

A comment on ‘Crystallography and migration mechanisms of planar interface boundaries’ *Acta Materialia*, 52, 795–807 (2004) by J. F. Nie

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Abstract

In a recent paper by Nie, it was claimed that there is no two-dimensional continuity of lattice planes across the invariant line. However, it is a property of an invariant line strain that any planes related by the transformation strain must exhibit continuity across the invariant line. This note indicates that the Nie’s incorrect conclusion is due to his definition of the shear strain that is different from the standard matrix method.

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Edge-to-edge matching of lattice planes has been considered to be a crystallographic feature of interphase interfaces or habit planes in various phase transformation systems [1–5]. In a recent publication [4], Nie presented a set of analytical formulae to describe the geometry of planar interfaces in terms of plane edge matching, and claimed that many existing theoretical models were incapable of describing the interface, including the O-lattice model [6,7] which is well accepted as the most general geometrical theory for interfaces [8]. Nie [4] did not realize that matching of plane edges is a property of principal O-lattice planes, and that a plane containing O-lines must be parallel to at least two sets of Moiré planes associated with low index planes. Hence, at least two sets of planes must continue across the interface containing the O-lines, which are parallel to an invariant line. The corresponding orientation rela-

tionship (OR) between two phases and the orientation of the interface containing the O-lines can all be determined from standard O-lattice matrix calculations [7,9]. Although the original result was derived from a three-dimensional (3-D) analysis, the conclusion is equally valid in 2-D.

Nevertheless, Nie [4] stated that his geometrical formulae differ from those of the 2-D invariant line model, as defined by Xiao and Howe [10]. Nie concluded that “The implication of this difference is such that, for the general case of phase transformations, there is no two-dimensional continuity of lattice planes across the invariant line” (in the first conclusion in Ref. [4]). It follows from the properties of the invariant lines, that displacement between any pair of reciprocal lattice vectors related by an invariant line strain must lie in the zone axis of the invariant line [9]. Since such a displacement vector defines a set of Moiré planes formed by superimposing the planes related by the transformation strain [11], the above geometry ensures that the invariant line must lie in any Moiré planes, where there is continuity of the related lattice planes. Therefore, there should be

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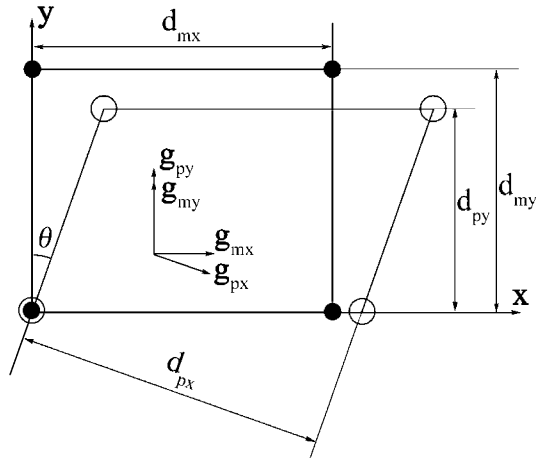


Fig. 1. A sketch of a 2-D deformation, following the formulation by Nie [4]. The solid and open circles represent the lattice points before and after the deformation, respectively. The reciprocal vectors for two pairs of planes related by the deformation are indicated.

no misfit between any pair of planes related by the transformation strain across the invariant line. This result is completely general, and can be readily demonstrated for the 2-D case, as follows.

Consider two planes of the parent lattice normal to axes x and y , denoted by the vectors \mathbf{g}_{mx} and \mathbf{g}_{my} , as specified in Fig. 1, which follows Nie's approach [4]. (All the vectors used in this context refer to column vectors unless otherwise noted and row vectors are defined with a transpose operation, denoted by '.) These planes can be indexed simply with $(1/d_{mx} \ 0)$ and $(0 \ 1/d_{my})$, where d_{mx} and d_{my} are the spacings of planes \mathbf{g}_{mx} and \mathbf{g}_{my} , respectively. In an invariant line condition, the transformation matrix \mathbf{A} must satisfy

$$\mathbf{A}\mathbf{x}_i = \mathbf{x}_i, \quad (1)$$

where \mathbf{x}_i is the invariant line. (All the vector and matrix components in this and subsequent equations are expressed in the reference Cartesian space.) The planes in the product phase, \mathbf{g}_{px} and \mathbf{g}_{py} , are related to \mathbf{g}_{mx} and \mathbf{g}_{my} by [12]

