of $\mathbf{G}_1$ and $\mathbf{G}_1'$ with their respective "$\sqrt{\mathbf{G}}$" allows $\mathbf{G}_1$ and $\mathbf{G}_1'$ to make equal angle [given in equation (10)] with its respective "$\sqrt{\mathbf{G}_1}$". In a similar manner, the vectors $\mathbf{G}_2$ and $\mathbf{G}_2'$ are related to their respective "$\sqrt{\mathbf{G}_1}$" vectors. This implies that each of the sub-lattice units formed by the pair of vectors $\mathbf{G}_1$, $\mathbf{G}_2$ and $\mathbf{G}_1'$, $\mathbf{G}_2'$ have their own related sub-lattice unit formed by respective $\sqrt{\mathbf{G}}$ vectors. The situation is also illustrated in Figure 1 for the [001] projected square lattice network of a primitive cubic crystal. It can be seen that each of the sub-lattices (OABC, OA'B'C'**)** that are formed by respective pair of vectors ($\mathbf{G}_1$, $\mathbf{G}_2$ and $\mathbf{G}_1'$, $\mathbf{G}_2$) has its respective "$\sqrt{\mathbf{G}}$" sub-lattice unit outlined (OPQR and OP'Q'R'**)** formed by pairs of vectors ($\sqrt{\mathbf{G}_1}$, $\sqrt{\mathbf{G}_2}$ and $\sqrt{\mathbf{G}_1'}$,$\sqrt{\mathbf{G}_2'}$). The $\sqrt{\mathbf{G}_1}$ for this lattice network is resulted from axial ratio, *m*=1, and unique values of S' = 2, T' = 1 and assumes the value of $\sqrt{5}$.

V. SUPERPOSITION OF THE SGV FROM ONE CRYSTAL TO THE AXIAL POSITION VECTOR ASSOCIATED TO AN IDENTICAL SGV OF ANOTHER CRYSTAL FORMS CSLS

Any two-dimensional lattices of a cubic crystal can be a considered as dichromatic patterns of two identical lattice networks that are superimposed on top of each other. The constituting crystals in such a dichromatic pattern have their sub-lattices [formed by the pair of vectors $\mathbf{G}_1$, $\mathbf{G}_2$; $\mathbf{G}_1'$, $\mathbf{G}_2'$; $\sqrt{\mathbf{G}_1}$, $\sqrt{\mathbf{G}_2}$ and $\sqrt{\mathbf{G}_1}'$, $\sqrt{\mathbf{G}_2}'$ (originated from a unique SGV as well as its various unique properties discussed earlier)] appearing as superimposed. Beginning from such a dichromatic pattern a mutual rigid body rotation about the common rotation axis of the constituting lattices can bring the unique $\mathbf{G}_1$ vector of one lattice to coincide only with $\mathbf{G}_1'$ vector of the other constituting lattice. The reason is that both of these vectors, owing to related unique S and T values, are equal in magnitude. The amount of this rotation is the same as that needed for bringing the SGV of a single lattice network to its respective axial position vector and is given in equation (6). Similar uniqueness in the value of S' and T' in the square root of $\sqrt{\mathbf{G}_1}$ and the existence of identical angles between SGV ($\mathbf{G}_1$) and the square root of SGV ($\sqrt{\mathbf{G}_1}$), as well between axial position vector $\mathbf{G}_1'$ and the square root of axial position vector $\sqrt{\mathbf{G}_1}'$, can bring a simultaneous coincidence of $\sqrt{\mathbf{G}_1}$ of same lattices to only the $\sqrt{\mathbf{G}_1}'$ of other lattices. Hence, for a specific Σ a particular pair of SGV and its square root vector can only assume coincidence during mutual rotation of the SGV and form super-lattices. Other position vectors do not have such uniqueness in the values of S, T, S' and T', and therefore, are unable to coincide in similar manner to form super-lattices. Under this circumstance, sub-lattice units formed by SGV and its co-planar normal (i.e. $\mathbf{G}_1$, $\mathbf{G}_2$) as well as by the square root of SGV and its coplanar normal (i.e. $\sqrt{\mathbf{G}_1}$, $\sqrt{\mathbf{G}_2}$) of one crystal superimpose only on the sub-lattice formed by axial position vectors (i.e. $\mathbf{G}_1'$, $\mathbf{G}_2'$) as well as by the square root of the axial position vector (i.e. $\sqrt{\mathbf{G}_1}'$, $\sqrt{\mathbf{G}_2}'$) of the other crystal.

