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# Crystallogeometrical Approach to Stacking-Fault Analysis in Ordered Alloys

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**Abstract**

Stacking faults (SFs) and antiphase boundaries (APBs) in an $n$-dimensional ordered alloy with arbitrary primitive cell are analysed from the crystallogeometrical standpoint. The general definition of a SF is given based on the concept of the boundary displacement lattice. The method of enumeration of all possible SFs of a given orientation is proposed. Finally, the energy of an unrelaxed SF is written in terms of the pair-potential functions. The proposed method may be implied as an efficient way of energy estimation and structural analysis of SFs.

## 1. Introduction

The ordered alloys and intermetallics show plastic behaviour that differs significantly from that of pure metals (Stoloff, 1971; Yamaguchi *et al.*, 1981). From an industrial standpoint, the most important anomaly is the increase in yield stress with increasing temperature, first noted for $Ni_3Al$ by Westbrook (1957), and then observed for many ordered alloys. Much effort has been directed toward finding explanations for this anomaly (Yamaguchi *et al.*, 1981; Hirsch, 1992). Transmission electron microscopy (for example, Veyssiere & Noebe, 1992) and *in situ* observations (*e.g.* Molenat & Caillard, 1991) of superdislocations gave some information that has been used to improve the current models describing the anomaly (*e.g.* Paidar *et al.*, 1992). It is believed that this yield stress temperature anomaly is attributable to the specific structure of the superdislocations. They are dissociated into two or more superpartials connected by an APB or an intrinsic SF or a complex SF consisting of an APB and an intrinsic SF (Yamaguchi *et al.*, 1981; Trinckauf & Nembach, 1992). Such a structure of dislocations leads to their relatively low mobility in some slip planes and some directions. The magnitude and orientation dependence of the energy of planar defects, listed above, strongly affect the properties of the superdislocations. For this reason, the plastic deformation models that have been developed to explain the anomalous flow behaviour require good estimations of the energies of planar defects of different orientations.

The first analytical expression of the APB energy in terms of the pair potentials was derived by Flinn (1960). In that expression, the change in the number and type of the pair interatomic bonds was taken into account only for the first or second coordination shell. Then the analogous expressions usually for two or three coordination shells were derived by many authors (*e.g.* Pandey & Krishna, 1975, 1976; Yamaguchi *et al.*, 1981). Such kinds of expressions, in spite of their simplicity, were successfully used in the development of the theories of plastic deformation in ordered alloys. Later, experimental investigations (Douin *et al.*, 1986) showed that APBs and SFs in orientations with rather high Miller indices are also important. For such defects, the pair bonds in the larger number of coordination shells must be taken into account (Starostenkov & Kirienko, 1994). The derivation of such formulae requires the assistance of a computer and is impossible without generalization of the calculation procedure.

The expressions of the energies of defects mentioned above do not take into account the atomic relaxation near the defect. In essence, the energy of the defect is judged from the difference in the number and type of pair interatomic bonds in perfect and defect crystals. That is why we call this approach a crystallogeometrical one. The approach sometimes cannot give a reliable estimation of the energy of a planar defect but, for the spectrum of defects that differ, for example, by their orientation, this model often gives quite good estimations of relative energies (Starostenkov & Kirienko, 1994).

The APB is the so-called coherent planar defect, which does not destroy the lattice of the alloy but only changes a specific order in the arrangement of the atoms of different types in the lattice points. Other types of planar defects such as a SF, a twin boundary or a special grain boundary give the examples of partly coherent defects. They destroy the lattice of a crystal

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but a sublattice of the lattice is preserved. It would appear reasonable that the accuracy of the crystallogeometrical approach increases with the degree of coherence of the defect.

For coherent or partly coherent planar defects, the different lattice models are useful concepts for the description of the geometrical relationship between two adjacent parts of a crystal. For grain boundaries with relatively small $\Sigma$ and for some other planar defects, the 0-lattice, the coincidence site lattice and the displacement shift lattice (Bollmann, 1967, 1970; Chadwick & Smith, 1976) play an important role. For the description of all possible structure defects in grain boundaries, the grain-boundary displacement (GBD) lattice was proposed by Orlov *et al.* (1975).

In the present paper, the crystallogeometrical approach derived earlier for some other planar and one-dimensional defects in superlattices (Starostenkov *et al.*, 1993*a*, 1994; Dmitriev *et al.*, 1995) was expanded for SFs. The simplest case for analysis is the case of a coherent defect. Here the idea of reducing the analysis of a noncoherent or a partly coherent defect to analysis of a coherent one (Bollmann, 1967, 1970) was employed. This reduction can be performed if a lattice that contains all the nodes of the defected crystal is known.

The $(n-1)$-dimensional defect in an $n$-dimensional crystal was considered. This gives a common approach that can be easily applied to both cases of practical importance, namely to the planar defects in a real three-dimensional crystal and to the linear defects in a two-dimensional model of a real crystal.

The remainder of the paper is organized as follows. The basic definitions of an $n$-dimensional lattice (Conway & Sloane, 1993) and superlattice are recalled in §2. Then the solution of some auxiliary crystallographic problems is presented in §3. The definition of a SF, enumeration of SFs with given orientation and the derivation of the SF energy expression are presented in §4. Finally, §5 contains an example of SF analysis in the superlattice $L1_0$.

## 2. Geometry of a lattice and a superlattice

One of the convenient ways of describing crystal geometry in $n$-dimensional Euclidean space $E^n$ is the lattice $\Lambda^q$, where $q \in \{0, 1, \ldots, n\}$. $\Lambda^q$ is a set of vectors such as

$$\mathbf{x} = \sum_{i=1}^{q} f_i \mathbf{v}_i, \tag{1}$$

where $f_i$ are integers and $\mathbf{v}_i$ are a linearly independent set of vectors. The lattice $\Lambda^q$ is uniquely determined by the vectors $\mathbf{v}_i$, which are called a basis or generator vectors of $\Lambda^q$.

