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The Prediction of Twinning Modes in Metal Crystals

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A new crystallographic analysis of deformation twinning in multiple lattices is developed. This enables the operative twinning modes to be predicted for all metal crystals, including α-uranium. Reasons are given for the non-appearance of certain modes expected theoretically.

Introduction

Deformation twinning of a crystal may be examined from two points of view, the macroscopic and the microscopic. On the macroscopic scale, twinning is achieved by a homogeneous shear parallel to the composition or twinning plane K_1, along a shear direction η_1. The plane perpendicular to K_1, passing through η_1, is termed the plane of shear. Associated with K_1, η_1 there exists a second undistorted plane K_2, cutting K_1 in a direction perpendicular to η_1 and cutting the plane of shear in a direction η_2. Twinned crystals are of two distinct kinds, referred to as first and second. In the former, K_1 is rational, and may be regarded as the plane of an imagined mirror which reflects the structure of the twin into that of the matrix. In the latter, K_1 is irrational, but η_1 is rational, and may be regarded as the direction of an imagined axis about which a rotation of 180° transforms the structure of the twin into that of the matrix. For any given mode

$$K_1 = (hkl),\ K_2 = (h'k'l'),\ \eta_1 = [uvw],\ \eta_2 = [u'v'w'],$$

there exists theoretically a conjugate or reciprocal mode

$$K_1 = (h'k'l'),\ K_2 = (hkl),\ \eta_1 = [u'v'w'],\ \eta_2 = [uvw],$$

involving the same macroscopic shear. From the macroscopic point of view, there should be nothing to choose between a mode and its conjugate, but in certain cases the latter has never been reported operative. The conjugates to the modes (9) and (10), of Table 1, have been reported operative: these are the only established examples in metals of twinning of the second kind.

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Nothing can be known directly of the twinning shear on the microscopic scale, and the only practicable method of progress is to guess at the most likely net displacements of the atoms. In simple lattices the problem is trivial, for the atoms have only to execute the macroscopic shear in order to arrive at their final positions. In multiple lattices the microscopic shear has necessarily a homogeneous component, which may be effectively identified with the macroscopic shear, together with inhomogeneous components which produce no macroscopic effects but merely serve to generate the twinned configuration. The resolution into the two components cannot be uniquely defined mathematically, a feature which constitutes the essential difficulty of the problem. Fortunately, however, a considerable degree of systematization may be effected by introducing a new concept, that of the semi-homogeneous shear, roughly described as a shear homogeneous on the finest possible scale compatible with producing a twinned configuration. This will be recognized as the closest possible analogue, indeed as the natural generalization, of the completely homogeneous shear assumed for simple lattices. With the restriction to semi-homogeneity, the microscopic shear corresponding to a given macroscopic shear can always be uniquely defined, and a quantitative crystallographic analysis of twinning becomes possible.

Given a rational composition plane K_1, but not the shear direction η_1, there exists an infinite number of possible semi-homogeneous shears parallel to K_1, each defining a hypothetical macroscopic twinning shear. Their properties may be examined by the technique of projecting the crystal on to K_1, and the following result has already been obtained (Jaswon & Dove, 1956): of all the macroscopic shears in question, the one along η_1 has the smallest magnitude. In the present paper, the analysis is extended to examine the factors which determine the choice of K_1. Given any crystal plane K, projecting on K enables us to deduce the semi-homogeneous shear of smallest homogeneous component parallel to K, the magnitude of this hypothetical shear being denoted $\mathscr{S}$. Now applying an inequality theorem proved in the text, we arrive at the following significant conclusion: for a given crystal structure, $\mathscr{S}$ attains a minimum value, S, on the planes of indices K_1 and K_2. Accordingly, the operative mode in a multiple lattice, as in a simple lattice, may be completely predicted by invoking a formal, geometrical requirement. The power of the method may be appreciated by the fact that it predicts eight modes in α-uranium with shear values falling between 0·2 and 0·3, five of which have so far been reported operative (Cahn, 1953; Lloyd & Chiswick, 1955). Several high shear modes seem to have been established in titanium (Liu & Steinberg, 1952; Rosi, Dube & Alexander, 1953; Rosi & Perkins, 1953) and cannot be accounted for on the present ideas: almost certainly, however, the formal geometrical factor is here completely dominated by the presence of interstitial impurities (Churchman, 1954). A surprising prediction is the mode (4) below for diamond, but the usual assignment (5) seems to be based on an unjustified deduction from the f.c.c. lattice. Unfortunately, deformation twinning has never been substantiated in diamond, so that no test of the theory is available in this instance.