$$\mathbf{g}_{px} = (\mathbf{A}^{-1})' \mathbf{g}_{mx}, \quad (2a)$$

and

$$\mathbf{g}_{py} = (\mathbf{A}^{-1})' \mathbf{g}_{my}. \quad (2b)$$

In the O-lattice formulation [7], Eq. (1) can be rewritten as

$$\mathbf{T}\mathbf{x}_i = \mathbf{0}, \quad (3a)$$

$$\mathbf{T} = \mathbf{I} - \mathbf{A}^{-1}, \quad (3b)$$

where \mathbf{T} is the 2×2 displacement matrix, and $\text{rank}(\mathbf{T}) = 1$. This implies that the two row vectors of \mathbf{T} , namely \mathbf{t}'_1 and \mathbf{t}'_2 are parallel to each other. In this case, the normal vectors of the Moiré planes corresponding to planes \mathbf{g}_{mx} and \mathbf{g}_{my} , can be expressed by

$$\Delta\mathbf{g}_x = \mathbf{g}_{mx} - \mathbf{g}_{px} = \mathbf{T}' \mathbf{g}_{mx} = (\mathbf{t}_1 \mathbf{t}_2) \begin{pmatrix} 1/d_{mx} \\ 0 \end{pmatrix} = \mathbf{t}_1/d_{mx}, \quad (4a)$$

and

$$\Delta\mathbf{g}_y = \mathbf{g}_{my} - \mathbf{g}_{py} = \mathbf{T}' \mathbf{g}_{my} = (\mathbf{t}_1 \mathbf{t}_2) \begin{pmatrix} 0 \\ 1/d_{my} \end{pmatrix} = \mathbf{t}_2/d_{my}. \quad (4b)$$

Since \mathbf{t}_1 and \mathbf{t}_2 are parallel, Eqs. (4a) and (4b) demonstrate that the two Moiré planes represented by $\Delta\mathbf{g}_x$ and $\Delta\mathbf{g}_y$ must be parallel. According to the geometric properties of Moiré planes [6], the edges of the planes \mathbf{g}_{mx} and \mathbf{g}_{px} , and the edges of the planes \mathbf{g}_{my} and \mathbf{g}_{py} should meet each other in the same plane that is normal to the $\Delta\mathbf{g}_x$ (or $\Delta\mathbf{g}_y$). For a more general set of edge-on planes in the parent lattice, \mathbf{g}_m , which can be expressed as the linear combination of the \mathbf{g}_{mx} and \mathbf{g}_{my} , the above conclusion remains valid because the corresponding $\Delta\mathbf{g}_m$ can always be expressed as the linear combination of the parallel \mathbf{t}_1 and \mathbf{t}_2 . Furthermore, since

$$\Delta\mathbf{g}'_m \mathbf{x}_i = \mathbf{g}'_m \mathbf{T}\mathbf{x}_i = 0, \quad (5)$$

the invariant line must lie in the Moiré planes formed by any pair of edge-on correlated planes. Therefore, the continuity of any edge-on planes across the invariant line always applies. This conclusion is quite different from that of Nie [4].

Why did Nie draw an opposite conclusion? His conclusion was based on the difference between the formulae he derived [4] and the corresponding results for the 2-D invariant line condition [10]. Comparing the continuity criterion derived by Nie's continuity criterion and the 2-D invariant line condition, we can show that the 'difference' between the two approaches lies in the definition of the shear strain, s . Fig. 2 shows a sketch of a general 2-D deformation consisting of a pure deformation and shear deformation. This deformation can be defined as [10]

$$\mathbf{B} = \begin{pmatrix} a & s_1 \\ & b \end{pmatrix}, \quad (6)$$

where a and b denote the pure strains along the x and y axes, respectively, while s_1 denotes the shear strain. Following Xiao and Howe's approach [10], let us consider a pair of vectors \mathbf{u} and \mathbf{v} in the unit cell of the parent and product lattices in Fig. 2. These vectors are related by

$$\mathbf{v} = \mathbf{B}\mathbf{u}. \quad (7)$$

In the 2-D coordinate system \mathbf{xOy} , $\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$ and $\mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$, as shown in Fig. 2. The following relationships therefore apply

$$v_1 = au_1 + s_1u_2, \quad (8a)$$

$$v_2 = bu_2. \quad (8b)$$

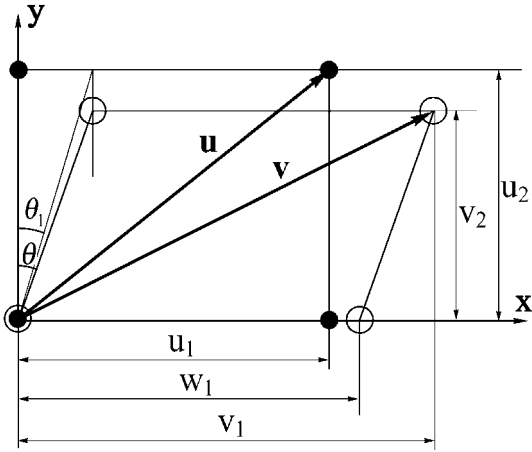


Fig. 2. A sketch of a general 2-D deformation, following the formulation by Xiao and Howe [10]. The solid and open circles represent the lattice points before and after the deformation, respectively. Two shear angles θ_1 , θ are specified to show the definition difference.