Let us define a matrix $\mathbf{V}$, rows of which are the coordinates of the vectors $\mathbf{v}_i$ in an orthonormal basis $\mathbf{e}_j$, $j = 1, \ldots, n$. Then (1) may be written as

$$\mathbf{x} = \mathbf{f}\mathbf{V}, \tag{2}$$

where $\mathbf{f}$ is an arbitrary vector with components $f_i$. The matrix $\mathbf{V}$ is called a generator matrix for the lattice $\Lambda^q$. The generator vectors $\mathbf{v}_i$ determine a primitive cell of the lattice with volume $[\det(\mathbf{V}\mathbf{V}^T)]^{1/2}$. For the case $n = q$, the volume is equal to the absolute value of $\det \mathbf{V}$. In further calculations, vectors $\mathbf{v}_i$ will be numbered in a way such that $\det \mathbf{V} > 0$.

For $q \geq 2$, there exist infinite possible ways of choosing the basis and the primitive cell for the lattice $\Lambda^q$. Two bases $\mathbf{u}_i$ and $\mathbf{v}_i$ generate the congruent lattices if and only if

$$\mathbf{U} = \mathbf{V}\mathbf{P}, \tag{3}$$

where $\mathbf{U}$, $\mathbf{V}$ are the generator matrices of bases $\mathbf{u}_i$, $\mathbf{v}_i$, respectively, and $\mathbf{P}$ is a unimodular matrix (all elements are integers and $\det \mathbf{P} = \pm 1$). The volume of the fundamental region does not depend on the basis.

Additionally to the lattice $\Lambda^q$, let us consider its translation $\Lambda^q + \mathbf{p}$ originated from the translation of all points of $\Lambda^q$ along the vector $\mathbf{p} \in E^n$. In the case when the translation vector $\mathbf{p} \notin \Lambda^q$, the created object is not a lattice but is called a packing.

Let the vectors $\mathbf{v}_i$ generate the lattice $\Lambda^n$ and the vectors $\mathbf{w}_i = K_i \mathbf{v}_i$ generate the lattice $\Omega^n$, where $K_i$ are positive integers. Obviously, the volumes of primitive cells of these lattices are related by the expression $\det \mathbf{W} = M \det \mathbf{V}$, where $\mathbf{W}$ is the generator matrix of lattice $\Omega^n$ and $M = \prod_{i=1}^{n} K_i$. All points of the lattice $\Lambda^n$ may be represented as the union of points of $M$ packings:

$$\Lambda^n = \bigcup_{m=1}^{M} (\Omega^n + \mathbf{g}_m), \tag{4}$$

where vectors $\mathbf{g}_m$ with respect to the basis $\mathbf{w}_i$ have the form

$$\mathbf{g}_m = (g_1/K_1, \ldots, g_n/K_n), \quad 0 \leq g_i \leq K_i - 1, \tag{5}$$

and they belong to the primitive cell of $\Omega^n$.

A superlattice $\Psi^n$ can be defined on the lattice $\Lambda^3$ by assigning some type of atoms $S_m$ to each packing:

$$\Psi^n = \bigcup_{m=1}^{M} (\Omega^n + \mathbf{g}_m)_{S_m}. \tag{6}$$

If instead of the basis $\mathbf{w}_i$ of the lattice $\Omega^n$ a new one is chosen, then the new fundamental region will contain exactly one lattice point from each packing $\Omega^n + \mathbf{g}_m$.

The translational cell of the superlattice $\Psi^n$ of a minimum volume will be called a primitive cell of the superlattice.

## 3. Solution of auxiliary tasks

### 3.1. *Separation of an n-dimensional superlattice into (n−1)-dimensional monoatomic packings*

Let us represent the superlattice $\Psi^n$ given by (6) as a union of $(n-1)$-dimensional monoatomic packings of given orientation. The orientation of $(n-1)$-dimensional packings will be defined by the hyperplane with Miller indices

$$(h_1 \ldots h_n) \tag{7}$$

with respect to the basis $\mathbf{w}_i$ of the lattice $\Omega^n$.

Let us choose for the lattice $\Omega^n$ the new basis $\mathbf{u}_i$ with the vectors $\mathbf{u}_1, \ldots, \mathbf{u}_{n-1}$ parallel to the hyperplane (7). Hereinafter, the hyperplane will be called the plane. The set of vectors $\mathbf{x} = (x_1, \ldots, x_n)$ parallel to the plane (7) satisfies the linear equation

$$h_1 x_1 + \ldots + h_n x_n = 0. \tag{8}$$

The general integer solution of (8) can be expressed as follows:

$$\mathbf{x}^{\mathrm{T}} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \mathbf{G} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_{n-1} y \end{pmatrix}, \tag{9}$$

where $\alpha_1, \ldots, \alpha_{n-1}$ are any integers, $\mathbf{G}$ is an $n \times (n-1)$ matrix of rank $n-1$ with appropriate integer elements. The method of finding the integer solutions to the linear system with integer coefficients was described, for example, by Shapiro (1979).

The components of vectors $\mathbf{u}_1, \ldots, \mathbf{u}_{n-1}$ of the required basis $\mathbf{u}_i$ can be defined with respect to the basis $\mathbf{w}_i$ as the corresponding columns of matrix $\mathbf{G}$. The last vector $\mathbf{u}_n$ can be found from the condition

$$\det \mathbf{U} = \det \mathbf{W}, \tag{10}$$

where $\mathbf{U}$ is the new generator matrix of $\Omega^n$.

The representation of $\Psi^n$ as a union of $(n-1)$-dimensional monatomic packings is given by

$$\Psi^n = \bigcup_{m=1}^{M} \bigcup_{k=-\infty}^{\infty} (\Omega^{n-1} + k\mathbf{u}_n + \mathbf{g}_m^*)_{S_m}, \tag{11}$$

where lattice $\Omega^{n-1}$ is generated by the vectors $\mathbf{u}_1, \ldots, \mathbf{u}_{n-1}$ and hence has orientation $(h_1 \ldots h_n)$. The components of vectors $\mathbf{g}_m^*$ with respect to the basis $\mathbf{u}_i$ can be calculated as $\mathbf{g}_m \mathbf{U}_*^{-1}$ (modulo 1), where the rows of matrix $\mathbf{U}_*$ are the components of vectors $\mathbf{u}_i$ with respect to the basis $\mathbf{w}_i$.