We now enumerate (Table 1) the *predicted* twinning modes of metal crystals, grouped as far as possible to bring out significant comparisons. To each mode there corresponds, of course, a conjugate which is understood. The designations X or Y refer only to modes in multiple lattices, and will be explained below.

Bismuth stands also for arsenic and antimony; diamond stands also for silicon and germanium, though here the formal geometrical factor may be dominated by the effect of impurities. Body-centred cubic metals, and β-tin, are referred to face-centred tetragonal unit cells; this facilitates comparison with indium, and indeed also with diamond and f.c.c. metals. Analysis indicates that twinning modes in a multiple lattice fall into two main classes, here denoted X and Y, depending on the mechanism of the inhomogeneous

Table 1

	K_1	K_2	η_1	η_2	S	Unit cell			
Bismuth	(110)	(001)	$[00\bar{1}]$	[110]	$\frac{2\sqrt{2w}}{\sqrt{(1+2w)}\sqrt{(1-w)}}$	F. c. rhombohedral	$w=\cos\alpha$	Y	(1)
Mercury	(110)	(001)	$[00\bar{1}]$	[110]		F. c. rhombohedral			(2)
C. p. h. metals	$(10\bar{1}2)$	$(10\bar{1}\bar{2})$	$[\bar{1}011]$	$[10\bar{1}1]$	$\frac{q^2-3}{\sqrt{3}q}$	Hexagonal	$q=c/a$	X	(3)
Diamond	(111)	$(11\bar{3})$	$[\bar{1}\bar{1}2]$	[332]	$1/2\sqrt{2}$	F. c. cubic	$q=1$	X	(4)
F. c. c. metals	(111)	$(11\bar{1})$	$[11\bar{2}]$	[112]	$1/\sqrt{2}$	F. c. cubic	$q=1$		(5)
β-Tin	(331)*	$(\bar{1}\bar{1}1)$	$[\bar{1}\bar{1}6]$	[112]	$(1-6q^2)/2\sqrt{2}q$	F. c. tetragonal	$q=0{\cdot}383$	X	(6)
Indium	(101)	$(10\bar{1})$	$[10\bar{1}]$	[101]	$(q^2-1)/q$	F. c. tetragonal	$q=1{\cdot}078$		(7)
B. c. c. metals	(101)*	$(10\bar{1})$	$[10\bar{1}]$	[101]	$1/\sqrt{2}$	F. c. tetragonal	$q=1/\sqrt{2}$		(8)
α-Uranium	(111)	'$(1\bar{7}6)$'	'$[12\bar{3}]$'	$[5\bar{1}\bar{2}]$	0·214	Orthorhombic		Y	(9)
	(112)	'$(1\bar{7}2)$'	'$[3\bar{7}2]$'	[312]	0·227			X	(10)
	(021)	'$(\bar{1}\bar{1}, 1, 4)$'	'[100]'	[132]	0·286			X	(11)
	(130)	$(1\bar{1}0)$	$[3\bar{1}0]$	[110]	0·298			Y	(12)

* These reduce to the usually quoted indices on transforming to the conventional unit cells.

displacements. If a Y-mode is predicted for the crystal, this is the same as the predicted mode of the Bravais space lattice of the crystal; hence the comparison between bismuth and mercury (the latter provides a realization of the Bravais space lattice of the former). If an X-mode is predicted, this differs from the predicted mode of the Bravais space lattice, particularly in having a smaller shear value—hence the comparison between (4) and (5), and between (6) and (7) or (8). Not much significance, however, attaches to the latter comparisons since the relative dimensions of the unit cells are so markedly different.

Twinning of the second kind, with special reference to α-uranium, will be taken up in a later paper.