The situation is also depicted in Figure 1b. In the figure, sub-lattice due to SGV of magnitude 5 and related axial position vector of the two crystals after a mutual rotation of 36.9º are superimposed to form a super-lattice. This super-lattice is outlined in the figure as OABC. The super-lattice formed due to superposition of sub-lattices of the square root of SGV of the two crystals is also outlined in the figure as OPQR. Out of these two possible super-lattices the one (outlined as OPQR in Figure 1b) formed by the square root of SGV and its normal is smaller and therefore is the smallest super-lattice that can be formed for the specific SGV. This super-lattice is therefore the two-dimensional coincidence site lattice (CSL). The Σ, angle of rotation and rotation axis for the SGV just discussed can be directly obtained by the values of S, S', T, T′ and *m* of the constituting crystals. These values thus obtained enable the two-dimensional CSL designated by OPQR in Figure 1b to be termed as a [001] projected Σ=5 CSL of a primitive cubic crystal.

The larger super-lattice unit (outlined as OABC in Figure 1b) has the cell axes that have the magnitude of SGV resolved along two axial direction of the basic lattice network unit of the crystal. This allows either cell edge of this super-lattice unit to be made of Σ number of respective cell edge of the basic lattice network unit. Also in the earlier discussion it was revealed that that the area of the sub-lattice unit of each of the constituting crystals forming the two-dimensional CSL is Σ times larger than the area of the basic lattice unit. The super-lattice describing the two dimensional CSL is formed by two identical sub-lattice units each of which has an area that is Σ times larger than the area of its basic lattice unit. This implies that the area of the two-dimensional CSL is also Σ times larger than the area of the basic lattice unit of both participating crystals.

For $\Sigma = 9$, the SGV is the square vector of the prime integer 3. The SGV representing the square vector of this prime integer (3) yields S and T, which are the identical integral multiple of respective S and T found for the SGV of a prime integer, 3. This pair of SGV lies along the same direction, and therefore, represents the shortest position vector that lies along this common direction of the related lattice network. This characteristic of SGV, S and T, indicates that the method described above in constructing CSLs for $\Sigma = 9$ becomes non-operative even though the magnitude of the square root of SGV for $\Sigma = 9$ and its co-planar normal vector provides the two cell edges of the related zero layer CSL. However, the mathematical basis of the present process always allows the zero layer CSL derived from the SGV of a prime integer to assume a network of zero layer coincident lattices that is identical in shape to that which exists in the constituting crystals. In this respect, the network of <110> projected zero layer CSLs for $\Sigma = 3$ is rectangular and assumes an axial ratio of $\sqrt{2}$ and $2\sqrt{2}$ for fcc and bcc Bravais lattices of a cubic crystal, respectively. The same can be found true for the network of lattice units existing for this orientation of related constituting crystals. This identical shape characteristic for the unit of the lattice networks present both in CSL and constituting crystals allows for the deduction of a second order SGV that assumes the CSL unit to be the unit for the network of lattices. The second order SGV thus deduced can now yield second order CSLs by allowing the original lattice network of the participating crystals to assume an overall mutual rotation of 141°. This overall rotation of constituting crystals corresponds exactly to that needed to attain a $\Sigma = 9$ bi-crystal. The second order operation just described also yields the cell edges of the zero layer CSL for the $\Sigma = 9$ bi-crystal. Similar application of the process just described can give second-, third-, fourth-, etc. order zero layer CSLs from the zero-layer CSL of lowest prime integer. For example, the zero layer CSL for $\Sigma = 25$ and $\Sigma = 125$ can be obtained as the second- and third-order CSL from the zero-layer $\Sigma = 5$ CSL by the present method.

VI. CSL CELL PARAMETERS

Information provided so far reveals that for the construction of any two-dimensional CSL of a periodic bi-crystal, a determination of S and T by equation (5) for its SGV or S′ and T' for the square root of the SGV by equation (9) yields necessary information about the amount of mutual rotation the participating crystals have to undertake in order to achieve coincident sites. After completion of the required mutual rotation the value of S′ and T' obtained from equation (9) for the square root of the same SGV defines the coordinates of the vector that defines CSL cell lengths and crystal data, such as direction of CSL.