### 3.2. *A boundary displacement lattice*

To describe the special grain boundaries in metals, the GBD lattice was proposed by Orlov *et al.* (1975). The GBD lattice may be built for any given lattice and given plane whose orientation determines the orientation of the planar defect. The points of an $n$-dimensional GBD lattice are the intersection points of the $n-1$ sets of parallel planes (no two of sets have parallel planes) passing through the points of a given lattice and perpendicular to the given plane, with the set of parallel planes passing through the points of a given lattice and parallel to the given plane. The GBD lattice may be useful not only for the grain-boundary problem, for example, it may be used to obtain the general definition of a SF. For this reason, in the present paper, the GBD lattice will be called a boundary displacement lattice (BDL).

Let us find the BDL for given lattice $\Lambda^n$ and given plane $(h_1 \ldots h_n)$. The BDL will be denoted $\Lambda^n_{\mathrm{BDL}}(\Lambda^n, (h_1 \ldots h_n))$ or $\Lambda^n_{\mathrm{BDL}}$. The orientation of the plane $(h_1 \ldots h_n)$ is given with respect to the basis $\mathbf{v}_i$ of the lattice $\Lambda^n$.

The construction of the BDL with any given orientation of the plane $(h_1 \ldots h_n)$ is possible only if the generator matrix $\mathbf{V}$ of lattice $\Lambda^n$ can be represented in the form $\mathbf{V} = \rho \mathbf{V}'$, where $\rho$ is real and the components of matrix $\mathbf{V}'$ are rational numbers.

The construction of the BDL requires the following steps.

(i) The new basis $\mathbf{u}_i$ of the lattice $\Lambda^n$ should be chosen in such a manner that vectors $\mathbf{u}_1, \ldots, \mathbf{u}_{n-1}$ are parallel to the plane $(h_1 \ldots h_n)$ as was described in §3.1.

(ii) The orthogonal projection of the vector $\mathbf{u}_n$ on the plane $(h_1 \ldots h_n)$ should be found. The components of this projection with respect to the basis $\mathbf{u}_i$ can be written in the form

$$(c_1/d_1, \ldots, c_{n-1}/d_{n-1}, 0), \tag{12}$$

where $c_i/d_i$ are the irreducible fractions.

(iii) The generator vectors of the desired BDL are

$$\mathbf{t}_1 = (1/|d_1|)\mathbf{u}_1, \ldots, \mathbf{t}_{n-1} = (1/|d_{n-1}|)\mathbf{u}_{n-1}, \mathbf{t}_n = \mathbf{u}_n. \tag{13}$$

One can see that the lattice $\Lambda^n$ is a sublattice of $\Lambda^n_{\mathrm{BDL}}(\Lambda^n, (h_1 \ldots h_n))$.

## 4. Analysis of stacking faults

### 4.1. *Definition of a stacking fault*

In the literature, many definitions of SFs can be found (*e.g.* Hirth & Lothe, 1992). Unfortunately, the descriptions they provide are not general enough to be used for all types of structures. A general definition of a SF with orientation $(h_1 \ldots h_n)$ in the superlattice $\Psi^n$, not contradictory to the others, may be given as follows.

Let us consider two coincident interpenetrating copies of the superlattice $\Psi^n$ based on the lattice $\Lambda^n$ with the basis $\mathbf{v}_i$. Let us find $\Lambda^n_{\mathrm{BDL}}(\Lambda^n, (h_1 \ldots h_n))$ and translate one copy of the superlattice with respect to

another along the vector $\mathbf{g} \in \Lambda^n_{\mathrm{BDL}}$. The shifted superlattice is symbolized by $\hat{\Psi}^n$. The crystal with the SF is obtained by contact between $\Psi^n$ and $\hat{\Psi}^n$, the plane boundary between $\Psi^n$ and $\hat{\Psi}^n$ has orientation $(h_1 \dots h_n)$ and passes through the origin of the unshifted superlattice.

Notice that the APB is a particular case of the above definition when $\mathbf{g} \in \Lambda^n$. This definition itself is a particular case of the grain-boundary SF definition, given by Orlov *et al.* (1975). In some cases, a planar defect with the translation vector $\mathbf{g} \notin \Lambda^n_{\mathrm{BDL}}$ may be of interest. In this case, instead of the lattice $\Lambda^n_{\mathrm{BDL}}$ a lattice with smaller fundamental region that contains the wanted vector $\mathbf{g}$ has to be considered.

### 4.2. *Enumeration of stacking faults*

In pure metals, the number of SFs with orientations with low Miller indices is relatively small. In ordered alloys, this considerably increases owing to the presence of atoms of different types. Let us describe all the SFs of orientation $(h_1 \dots h_n)$ with different energy in the superlattice $\Psi^n$.

This problem has been solved for APBs (Indenbom & Loginov, 1987; Dmitriev *et al.*, 1995). According to the definition given in §4.1, the adjacent domains of a crystal containing a SF are relatively shifted by the vector $\mathbf{g} \in \Lambda^n_{\mathrm{BDL}}$. This means that nodes of both $\Psi^n$ and $\hat{\Psi}^n$ belong to $\Lambda^n_{\mathrm{BDL}}$. Let us assume that the points of the $\Lambda^n_{\mathrm{BDL}}$ that are not occupied by the atoms of either $\Psi^n$ or $\hat{\Psi}^n$ contain the atoms of type $O$. As a result, the SF becomes a coherent-type defect because it does not destroy the $\Lambda^n_{\mathrm{BDL}}$ and in this case the theory developed for the APBs can be applied.

The number of energetically different APBs of any given orientation in superlattice $\Psi^n$ cannot exceed $L-1$, where $L$ is the number of atoms inside the primitive cell of superlattice $\Psi^n$ (Dmitriev *et al.*, 1995). In the considered case, the number $L$ is equal to the number of points of $\Lambda^n_{\mathrm{BDL}}$ inside the primitive cell of superlattice $\Psi^n$.