The semi-homogeneous twinning shear

A multiple lattice may be regarded as consisting of two interpenetrating lattices, so that all the crystal planes occur in pairs. Using a convenient and obvious notation, successive parallel planes of the one lattice are denoted $\ldots \bar{2}a, \bar{1}a, 0a, 1a, 2a, \ldots$ and the corresponding successive parallel planes of the other lattice are denoted $\ldots \bar{2}b, \bar{1}b, 0b, 1b, 2b, \ldots$ as depicted in Fig. 1(i). Given a plane $0a$, there are two distinct

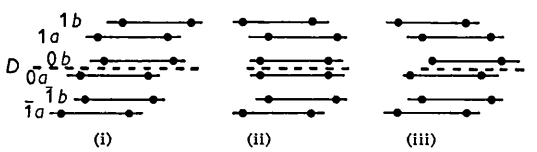

Fig. 1. (i) Untwinned crystal (schematic). (ii) Ideal twin configuration. This could hardly be tolerated for the narrow-gap possibility. (iii) Compromise position of $0a$, $0b$. This is more likely than (ii).

possibilities for the associated plane $0b$, namely the neighbouring plane separated by the wide gap and the neighbouring plane separated by the narrow gap. This leads to several possibilities for the detailed structure of K_1, all of which yield the same macroscopic results. As the mathematically simplest possibility, we identify K_1 with an imagined mirror plane midway between $0a, 0b$ (narrow gap), which reflects the twinned crystal into that of the matrix, as indicated by the broken line D in Fig. 1. In an ideal twin, $0a$ and $0b$ should be mirror images with respect to D, but such a configuration could hardly be tolerated energetically. It is much more likely that the equilibrium stacking of $0a, 0b$ is largely maintained, and that they assume a compromise position between twin and matrix as shown in Fig. 1(iii). Fuller discussion of the transition region is presented in a preceding paper (Jaswon & Dove, 1956).

As regards the net twinning displacements of the succeeding crystal planes $1a, 1b, 2a, 2b, \ldots$, we lay down the following general requirements for a semi-homogeneous shear:

1. The associated planes na, nb should become the images either of the $\bar{n}a, \bar{n}b$ respectively or of $\bar{n}b, \bar{n}a$ respectively, with respect to D as mirror plane. This is the most direct identification between twin and parent crystals that one can postulate.
2. The deformation should be homogeneous on the scale of succeeding units of pairs of planes $1a, 1b$; $2a, 2b$; $\ldots$, the finest scale possible in a multiple lattice. More precisely, the net twinning displacements $\mathbf{A}_n, \mathbf{B}_n$ of na, nb should have a homogeneous component $\frac{1}{2}(\mathbf{A}_n+\mathbf{B}_n)$ which is horizontal* and proportional to n.
3. The inhomogeneous components, or reshuffles, $\pm\frac{1}{2}(\mathbf{A}_n-\mathbf{B}_n)$ may be either horizontal or vertical*. Horizontal reshuffles should not amount to more than interatomic spacing along the most-closely-packed lattice direction of K_1. Vertical reshuffles are nothing more than an interchange on the levels of na and nb, in which case the stacking configuration of na, nb must be favourable for interchange.

These conditions can be realized in two distinct ways, effectively determined by the nature of the twinning displacements of $1a, 1b$. Most simply, the planes $1a, 1b$ may undergo the least possible common translation $\mathbf{T}'$ that carries them directly over $\bar{1}a, \bar{1}b$ respectively, whence they become the images of the latter by a vertical interchange (Y-mechanism). Alternatively, the planes $1a, 1b$ undergo the least possible purely horizontal displacements $\mathbf{T}+\mathbf{t}, \mathbf{T}-\mathbf{t}$ to become the images of $\bar{1}b, \bar{1}a$ respectively (X-mechanism). In either event, however, the translation $2\mathbf{T}$ or $2\mathbf{T}'$, as the case may be, carries $2a, 2b$ directly over $\bar{2}a, \bar{2}b$ respectively, whence they become the images of the latter by a vertical interchange. Further, according to the Y-mechanism, the reshuffles within succeeding units, without exception, follow essentially the pattern set by $1a, 1b$; according to the X-mechanism, the reshuffles are alternately horizontal and vertical, following the patterns set by $1a, 1b$ and $2a, 2b$ respectively (see Appendix). For a given rational composition plane, we expect the smaller of the vectors $\mathbf{T}, \mathbf{T}'$ to determine the twinning mechanism, and hence also the macroscopic shear. This is found to be the case. On the other hand, if the magnitudes T and T' are equal, or comparable, the decisive factor is then the relative feasibility of the reaction paths. For instance $T = T'$ in the case of the bismuth mode (1), but this is undoubtedly a Y-mode: the planes na, nb almost constitute a single plane of corrugated structure in which horizontal reshuffles could hardly be tolerated. It may be noted that the Y-mechanism implies an effectively homogeneous shear on the microscopic scale, a feature which suggests that Y-modes, if operative at all, should be operative very readily. This analysis is supported by two interesting facts:

* In the present context, horizontal and vertical mean parallel and perpendicular to K_1 respectively.

twinning occurs with remarkable facility in bismuth, where, as we have seen, the operative mode (1) is an ideal Y-mode; the α-uranium Y-mode (12) competes with the X-mode (10), even though $S_{(130)} = 0{\cdot}298$, $S_{(112)} = 0{\cdot}227$. Reaction-path analysis throws light on the non-appearance of the bismuth $K_1 = (001)$ mode, i.e. the conjugate to (1): parallel to (001), the corrugated plane na, nb must pass directly over the preceding plane, atom over atom, before reaching its final position, a factor which should decisively inhibit (001)-twinning compared with (110)-twinning.

According to the preceding considerations, the translation $2\mathbf{T}$ or $2\mathbf{T}'$, as the case may be, always carries $2a$ directly over $\bar{2}a$. Conversely, by projecting $2a$ on to $\bar{2}a$, we deduce at once the vector $\mathbf{Q}_0$ which is to be identified as either $2\mathbf{T}$ or $2\mathbf{T}'$. No further information is available from this projection alone, but in any case $\mathbf{Q}_0/2d$ should yield the magnitude and direction of the macroscopic shear. The method has been applied to all known composition planes, and gives the same results as obtained by the more fundamental analysis based on $1a$, $1b$. Its true importance, however, will emerge only in the next section. We remark here that the Bravais space lattice of the crystal may be formally produced by omitting all the b planes, in which case the succeeding lattice planes $1a$, $2a$, ..., na, ... undergo the twinning displacements $\mathbf{T}'$, $2\mathbf{T}'$, ..., $n\mathbf{T}'$, ... parallel to K_1. Bearing in mind that this set of displacements constitutes the homogeneous component of the crystal deformation if a Y-mechanism is operative, we are led to the conclusion given in the introduction.

The inequality theorem

We are now in a position to prove the central theorem of the present investigation. In Fig. 2 are drawn the traces of $\bar{2}a$, $0a$, $2a$, together with a lattice point P in plane $\bar{2}a$ and nearest neighbouring lattice point R in plane $2a$; the vector PR is referred to as $\mathscr{F}$. Plane $2a$ is carried directly over $\bar{2}a$ by undergoing the displacement $\mathbf{Q} = RR'$, where R' lies directly over P; $\mathbf{Q}$ is evidently the least possible displacement of this kind. If $\mathscr{S}$ is the hypothetical macroscopic twinning shear defined by $\mathbf{Q}$, we have

$$\mathscr{S}^2 = Q^2/4d^2, \quad \text{i.e.} \quad 1/d^2 = 4(\mathscr{S}^2+4)/\mathscr{F}^2,$$

where d is the interplanar spacing. Now replacing $\mathscr{F}$ by $\mathbf{E}$, where $\mathbf{E}$ is the shortest possible lattice vector (of the Bravais space lattice of the crystal), we arrive at the inequality

$$1/d^2 \leq 4(\mathscr{S}^2+4)/E^2,$$

satisfied by the $\mathscr{S}$, d of any set of crystal planes (hkl). As a corollary, for any prescribed value of $\mathscr{S}$, e.g. $\mathscr{S} = 1$, the inequality places a restriction on $1/d^2$, and hence on the indices (hkl) satisfying the inequality. This theorem should be compared with the analogous theorem for simple lattices, proved in the preceding paper.

