결정미소역학 (Crystal Mechanics)

Lecture 10 – Mechanical Twinning

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deformation twinning



Before and after deformation twinning

Type I twin can be visualized as simply a mirror image of the matrix, obtained with a hypothetical mirror situated in a characteristic crystallographic plane. The orientation of the twin may be visualized by imagining the matrix to be rotated by 180° about the pole of the composition plane. *Type II twin* may be thought of as having an orientation that would be obtained by rotating the matrix 180° about a characteristic axis, η_1 .

Deformation twins in Mo - 35%Re



unetched

etched



Geometry of mechanical twinning

Change in shape of hemisphere due to deformation twinning



Diagram showing how sphere is converted into ellipsoid by deformation twinning



The twinning elements



Diagram showing twinning elements consisting of planes K_1 and K_2 and directions η_1 and η_2

The twinning elements are not all independent



Twinning elements

Structure	K_1	<i>K</i> ₂	η_1	η_2	γ	
Fcc	(111)	(1 1-1)	[1 1-2]	[112]	$1/\sqrt{2}$	
Bcc	(112)	(-1-1 2)	[-1-1 1]	[111]	$1/\sqrt{2}$	
Нср						
Zn,Cd,Co,Mg, Zr,Ti,Be	(1 0-1 2)	(1 0-1-2)	[-1011]	[1 0-1 1]	$\frac{\left(c/a\right)^2 - 3}{\sqrt{3}(c/a)}$	
Co Re Zr Zr Graphite	$(1 1-2 1) \\ (1 1-2 1) \\ (1 1-2 1) \\ (1 1-2 2) \\ (1 1-2 1) $	(0001) (0001) (0001) (1 1-2 4) (0001)	[1 1-2-6] [1 1-2-6] [1 1-2-6] [1 1-2-3] [1 1-2-6]	[1 1-2 0] [1 1-2 0] [1 1-2 0] [2 2-4 3] [1 1-2 0]	- 0.63 0.23 -	
Mg	(1 0-1 1)	(-1013)	[-1012]	[3 0-3 2]	0.14	
Ti Ti	(1 1-2 2) (10-11)	(1 1-2 4) (-1013)	[1 1-2-3] [-1012]	[2 2-4 3] [3 0-3 2]	0.22 0.1	
α-U	(130)	(1-1 0)	[3-1 0]	[110]	0.299	
(orthorhombic)	(1-7 2)	(112)	[312]	[3-7 2]	0.228	
Fct	(101)	(1 0-1)	[1 0-1]	[101]	(c/a)-(a/c)	



twinning on atomic scale

Sketch of atomic positions in (111) plane of fcc crystal; atoms marked "A" all lie in same plane while those marked "B" and "C" lie in adjacent parallel planes. Vector BC=(1/6)[1 1 -2]





Diagram showing how stacking sequence of (111) planes in fcc crystal is changed by deformation twinning



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Stacking sequence of {112} planes in bcc crystal. (a) Two unit cells showing positions of atoms in (1-1 2) planes. (b) Traces of (1-1 2) planes on (110) projection: Atom sites marked by circles lie in plane of diagram; those marked by squares lie $a/\sqrt{2}$ above and below. (c) Atomic sites in (112) plane; sites marked "A", "B", "C", "D", "E" and "F" lie in successive (112) planes



stacking sequence of {112} planes in bcc crystal is changed by deformation twinning



Stacking sequence of {112} planes in B.C.C crystal

Transformation of crystallographic directions by twinning





Transformation of crystallographic directions by twinning

Coordinate axes x_i' of which x_3' is normal to composition



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		x_1	X_2	x_3	
	x'_1	<i>a</i> ₁₁	<i>a</i> ₁₂	<i>a</i> ₁₃	
	x'_2	a_{21}	<i>a</i> ₂₂	<i>a</i> ₂₃	
	x'_3	<i>a</i> ₃₁	<i>a</i> ₃₂	<i>a</i> ₃₃	
p'_1	7	$\begin{bmatrix} a_{11} \end{bmatrix}$	а	12	<i>a</i> ₁₃

$$\begin{bmatrix} p'_{2} \\ p'_{3} \end{bmatrix} = \begin{bmatrix} a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} p_{2} \\ p_{3} \end{bmatrix}$$

$$\begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{bmatrix} \begin{bmatrix} p_1' \\ p_2' \\ p_3' \end{bmatrix}$$