It is well known that the shift APB may not be formed in all orientations. The orientations in superlattice $\Psi^n$ where the shift APBs can be formed were derived by Starostenkov *et al.* (1993*b*). For those orientations, a SF is called a complex SF, otherwise it is called an intrinsic SF (Yamaguchi *et al.*, 1981).

### 4.3. *Energy of a stacking fault in the pair-potential approximation*

The energy of a SF in the superlattice $\Psi^n$ will be calculated under the assumption that interatomic interactions may be described by the pair interatomic potentials.

Let the position of two atoms of types $A$ and $B$ be defined by radius vectors $\mathbf{r}_A$ and $\mathbf{r}_B$, respectively. Let us assume that the pair interatomic potentials $\varphi_{AB}(|\mathbf{r}_A - \mathbf{r}_B|)$ are given. By the energy of interaction of packings, we imply the work required to move them away by an infinite distance. If either or both $A$ and $B$ atoms are atoms of type $O$, then $\varphi_{AB}(|\mathbf{r}_A - \mathbf{r}_B|) \equiv 0$.

We have a given superlattice $\Psi^n$ defined on the lattice $\Lambda^n$ as in (6) and given plane $(h_1 \dots h_n)$ with respect to the basis $\mathbf{v}_i$ or $(K_1 h_1 \dots K_n h_n)$ with respect to the basis $\mathbf{w}_i$. Derivation of the energy of the SF is as follows.

The first step is to find the generator vectors $\mathbf{t}_i$ of $\Lambda^n_{\mathrm{BDL}}(\Lambda^n, (h_1 \dots h_n))$ (see §3.2). Then the superlattice $\Psi^n$ should be redefined on the $\Lambda^n_{\mathrm{BDL}}$ by adding some packings of type $O$. The number of atoms inside the primitive cell of superlattice $\Psi^n$, including atoms of type $O$, is

$$L = \det \mathbf{W} / \det \mathbf{T}, \tag{14}$$

where $\mathbf{W}$ and $\mathbf{T}$ are the generator matrices of lattices $\Omega^n$ and $\Lambda^n_{\mathrm{BDL}}$, respectively. Then, (6) may be rewritten as

$$\Psi^n = \bigcup_{l=1}^{L} (\Omega^n + \mathbf{g}_l)_{S_l}. \tag{15}$$

Equation (15) differs from (6) only by the presence of $L - M$ packings of type $O$ that do not affect the energy of the crystal.

The following step is to separate the crystal (15) into $(n-1)$-dimensional monoatomic packings of given orientation $(K_1 h_1 \dots K_n h_n)$. For this purpose, let us choose a new basis $\mathbf{z}_i$ of the lattice $\Omega^n$ instead of $\mathbf{w}_i$ such that vectors $\mathbf{z}_1, \dots, \mathbf{z}_{n-1}$ are parallel to the given plane $(K_1 h_1 \dots K_n h_n)$ and $\mathbf{z}_n$ is chosen from the condition $\det \mathbf{Z} = \det \mathbf{W}$, where $\mathbf{Z}$ is the generator matrix of the new basis. The desired representation is given by

$$\Psi^n = \bigcup_{l=1}^{L} \bigcup_{k=-\infty}^{\infty} (\Omega^{n-1} + k\mathbf{z}_n + \mathbf{g}_l^*)_{S_l}, \tag{16}$$

where lattice $\Omega^{n-1}$ is generated by vectors $\mathbf{z}_1, \dots, \mathbf{z}_{n-1}$. The components of vectors $\mathbf{g}_l^*$ with respect to the basis $\mathbf{z}_i$ can be calculated as $\mathbf{g}_l \mathbf{Z}_*^{-1}$ (modulo 1), where the rows of matrix $\mathbf{Z}_*$ are the components of vectors $\mathbf{z}_i$ with respect to the basis $\mathbf{w}_i$.

According to the definition of SF given in §4.1, let us consider two coincident interpenetrating copies of crystal $\Psi^n$ given by (16), one of which will be marked $\hat{\Psi}^n$. Then let us translate the crystal $\hat{\Psi}^n$ along a vector $\mathbf{g}_l^* \in \Lambda^n_{\mathrm{BDL}}$. As a result, the sorts of packings $S_l$ will be changed to $D_l$ ones. The plane $(K_1 h_1 \dots K_n h_n)$ divides the crystals on the half-crystals:

$$\Psi^n = \Psi^n_- \cup \Psi^n_+ \quad \text{and} \quad \hat{\Psi}^n = \hat{\Psi}^n_- \cup \hat{\Psi}^n_+, \tag{17}$$

where

$$\begin{aligned}\Psi_-^n &= \bigcup_{l=1}^{L}\bigcup_{k=-\infty}^{-1}(\Omega^{n-1}+k\mathbf{z}_n+\mathbf{g}_l^*)_{S_l}\\ \Psi_+^n &= \bigcup_{l=1}^{L}\bigcup_{k=0}^{\infty}(\Omega^{n-1}+k\mathbf{z}_n+\mathbf{g}_l^*)_{S_l}\\ \hat{\Psi}_-^n &= \bigcup_{l=1}^{L}\bigcup_{k=-\infty}^{-1}(\Omega^{n-1}+k\mathbf{z}_n+\mathbf{g}_l^*)_{D_l}\\ \hat{\Psi}_+^n &= \bigcup_{l=1}^{L}\bigcup_{k=0}^{\infty}(\Omega^{n-1}+k\mathbf{z}_n+\mathbf{g}_l^*)_{D_l}.\end{aligned} \tag{18}$$

The defect crystal is $\Psi_-^n \cup \hat{\Psi}_+^n$.

The energy of a SF can be calculated as the difference

$$E_{SF} = E(\Psi_-^n \Leftrightarrow \hat{\Psi}_+^n) - E(\Psi_-^n \Leftrightarrow \Psi_+^n), \tag{19}$$

where the minuend is the energy of interaction of half-crystals in the defect crystals and the subtrahend is that for the ideal crystal.