Actual determination of the cell parameters of the two-dimensional CSL thus formed requires the dimension of the magnitude of the unit cell vectors along the axial edges of the lattice network unit. For example, for the <110> projection of

the body centered cubic crystal, the magnitude of the unit cell vector has the dimension of the cell parameter *a* of the unit cell. Taking account of this dimension in the magnitude of the unit cell vector and the ratio, $m=\sqrt{2}$, the resulting two-dimensional CSL for this <110> projection is found to posses cell parameters of $(a/2\sqrt{\mathbf{G}_1})$ and $a/\sqrt{2}(\mathbf{G}_2)$. On the other hand, if the crystal is face centered cubic then the magnitude of the unit cell vector has the dimension of $a/\sqrt{2}$, and the resulting cell parameters of two-dimensional CSL in this orientation becomes $a(\sqrt{\mathbf{G}_1})$ and $a/\sqrt{2}(\sqrt{\mathbf{G}_1})$. Hence, determining the CSL cell parameter by this method requires the knowledge of the type of cell parameters of the basic unit of lattice network used for calculating the SGV for the bi-crystal. In the instance where SGV is calculated on the basis of the entire cell dimensions of the unit of lattice network, the cell parameters ($\mathbf{a}_{(CSL)}$), ($\mathbf{b}_{(CSL)}$) of the two-dimensional CSL can then be calculated by the following relationships:

$\mathbf{a}_{(CSL)}$ = [Square root of the magnitude of SGV(Σ)] × [related cell parameter of the unit of lattice network expressed in terms of the lattice parameter (a) of the crystal (15)

$\mathbf{b}_{(CSL)}$ = [Square root of the magnitude of the vector normal to SGV (Σ)] × [related cell parameter of the unit of lattice network expressed in terms of the lattice parameter (a) of the crystal] (16)

For other instances, where the SGV is calculated on the basis that the magnitude of each participating cell edge is one-half of that which exists for the unit of the lattice network, the term in the parenthesis of equation (15) and (16) has to be divided by two. A stereogram and zone law along rotation axis of the crystal can provide information on the type and cell edges of the orthogonal unit of the lattice network the crystal assumes along a plane that is normal to the rotation axis. The information thus obtained can be used to determine the cell parameters and direction of the cell parameters of the resulting two-dimensional CSL. In this context it is worth noting that the present process yields only orthogonal two-dimensional CSLs. This form of two-dimensional orthogonal CSL is correct for all orientations of a cubic crystal. However, along a <111> orientation the lattices of cubic crystals also assume a hexagonal close packed system. Under such a situation, the lattice parameters of two-dimensional CSLs described in terms of a two-dimensional ortho-hexagonal (O-H) co-ordinate system can be expressed in terms of the two-dimensional hexagonal co-ordinate system by the following relationships:

$$\mathbf{a}_{(CSL)\,O\text{-}H} = a\sqrt{3}/2\,\mathbf{i} + a/2\,\boldsymbol{j},\quad \mathbf{b}_{(CSL)\,O\text{-}H} = a\sqrt{3}/2\,\mathbf{i} + a\sqrt{3}/2\,\mathbf{j} \qquad (17)$$

where *a* is axial length in hexagonal form ***i*** and ***j*** are the unit vectors along hexagonal direction. However, in either co-ordinate system the area of the two-dimensional CSL is Σ times larger than the area of the basic lattice unit of both participating crystals. The cell parameters of two-dimensional CSLs formed by the SGV with magnitude (Σ value) ranging from 1 to 13 are listed in Table 1. The addition of a third axis along the rotation axis of these two-dimensional CSL yields the desired three dimensional CSL.

VII. CONCLUSIONS

The present process uses a completely independent geometrical approach for constructing the CSLs of cubic crystals, and yields the CSL corresponded to every Σ value. Since, a cubic crystal cannot yield every Σ for its single orientation; the process can only yield only a few CSL units around a common rotation axis of the participating crystals. The process is simple and requires a prior knowledge of whether the orthogonal lattice network unit normal to rotation axis of the bi-crystal is primitive or centered.

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