If plane $\bar{2}a$ has the equation $hx+ky+lz = 0$, then $2a$ has the equation $hx+ky+lz = 4$. Accordingly, regarding P as the origin, and writing $\mathscr{F} = [\mathscr{F}_x, \mathscr{F}_y, \mathscr{F}_z]$, we have $h\mathscr{F}_x+k\mathscr{F}_y+l\mathscr{F}_z = 4$. Of all the possible solutions of the equation $hx+hy+lz = 4$, the solution $\mathscr{F}_x, \mathscr{F}_y, \mathscr{F}_z$ defines the vector of shortest length, which property may be used as a means of identifying it. Once $\mathscr{F}$ is known for a given set of planes, we may write

$$-\mathbf{Q} = \mathscr{F}-4\mathbf{d}, \quad \mathscr{S}^2 = \mathscr{F}^2/4d^2-4\,.$$

Alternatively, of course, $\mathbf{Q}$ may be found directly by projecting $2a$ on to $\bar{2}a$, as described above. In the case of the operative twinning plane K_1, we write $\mathscr{F} = \mathscr{F}_0$, $\mathbf{Q} = \mathbf{Q}_0$: our results show that η_2, η_1 have the directions of $\mathscr{F}_0$, $\mathbf{Q}_0$ respectively.

In the diamond structure,

$$\mathbf{E} = [\tfrac{1}{2}, \tfrac{1}{2}, 0], \quad E^2 = \tfrac{1}{2};$$

also

(i) $1/d^2 = h^2+k^2+l^2$ if h, k, l are all odd,
(ii) $1/d^2 = 4(h^2+k^2+l^2)$ if h, k, l are not all odd.

Accordingly, setting $\mathscr{S} = 1$, the inequality assumes the form

(i) $h^2+k^2+l^2 < 40$ if h, k, l are all odd,
(ii) $h^2+k^2+l^2 < 10$ if h, k, l are not all odd.

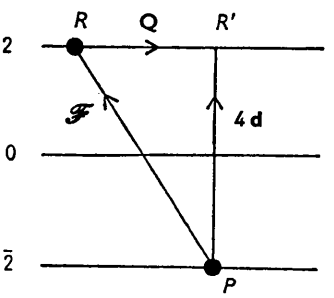

Fig. 2.

Table 2

hkl	$h^2+k^2+l^2$	$\mathscr{F}$	$\mathscr{S}$	hkl	$h^2+k^2+l^2$	$\mathscr{F}$	$\mathscr{S}$
111	3	$\frac{3}{2}, \frac{3}{2}, 1$	$1/2\sqrt{2}$	100	1	2, 0, 0	0
113	11	$\frac{1}{2}, \frac{1}{2}, 1$	$1/2\sqrt{2}$	110	2	1, 1, 0	0
133	19	$1, \frac{1}{2}, \frac{1}{2}$	$5/2\sqrt{2}$	120	5	0, 1, 0	1
115	27	$1, \frac{1}{2}, \frac{1}{2}$	$7/2\sqrt{2}$	112	6	0, 0, 1	$\sqrt{2}$
135	35	$0, \frac{1}{2}, \frac{1}{2}$	$\sqrt{3}/2\sqrt{2}$	122	9	$0, \frac{1}{2}, \frac{1}{2}$	$1/\sqrt{2}$

The possibilities to be considered are set forth in Table 2. From this, and similar tables appropriate to other cases, we deduce the results quoted in the introduction.

The conjugate to the modes (6) and (12) have never been reported operative, but both planes in question happen to function as slip planes. It could be argued that too much significance need not be attached to this effect, since the b.c.c. (112) plane functions both as a slip and as a twinning plane. The argument is not conclusive, though, for it has been pointed out by Chalmers & Martius (1952) that slip on the system (121) $[1\bar{1}1]$ may be resolved into slip of equal amounts on the systems (110) $[1\bar{1}1]$, (011) $[1\bar{1}1]$—an interpretation consistent with the zigzag nature of the surface traces often observed with {112} slip. Accepting the view that the b.c.c. (112) plane is primarily a twinning plane, there are no exceptions to the rule, most strikingly exemplified by the f.c.c. {111} system, that twinning is inhibited by slip. The physical significance of the rule, and of the 'least shear' criterion, is most probably to be understood in terms of the theory of dislocations, but this aspect falls outside the scope of the present analysis.