 $\langle \downarrow \downarrow \rangle$

 $\parallel p_1$

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Transformation of crystallographic directions by twinning¹

Coordinate axes x_i of which x_3 is normal to composition plane of twin



refer the vector to the conventional reference axes x_i within the twin referred to the axes x_i^T .

$$\begin{bmatrix} p_1^T \\ p_2^T \\ p_3^T \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} p_1' \\ p_2' \\ p_3' \end{bmatrix} = \begin{bmatrix} -a_{11} & -a_{12} & -a_{13} \\ -a_{21} & -a_{22} & -a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$

Transformation
matrix $\begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{bmatrix}$

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{bmatrix} \begin{bmatrix} p_1^T \\ p_2^T \\ p_3^T \end{bmatrix} = \begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{bmatrix} \begin{bmatrix} -a_{11} & -a_{12} & -a_{13} \\ -a_{21} & -a_{22} & -a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$

$$= \begin{bmatrix} (2a_{31}^{2} - 1) & 2a_{31}a_{32} & 2a_{31}a_{33} \\ 2a_{32}a_{31} & (2a_{32}^{2} - 1) & 2a_{32}a_{33} \\ 2a_{33}a_{31} & 2a_{33}a_{32} & (2a_{33}^{2} - 1) \end{bmatrix} \begin{bmatrix} p_{1} \\ p_{2} \\ p_{3} \end{bmatrix} \begin{bmatrix} a_{11}^{2} + a_{12}^{2} + a_{13}^{2} = 1 & a_{11}a_{21} + a_{12}a_{22} + a_{13}a_{23} = 0 \\ a_{21}^{2} + a_{22}^{2} + a_{23}^{2} = 1 & a_{11}a_{31} + a_{12}a_{32} + a_{13}a_{33} = 0 \\ a_{31}^{2} + a_{32}^{2} + a_{33}^{2} = 1 & a_{21}a_{31} + a_{22}a_{32} + a_{23}a_{33} = 0 \\ a_{31}^{2} + a_{32}^{2} + a_{33}^{2} = 1 & a_{21}a_{31} + a_{22}a_{32} + a_{23}a_{33} = 0 \\ \end{bmatrix}$$

Suppose that an fcc crystal is stressed along [144], and a thin deformation twin is created with (111) as its plane. Along what direction within the twin does the applied stress act?

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} = \begin{bmatrix} (2a_{31}^2 - 1) & 2a_{31}a_{32} & 2a_{31}a_{33} \\ 2a_{32}a_{31} & (2a_{32}^2 - 1) & 2a_{32}a_{33} \\ 2a_{33}a_{31} & 2a_{33}a_{32} & (2a_{33}^2 - 1) \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$

P:[144]
$$x_3^T = [111]$$
 $a_{31} = a_{32} = a_{33} = 1/\sqrt{3}$

The twin crystal is stressed in the [522] direction.

$$\langle \downarrow \downarrow \rangle$$

A bcc crystal contains a twin with a (112) composition plane, and it is sliced parallel to the (001) plane, and thinned for examination in the electron microscope. Along which plane within the twin has the slice been taken?

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} = \begin{bmatrix} (2a_{31}^2 - 1) & 2a_{31}a_{32} & 2a_{31}a_{33} \\ 2a_{32}a_{31} & (2a_{32}^2 - 1) & 2a_{32}a_{33} \\ 2a_{33}a_{31} & 2a_{33}a_{32} & (2a_{33}^2 - 1) \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$

P:[001]
$$x_3^T = [112]$$

 $a_{31} = 1/\sqrt{6}, \ a_{32} = 1/\sqrt{6}, \ a_{33} = 2/\sqrt{6}$

the (221) plane

Transformation of a vector that is sheared during twinning

Direction of interest in general becomes reoriented by deformation twinning. x_3' is normal to K_1 and x_2' lies parallel to η_1