The energy of a SF $(K_1h_1 \dots K_nh_n)$ per unit area formed by translation of the crystal $\hat{\Psi}^n$ with respect to the crystal $\Psi^n$ along the vector $\mathbf{g}_l^*$ is

$$E_{SF}(\mathbf{g}_l^*) = (1/H)\sum \varphi_{S_{l_1}D_{l_2}}(|\mathbf{qZ}|) - (1/H)\sum \varphi_{S_{l_1}S_{l_2}}(|\mathbf{qZ}|), \tag{20}$$

where

$$\sum = \sum_{l_1,l_2=1}^{L}\sum_{k_1,\dots,k_{n-1}=-\infty}^{\infty}\sum_{k_n=-\infty}^{-1}\sum_{k_{n+1}=0}^{\infty}, \tag{21}$$

$$\mathbf{q} = \mathbf{g}_{l_1}^* - \mathbf{g}_{l_2}^* + (k_1, \dots, k_{n-1}, k_n - k_{n+1}), \tag{22}$$

$H = [\det(\mathbf{Z}_n\mathbf{Z}_n^{\mathrm{T}})]^{1/2}$, $\mathbf{Z}_n$ is the generator matrix of the $(n-1)$-dimensional lattice with generator vectors $\mathbf{z}_1, \dots, \mathbf{z}_{n-1}$.

To make (20) convenient for practical calculations, it is necessary to find the ranges of the integer-valued indexes $k_j$ sufficient for taking into account all bonds of length not greater than $R$, where $R$ is the cut-off radius of the pair potentials. It is enough to consider $-P_j \le k_j \le P_j$, $j = 1, \dots, n-1$; $-P_n \le k_n \le -1$; $0 \le k_{n+1} \le P_n$; where

$$P_j = \lfloor R[\det(\mathbf{Z}_j\mathbf{Z}_j^{\mathrm{T}})]^{1/2}/\det\mathbf{Z}\rfloor + 1, \quad j = 1, \dots, n; \tag{23}$$

$\mathbf{Z}_j$ is the generator matrix of an $(n-1)$-dimensional lattice generated by vectors $\mathbf{z}_1, \dots, \mathbf{z}_{j-1}, \mathbf{z}_{j+1}, \dots, \mathbf{z}_n$; $\lfloor x \rfloor$ is the integer part of $x$.

## 5. Example

As an illustration, let us derive the expression for the energies of all possible SFs with orientation parallel to close-packed planes in the superlattice $L1_0$. The superlattice $L1_0$ is based on the f.c.c. lattice and successive (001) planes are alternately occupied by atoms of one species. We label the f.c.c. lattice with the lattice parameter $a$ and the superlattice $L1_0$ as $\Lambda^3$ and $\Psi^3$, respectively. The generator matrix $\mathbf{V}$ of the lattice $\Lambda^3$ can be chosen as

$$\mathbf{V} = \frac{a}{2}\begin{bmatrix}2 & 0 & 0\\ 1 & 1 & 0\\ 1 & 0 & 1\end{bmatrix}, \tag{24}$$

hence the generator vectors of $\Lambda^3$ with respect to the orthonormal basis $\mathbf{e}_i$ are $\mathbf{v}_1 = (a, 0, 0)$, $\mathbf{v}_2 = (a/2, a/2, 0)$, $\mathbf{v}_3 = (a/2, 0, a/2)$ (see Fig. 1).

The superlattice $L1_0$ can be defined as in §2 by choosing $K_1 = 1$, $K_2 = 1$, $K_3 = 2$. Then $M = 2$ and (6) becomes

$$\Psi^3 = \bigcup_{m=1}^{2}(\Omega^3 + \mathbf{g}_m)_{S_m}, \tag{25}$$

where the lattice $\Omega^3$ has generator vectors $\mathbf{w}_1 = \mathbf{v}_1$, $\mathbf{w}_2 = \mathbf{v}_2$, $\mathbf{w}_3 = 2\mathbf{v}_3$, translation vectors of packings are $\mathbf{g}_1 = \mathbf{0}$, $\mathbf{g}_2 = \mathbf{v}_3$ and the two sorts of packings are $S_1 = A$, $S_2 = B$.

The close-packed planes with respect to the basis $\mathbf{v}_i$ are (111). Let us turn now to the derivation of the boundary displacement lattice $\Lambda^3_{BDL}(\Lambda^3, (111))$. First, the new basis $\mathbf{u}_i$ of the lattice $\Lambda^3$ with vectors $\mathbf{u}_1$, $\mathbf{u}_2$ parallel to the plane (111) should be found. In doing this, we are guided by the algorithm described in §3.1. Equation (8) takes the form

$$x_1 + x_2 + x_3 = 0 \tag{26}$$

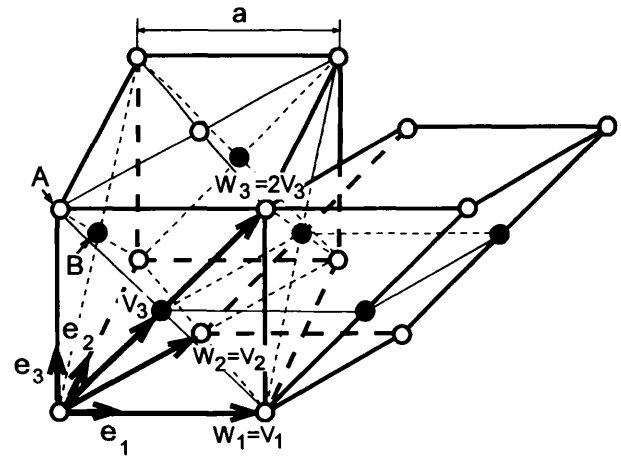


Fig. 1. Superlattice $L1_0$ or $\Psi^3$. Vectors $\mathbf{v}_i$ generate the f.c.c. lattice or lattice $\Lambda^3$. Vectors $\mathbf{w}_i$ define the primitive cell of the superlattice.

and its general solution is

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -1 & -1 \end{bmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}, \tag{27}$$

where $\alpha_1$, $\alpha_2$ are any integers. Consequently,

$$\mathbf{u}_1 = (1, 0, -1), \quad \mathbf{u}_2 = (0, 1, -1). \tag{28}$$

Condition $\det \mathbf{U} = \det \mathbf{V}$, where $\mathbf{U}$, $\mathbf{V}$ are two generator matrices of the lattice $\Lambda^3$, gives

$$\mathbf{u}_3 = (1, 0, 0). \tag{29}$$

Note that vectors $\mathbf{u}_i$ are given by equations (28) and (29) with respect to the basis $\mathbf{v}_i$.