APPENDIX

By definition, the translation $\mathbf{T}'$ carries plane $1a$ directly over $\bar{1}a$. Accordingly, if $2\mathbf{t}_{aa}$ is the shift* from $\bar{1}a$ to $1a$, we have,

$$2\mathbf{t}_{aa}+\mathbf{T}' = \mathbf{L} \qquad (1)$$

where $\mathbf{L}$ is a lattice vector parallel to K_1. Multiplying by n gives

$$2n\mathbf{t}_{aa}+n\mathbf{T}' = n\mathbf{L}; \qquad (2)$$

hence, noting that $2n\mathbf{t}_{aa}$ is the shift from $\bar{n}a$ to na, and that $n\mathbf{L}$ is a lattice vector parallel to K_1, equation (2) shows that $n\mathbf{T}'$ carries na directly over $\bar{n}a$ (and hence also nb directly over $\bar{n}b$).

By definition, the translations $\mathbf{T}+\mathbf{t}$, $\mathbf{T}-\mathbf{t}$ carry $1a$, $1b$ directly over $\bar{1}b$, $\bar{1}a$ respectively. Accordingly, if $\mathbf{t}_{ab}$ is the shift from $1a$ to $1b$, and $2\mathbf{t}_{bb}$ $(= 2\mathbf{t}_{aa})$ is the shift from $\bar{1}b$ to $1b$, we have

$$(2\mathbf{t}_{bb}-\mathbf{t}_{ab})+(\mathbf{T}+\mathbf{t}) = \mathbf{L}_a\,, \qquad (3)$$

$$(2\mathbf{t}_{aa}+\mathbf{t}_{ab})+(\mathbf{T}-\mathbf{t}) = \mathbf{L}_b\,, \qquad (4)$$

where $\mathbf{L}_a$, $\mathbf{L}_b$ are lattice vectors parallel to K_1. Adding (3) and (4) gives

$$4\mathbf{t}_{aa}+2\mathbf{T} = \mathbf{L}_a+\mathbf{L}_b; \qquad (5)$$

hence, bearing in mind that $4\mathbf{t}_{aa}$ is the shift from $\bar{2}a$ to $2a$, and that $\mathbf{L}_a+\mathbf{L}_b$ is a lattice vector parallel to K_1, equation (5) shows that $2\mathbf{T}$ carries $2a$ directly over $\bar{2}a$. Multiplying (5) by n shows that $2n\mathbf{T}$ carries $2na$ directly over $\bar{2}na$ (and hence also $2nb$ directly over $\bar{2}nb$).

Multiplying (3) and (4) by n, and rearranging terms, we obtain

$$(2n\mathbf{t}_{bb}-\mathbf{t}_{ab})+n\mathbf{T}+\mathbf{t}_n = n\mathbf{L}_a\,, \qquad (6)$$

$$(2n\mathbf{t}_{aa}+\mathbf{t}_{ab})+n\mathbf{T}-\mathbf{t}_n = n\mathbf{L}_b\,, \qquad (7)$$

where $\mathbf{t}_n = n\mathbf{t}-(n-1)\mathbf{t}_{ab}$. Noting that $2n\mathbf{t}_{bb}-\mathbf{t}_{ab}$, $2n\mathbf{t}_{aa}+\mathbf{t}_{ab}$ are the shifts from $\bar{n}b$, $\bar{n}a$ to na, nb respectively, equations (6) and (7) show that na, nb may become the images of $\bar{n}b$, $\bar{n}a$ by undergoing a common translation $n\mathbf{T}$ accompanied by horizontal reshuffles $\mathbf{t}_n$, $-\mathbf{t}_n$. This result holds for all values of n, but when n is even the interchange mechanism of the preceding paragraph is more likely. Evidently, $\mathbf{t}_n$ may be replaced by $(\mathbf{t}_n-\mathbf{L}_n)$, where $\mathbf{L}_n$ is any lattice vector parallel to K_1; on choosing $\mathbf{L}_n$ suitably, we may arrange for $|\mathbf{t}_n-\mathbf{L}_n|$ not to exceed an interatomic spacing along the most-close-packed lattice direction of K_1.

* The shift $2\mathbf{t}_{aa}$ may be defined as the component, parallel to $\bar{1}a$, of the vector joining a lattice point of $\bar{1}a$ to the nearest neighbouring lattice point of $1a$. Similarly for the shifts $2\mathbf{t}_{bb}$, $\mathbf{t}_{ab}$ mentioned subsequently.

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