Let us set $w_1 = au_1$ as specified in Fig. 2. Then one can express the pure strains and the shear strain as

$$a = w_1/u_1, \tag{9a}$$

$$b = v_2/u_2, \tag{9b}$$

$$s_1 = (v_1 - w_1)/u_2. \tag{9c}$$

These expressions are in accord with the definition by Xiao and Howe [10]. s_1 can also be expressed in terms of the shear angle θ_1 , i.e. $s_1 = tg\theta_1$ as evaluated by the shear displacement per unit distance in the parent phase from the plane passing through the origin, an approach that is consistent with the convention of the phenomenological theory of martensitic crystallography [13].

In contrast, Nie [4] formulated the 2-D deformation in terms of the plane spacings of d_{mx} , d_{my} , d_{px} , d_{py} . The angle describing the shear component, θ , is defined in the product phase, as shown in Figs. 1 and 2. The three parameters for the 2-D deformation defined by Nie [4] were given as

$$\varepsilon_x = d_{px}/(d_{mx} \cos \theta), \tag{10a}$$

$$\varepsilon_y = d_{py}/d_{my}, \tag{10b}$$

$$s = tg\theta. \tag{10c}$$

Comparing the definitions in Eqs. (9) and (10), and the geometry in Figs. 1 and 2, one can establish the following relationships

$$a = \varepsilon_x, \tag{11a}$$

$$b = \varepsilon_y, \tag{11b}$$

$$s_1 = tg\theta = btg\theta = s\varepsilon_y. \tag{11c}$$

The difference between θ_1 and θ is specified in Fig. 2. The two sets of parameter definitions have been used

in further expressions by Nie [4] and Xiao and Howe [10]. The formulae for determining the rotation angle φ for the plane continuity [4] and ϕ for an invariant line in 2-D [10] are given in the Appendix A.

Clearly, the expressions by Nie [4] and by Xiao and Howe [10] are different, but they are self-consistent with the definitions. However, Nie also applied the parameters defined in Eq. (10) to form a following matrix expression for the transformation strain [4],

$$S = \begin{pmatrix} \varepsilon_x & s \\ & \varepsilon_y \end{pmatrix}, \tag{12}$$

though he did not apply this matrix in the formulation. While Eq. (12) is apparently similar with Eq. (6), the definition of the shear strain, s , is clearly in conflict with the standard transformation matrix in Eq. (6). By setting $s = s_1 = 0.3$, Nie presented the difference in the predictions of the OR and the habit plane from his formulae [4] and those from Xiao and Howe [10] in Fig. 7 of Ref. [4]. Based on this difference, Nie concluded there is no 2-D continuity of lattice plane across the invariant line. However, the difference in the definition of the shear component of the transformation strain in Eq. (11c) should be taken into consideration. With the substitution of the correct value of the shear strain for comparisons ($s_1 = s\varepsilon_y$ instead of s), Nie's expression for the OR is completely equivalent to that of Xiao and Howe [10], as can be seen in Appendix A. Similarly, the orientation of the habit plane should also be equivalent. It is not surprising that the different definitions have lead to the incorrect results in Fig. 7 of Ref. [4].

In summary, it is a property of an invariant line strain that any planes related by the transformation strain must exhibit continuity across the invariant line. With a known rotation axis, parallelism of Moiré planes can be determined with 2-D models, such as that by Nie [4] and Xiao and Howe [10]. The 3-D O-line model is more general because it does not place a prerequisite on the rotation axis which is usually parallel to a pair of rational directions. Of course, the O-line model is also applicable to the cases when the rotation axis is fixed. The 'difference' between the 2-D 'edge-to-edge' model and the 2-D invariant line model pointed out by Nie is due to the difference in the definition of the shear angle by Nie from the one in a standard matrix formula. Nie did not appreciate this difference, and as a result came to the wrong conclusion about the properties of the invariant line.

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Appendix A

In Nie's formulation [4], the product lattice has to rotate about the z axis by an angle to satisfy the condition of 2-D 'edge-to-edge' matching. The rotation angle ϕ was given by (Eq. 9 of Ref. [4])

$$\cos \phi = \frac{(1 + \varepsilon_x \varepsilon_y)(\varepsilon_x + \varepsilon_y) + s \varepsilon_y \sqrt{s^2 \varepsilon_y^2 - (\varepsilon_x^2 - 1)(\varepsilon_y^2 - 1)}}{(\varepsilon_x + \varepsilon_y)^2 + s^2 \varepsilon_y^2}.$$

Similarly, in the 2-D invariant line model by Xiao and Howe, the product lattice also has to rotate by an angle ϕ to produce a 2-D invariant line. The rotation ϕ was determined as (Eq. 8 of Ref. [10])

$$\cos \phi = \frac{(1 + ab)(a + b) + s_1 \sqrt{s_1^2 - (a^2 - 1)(b^2 - 1)}}{(a + b)^2 + s_1^2}$$

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