The following step is to find the $\mathbf{u}$ components of the orthogonal projection of the vector $\mathbf{u}_3$ on the plane (26). One obtains:

$$\left(\tfrac{4}{3}, -\tfrac{2}{3}, 0\right) \tag{30}$$

and thus the basis of $\Lambda^3_{\mathrm{BDL}}(\Lambda^3, (111))$ can be written as

$$\mathbf{t}_1 = \tfrac{1}{3}\mathbf{u}_1, \quad \mathbf{t}_2 = \tfrac{1}{3}\mathbf{u}_2, \quad \mathbf{t}_3 = \mathbf{u}_3. \tag{31}$$

Recall that the superlattice $\mathrm{L1}_0$ (25) was defined on the lattice $\Lambda^3$. Lattice $\Lambda^3$ is a sublattice of the lattice $\Lambda^3_{\mathrm{BDL}}$ so one can define the superlattice $\mathrm{L1}_0$ on the lattice $\Lambda^3_{\mathrm{BDL}}$ by assigning to the packings that are not occupied atoms of type $O$. The $\mathbf{e}$ coordinates of vectors $\mathbf{w}_i$ and $\mathbf{t}_i$ are obtained from $\mathbf{v}$ coordinates by multiplying by matrix $\mathbf{V}$. As a result, the generator matrices of $\Omega^3$ and $\Lambda^3_{\mathrm{BDL}}$ are

$$\mathbf{W} = \frac{a}{2}\begin{bmatrix} 2 & 0 & 0 \\ 1 & 1 & 0 \\ 2 & 0 & 2 \end{bmatrix}, \quad \mathbf{T} = \frac{a}{6}\begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ 6 & 0 & 0 \end{bmatrix}, \tag{32}$$

respectively, then $L = \det \mathbf{W}/\det \mathbf{T} = 18$. Equation (25) can be written as

$$\Psi^3 = \bigcup_{l=1}^{18} (\Omega^3 + \mathbf{g}_l)_{S_l}, \tag{33}$$

where the lattice $\Omega^3$ has generator vectors $\mathbf{w}_i$, translation vectors of packings with respect to the basis $\mathbf{w}_i$ are

$$\begin{aligned}
&\mathbf{g}_1 = (0, 0, 0), \quad \mathbf{g}_2 = (0, 0, \tfrac{1}{2}), \quad \mathbf{g}_3 = (0, \tfrac{1}{3}, \tfrac{1}{3}), \\
&\mathbf{g}_4 = (\tfrac{1}{3}, 0, \tfrac{1}{3}), \quad \mathbf{g}_5 = (0, \tfrac{2}{3}, \tfrac{1}{6}), \quad \mathbf{g}_6 = (\tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{6}), \\
&\mathbf{g}_7 = (\tfrac{2}{3}, 0, \tfrac{1}{6}), \quad \mathbf{g}_8 = (\tfrac{1}{3}, \tfrac{2}{3}, 0), \quad \mathbf{g}_9 = (\tfrac{2}{3}, \tfrac{1}{3}, 0), \\
&\mathbf{g}_{10} = (0, \tfrac{1}{3}, \tfrac{5}{6}), \quad \mathbf{g}_{11} = (\tfrac{1}{3}, 0, \tfrac{5}{6}), \quad \mathbf{g}_{12} = (0, \tfrac{2}{3}, \tfrac{2}{3}), \\
&\mathbf{g}_{13} = (\tfrac{1}{3}, \tfrac{1}{3}, \tfrac{2}{3}), \quad \mathbf{g}_{14} = (\tfrac{2}{3}, 0, \tfrac{2}{3}), \quad \mathbf{g}_{15} = (\tfrac{1}{3}, \tfrac{2}{3}, \tfrac{1}{2}), \\
&\mathbf{g}_{16} = (\tfrac{2}{3}, \tfrac{1}{3}, \tfrac{1}{2}), \quad \mathbf{g}_{17} = (\tfrac{2}{3}, \tfrac{2}{3}, \tfrac{1}{3}), \quad \mathbf{g}_{18} = (\tfrac{2}{3}, \tfrac{2}{3}, \tfrac{5}{6}).
\end{aligned} \tag{34}$$

and the sorts of packings are $S_1 = A$, $S_2 = B$, $S_3 - S_{18} = O$ (see Fig. 2). Information about the sorts of packings can be written as follows:

$$ABOOOOOOOOOOOOOOO. \tag{35}$$

The primitive cell of superlattice (33) contains $L = 18$ atoms. It means that the number of SFs (111) with different energy is no more than $L - 1 = 17$ because the translation along the vector $\mathbf{g}_1 = \mathbf{0}$ does not produce a defect.

Now we turn to calculation of the energies of all possible 17 SFs (111).