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The components q_i of the new orientation referred to the matrix axes

$$\begin{bmatrix} q_1' \\ q_2' \\ q_3' \end{bmatrix} = \begin{bmatrix} p_1' \\ p_2' \\ p_3' \end{bmatrix} + \begin{bmatrix} 0 \\ \gamma p_3' \\ 0 \end{bmatrix}$$
$$= \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix} + \gamma \begin{bmatrix} 0 & 0 & 0 \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$
$$= \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} + \gamma a_{31} & a_{22} + \gamma a_{32} & a_{23} + \gamma a_{33} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$



$$\begin{bmatrix} q_1' \\ q_2' \\ q_3' \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} + \gamma a_{31} & a_{22} + \gamma a_{32} & a_{23} + \gamma a_{33} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$

$$\begin{bmatrix} q_1^T \\ q_2^T \\ q_3^T \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} q_1' \\ q_2' \\ q_3' \end{bmatrix}$$



$$\begin{bmatrix} q_1^T \\ q_2^T \\ q_3^T \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} + \gamma a_{31} & a_{22} + \gamma a_{32} & a_{23} + \gamma a_{33} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$
$$\begin{bmatrix} q_1^T \\ q_2^T \\ q_3^T \end{bmatrix} = \begin{bmatrix} -a_{11} & -a_{12} & -a_{13} \\ -a_{21} - \gamma a_{31} & -a_{22} - \gamma a_{32} & -a_{23} - \gamma a_{33} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$

$$\begin{bmatrix} t_1 \\ t_2 \\ t_3 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{bmatrix} \begin{bmatrix} q_1^T \\ q_2^T \\ q_3^T \end{bmatrix}$$

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The orientation component t_k referred to x_k axes

$$\begin{bmatrix} t_1 \\ t_2 \\ t_3 \end{bmatrix} = -\begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix} - \gamma \begin{bmatrix} a_{21}a_{31} & a_{21}a_{32} & a_{21}a_{33} \\ a_{22}a_{31} & a_{22}a_{32} & a_{22}a_{33} \\ a_{23}a_{31} & a_{23}a_{32} & a_{23}a_{33} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix} + 2 \begin{bmatrix} a_{31}a_{31} & a_{31}a_{32} & a_{31}a_{33} \\ a_{32}a_{31} & a_{32}a_{32} & a_{32}a_{33} \\ a_{33}a_{31} & a_{33}a_{32} & a_{33}a_{33} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$

In general, the length and crystallographic character of p are changed by deformation twinning, as may be seen by comparing [p] and [t].

Consider a carbon atom located at the interstitial site (0,0,1/2) within the body centered cubic structure cell. If the crystal undergoes deformation twinning with (112) as the composition plane and [-1-1 1] as the shear direction, in which kind of interstitial site is the carbon atom located after twinning (assuming that the crystal undergoes a homogeneous shear)?



 $P = [0, 0, \frac{1}{2}]$ $X_2' = [-1 - 1 1]$ X₃'=[112] $a_{21} = -1/\sqrt{3}$ $a_{31} = 1/\sqrt{6}$ $a_{22} = -1/\sqrt{3}$ $a_{32} = 1/\sqrt{6}$ $a_{23} = 1/\sqrt{3}$ $a_{23} = 2/\sqrt{6}$

[t] = (1/2, 1/2, 0)



This point is the midpoint of a cube face, which in the bcc lattice x_1 is crystallographically equivalent to the midpoint of a cube edge. We conclude, then, that the crystallographic nature of the interstitial site (0, 0, 1/2) is unchanged by twinning.



$[t] = [1/2 \ 0 \ 0]$

After twinning



[-¹/₄ ¹/₄ ¹/₄]

after twinning it has the coordinates (-1/4, 1/4, 1/4), i.e. directly between the most closely spaced lattice points interstitial atom, so we assume that the carbon atom performs some kind of shuffle during twinning, so as to end up in a conventional interstitial site. Similarly, the (0, 1/2, 0) site is transformed to (1/4, -1/4, 1/4) by twinning.



The deformation due to mechanical twin can be expressed by twinned volume fraction.