Instead of the basis $\mathbf{w}_i$, the new one $\mathbf{z}_i$ will be chosen in such a manner that $\mathbf{z}_1$ and $\mathbf{z}_2$ are parallel to the close-packed planes. The close-packed planes in the basis $\mathbf{w}_i$ are $(K_1 K_2 2K_3) = (112)$. The equation

$$x_1 + x_2 + 2x_3 = 0 \tag{36}$$

has the general solution

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{bmatrix} -1 & -2 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}, \tag{37}$$

where $\alpha_1$, $\alpha_2$ are any integers and therefore

$$\mathbf{z}_1 = (-1, 1, 0), \quad \mathbf{z}_2 = (-2, 0, 1). \tag{38}$$

Condition $\det \mathbf{Z} = \det \mathbf{W}$, where $\mathbf{Z}$, $\mathbf{W}$ are two generator matrices of the lattice $\Omega^3$, gives

$$\mathbf{z}_3 = (-1, 0, 1). \tag{39}$$

Vectors $\mathbf{z}_i$ are given by (38) and (39) with respect to the basis $\mathbf{w}_i$. Vectors $\mathbf{z}_i$ with respect to the basis $\mathbf{e}_i$ give the rows of the generator matrix

$$\mathbf{Z} = \frac{a}{2}\begin{bmatrix} -1 & 1 & 0 \\ -2 & 0 & 2 \\ 0 & 0 & 2 \end{bmatrix}. \tag{40}$$

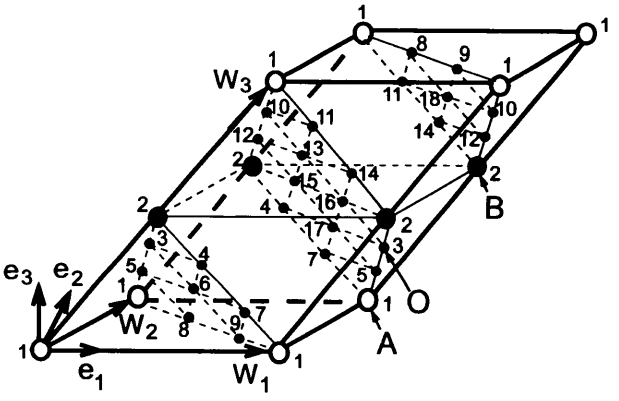


Fig. 2. The primitive cell of superlattice $\Psi^3$ with additional packings of sort $O$, which locate at the points of $\Lambda^3_{\mathrm{BDL}}(\Lambda^3, (111))$.

Rows of the matrix

$$\mathbf{Z}_* = \begin{bmatrix} -1 & 1 & 0 \\ -2 & 0 & 1 \\ -1 & 0 & 1 \end{bmatrix} \tag{41}$$

are the **w** coordinates of vectors $\mathbf{z}_i$. The **z** coordinates of vectors (34) can be obtained from the $w$ coordinates as follows [$\mathbf{g}_l^* = \mathbf{g}_l \mathbf{Z}_*^{-1}$ (modulo 1)]:

$$\begin{aligned}
&\mathbf{g}_1^* = (0,0,0), \quad \mathbf{g}_2^* = (0,\tfrac{1}{2},0), \quad \mathbf{g}_3^* = (\tfrac{1}{3},\tfrac{1}{3},0),\\
&\mathbf{g}_4^* = (0,\tfrac{1}{3},0), \quad \mathbf{g}_5^* = (\tfrac{2}{3},\tfrac{1}{6},0), \quad \mathbf{g}_6^* = (\tfrac{1}{3},\tfrac{1}{6},0),\\
&\mathbf{g}_7^* = (0,\tfrac{1}{6},0), \quad \mathbf{g}_8^* = (\tfrac{2}{3},0,0), \quad \mathbf{g}_9^* = (\tfrac{1}{3},0,0),\\
&\mathbf{g}_{10}^* = (\tfrac{1}{3},\tfrac{5}{6},0), \quad \mathbf{g}_{11}^* = (0,\tfrac{5}{6},0), \quad \mathbf{g}_{12}^* = (\tfrac{2}{3},\tfrac{2}{3},0),\\
&\mathbf{g}_{13}^* = (\tfrac{1}{3},\tfrac{2}{3},0), \quad \mathbf{g}_{14}^* = (0,\tfrac{2}{3},0), \quad \mathbf{g}_{15}^* = (\tfrac{2}{3},\tfrac{1}{2},0),\\
&\mathbf{g}_{16}^* = (\tfrac{1}{3},\tfrac{1}{2},0), \quad \mathbf{g}_{17}^* = (\tfrac{2}{3},\tfrac{1}{3},0), \quad \mathbf{g}_{18}^* = (\tfrac{2}{3},\tfrac{5}{6},0).
\end{aligned} \tag{42}$$

The superlattice (33) can be presented as a union of two-dimensional packings with orientation (111):

$$\Psi^3 = \bigcup_{l=1}^{18} \bigcup_{k=-\infty}^{\infty} (\Omega^2 + k\mathbf{z}_3 + \mathbf{g}_l^*)_{S_l}. \tag{43}$$

A close-packed plane is shown in Fig. 3. The volume of the new primitive cell of superlattice $\Psi^3$ is shown together with the nodes of type $O$.

Translation of the superlattice (43) along the vector $\mathbf{g}_l^*$ changes the typess of packing as follows:

$$\begin{aligned}
&\mathbf{g}_1^* : ABOOOOOOOOOOOOOOO,\\
&\mathbf{g}_2^* : BAOOOOOOOOOOOOOOO,\\
&\mathbf{g}_3^* : OOAOOOOOOBOOOOOOO,\\
&\mathbf{g}_4^* : OOOAOOOOOOBOOOOOO,\\
&\mathbf{g}_5^* : OOOOAOOOOOOBOOOOO,\\
&\mathbf{g}_6^* : OOOOOAOOOOOOBOOOO,\\
&\mathbf{g}_7^* : OOOOOOAOOOOOOBOOO,\\
&\mathbf{g}_8^* : OOOOOOOAOOOOOOBOO,\\
&\mathbf{g}_9^* : OOOOOOOOAOOOOOOBO,\\
&\mathbf{g}_{10}^* : OOBOOOOOOAOOOOOOO,\\
&\mathbf{g}_{11}^* : OOOBOOOOOOAOOOOOO,\\
&\mathbf{g}_{12}^* : OOOOBOOOOOOAOOOOO,\\
&\mathbf{g}_{13}^* : OOOOOBOOOOOOAOOOO,\\
&\mathbf{g}_{14}^* : OOOOOOBOOOOOOAOOO,\\
&\mathbf{g}_{15}^* : OOOOOOOBOOOOOOAOO,\\
&\mathbf{g}_{16}^* : OOOOOOOOBOOOOOOAO,\\
&\mathbf{g}_{17}^* : OOOOOOOOOOOOOOOAB,\\
&\mathbf{g}_{18}^* : OOOOOOOOOOOOOOOBA.
\end{aligned} \tag{44}$$

The energy of a SF per unit area, formed by translation of the crystal $\hat{\Psi}^n$ with respect to the crystal $\Psi^n$ along the vector $\mathbf{g}_l^*$ is

$$E_{\mathrm{SF}}(\mathbf{g}_l^*) = (1/H)\sum \varphi_{S_{l_1} D_{l_2}}(|\mathbf{qZ}|) - (1/H)\sum \varphi_{S_{l_1} S_{l_2}}(|\mathbf{qZ}|), \tag{45}$$

where

$$\sum = \sum_{l_1,l_2=1}^{18} \sum_{k_1=-P_1}^{P_1} \sum_{k_2=-P_2}^{P_2} \sum_{k_3=-P_3}^{-1} \sum_{k_4=0}^{P_3}, \tag{46}$$

$$\mathbf{q} = \mathbf{g}_{l_1}^* - \mathbf{g}_{l_2}^* + (k_1, k_2, k_3 - k_4), \tag{47}$$

$$\mathbf{Z}_1 = \frac{a}{2}\begin{bmatrix} -2 & 0 & 2 \\ 0 & 0 & 2 \end{bmatrix}, \quad \mathbf{Z}_2 = \frac{a}{2}\begin{bmatrix} -1 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix},$$
$$\mathbf{Z}_3 = \frac{a}{2}\begin{bmatrix} -1 & 1 & 0 \\ -2 & 0 & 2 \end{bmatrix}, \tag{48}$$

$$H = [\det(\mathbf{Z}_3 \mathbf{Z}_3^T)]^{1/2} = (3^{1/2}/2)a^2. \tag{49}$$

The cut-off radius of the potentials is $R = a \times 2^{1/2}$, then, according to (23), the limits of the sums in (46) are

$$P_1 = \lfloor 2 \times 2^{1/2} \rfloor + 1 = 3, \quad P_2 = \lfloor 2 \rfloor + 1 = 3,$$
$$P_3 = \lfloor 6^{1/2} \rfloor + 1 = 3. \tag{50}$$

Sorts of packings $S_{l_1}$, $S_{l_2}$ in (45) are given by (35), sorts $D_{l_2}$ are given by one of the set (44) for corresponding translation vector $\mathbf{g}_l^*$.

Equation (45), in view of (44) and (46)–(50), gives, for example

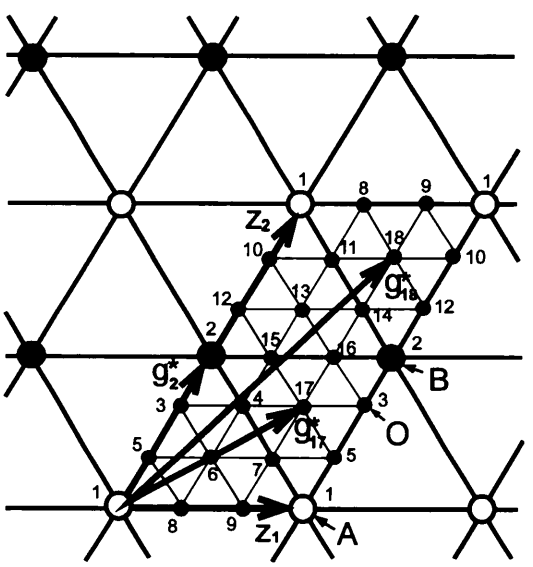


Fig. 3. A close-packed plane of superlattice $\Psi^3$ with additional packings of sort $O$.

$$E_{SF}(\mathbf{g}_2^*) = (2/3^{1/2}a^2)[-\omega(r_7) + 3\omega(r_{13}) - 4\omega(r_{19}) + 6\omega(r_{24})], \quad (51)$$

$$E_{SF}(\mathbf{g}_{17}^*) = (2/3^{1/2}a^2)[2\Delta(r_{17}) - 4\omega(r_{19}) - 6\Delta(r_{19}) + 8\omega(r_{22}) + 12\Delta(r_{22}) - 6\Delta(r_{24})], \quad (52)$$

$$E_{SF}(\mathbf{g}_{18}^*) = (2/3^{1/2}a^2)[-\omega(r_7) + 3\omega(r_{13}) + 2\omega(r_{17}) + 2\Delta(r_{17}) - 6\omega(r_{19}) - 6\Delta(r_{19}) + 4\omega(r_{22}) + 12\Delta(r_{22}) - 6\Delta(r_{24})], \quad (53)$$

where $\omega(r) = -\varphi_{AA}(r) + 2\varphi_{AB}(r) - \varphi_{BB}(r)$, $\Delta(r) = \varphi_{AA}(r) + \varphi_{BB}(r)$, $r_7 = (a/6)(18)^{1/2}$, $r_{13} = (a/6)(36)^{1/2}$, $r_{17} = (a/6)(48)^{1/2}$, $r_{19} = (a/6)(54)^{1/2}$, $r_{22} = (a/6)(66)^{1/2}$, $r_{24} = (a/6)(72)^{1/2}$. Translation vectors $\mathbf{g}_2^*$, $\mathbf{g}_{17}^*$ and $\mathbf{g}_{18}^*$ are shown in Fig. 3.

Actually, the defect obtained by translation along the vector $\mathbf{g}_2^* \in \Lambda^3$ is not a SF but it is an APB. The energy of this defect is expressed in terms of parameter $\omega$, which is to say that this defect does not destroy the lattice $\Lambda^3$.

The other two translations produce the defects that are truly SFs. One might expect that energy $E_{SF}(\mathbf{g}_{18}^*)$ is larger than energy $E_{SF}(\mathbf{g}_{17}^*)$ because the latter defect does not change the types of atoms at the coordination shells with smallest radii, namely, $r_7$ and $r_{13}$.

## 6. Summary

The definition of grain-boundary SFs given for pure metals by Orlov *et al.* (1975) was adopted to define a SF in an arbitrary ordered alloy. The problems of enumeration of all possible SFs of given orientation as well as the derivation of the analytical expression for SF energy in terms of pair potentials were solved.

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