Diffraction contrast imaging

Lecture 12 Part 2

Review: Planar faults
Strain fields - generally
Dislocations
Coherent precipitates

Strain fields

As with planar faults, strain fields also introduce changes in the location of atoms within the crystal

In other words, any strain field introduces an $\vec{R}(\vec{r}_n{}')$, where:

$$\vec{r}_n{}' = \vec{r}_n + \vec{R}_n$$

Location of defective unit cell → $\vec{r}_n{}'$

Regular lattice positions → $\vec{r}_n$

Displacement function → $\vec{R}_n$

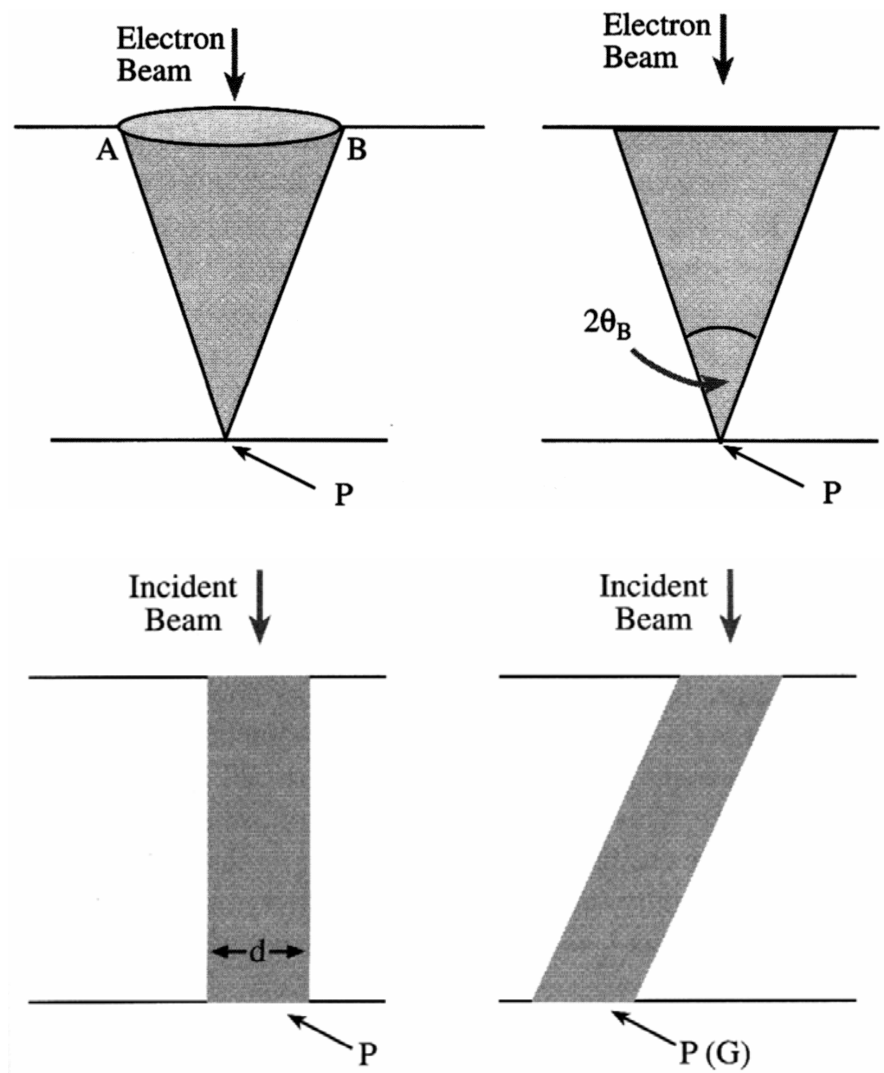
With planar faults, the shift between one lattice and the next is single valued

What happens if the strain field is continuous?

Calculating dislocation contrast

We use the "column approximation"

This is where we said we'd ignore variations in dz with changes in z



Modification of H-W Eqns

Possible to re-write the H-W Eqns in a different form, which incorporates a continuous $\vec{R}(\vec{r}_n{}')$

Use a different substitution of variables than in previous derivation (planar case)

Yields:

$$\frac{d\phi_o}{dz} = \frac{\pi i}{\xi_o}\phi_g$$

and

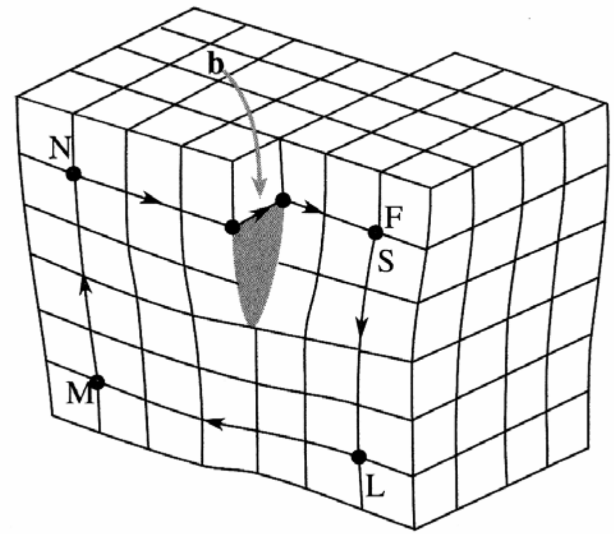
$$\frac{d\phi_g}{dz} = \frac{\pi i}{\xi_g}\phi_o + \left[2\pi i\left(sz + \vec{g}\cdot\frac{d\vec{R}}{dz}\right)\right]\phi_g = \frac{\pi i}{\xi_g}\phi_o + 2\pi i s_R \phi_g$$

$$s_R = sz + \vec{g}\cdot\frac{d\vec{R}}{dz}$$

Dislocations

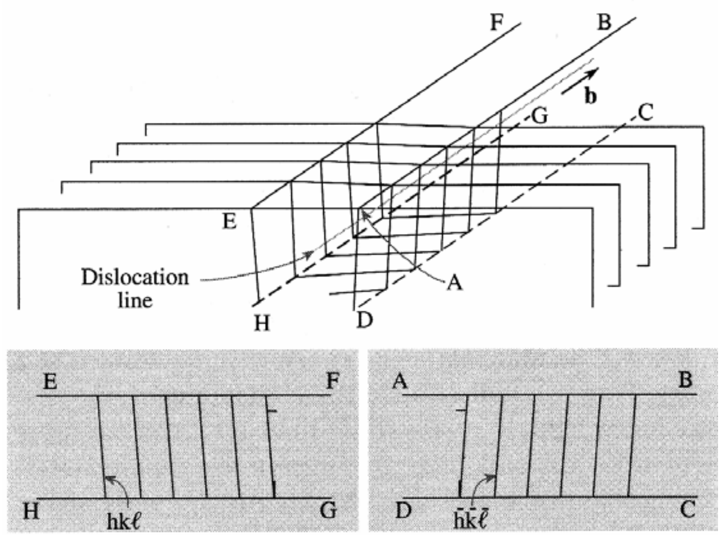
Screw dislocation

- $\vec{b} \parallel \vec{u}$
- Can slip along any plane
- Again, we image the strain field



Mixed dislocation

- $\vec{b}$ neither perpendicular nor parallel to $\vec{u}$
- Thus, each mixed dislocation can be resolved into edge components and screw components



Calculating dislocation contrast

So, divide the sample into narrow columns

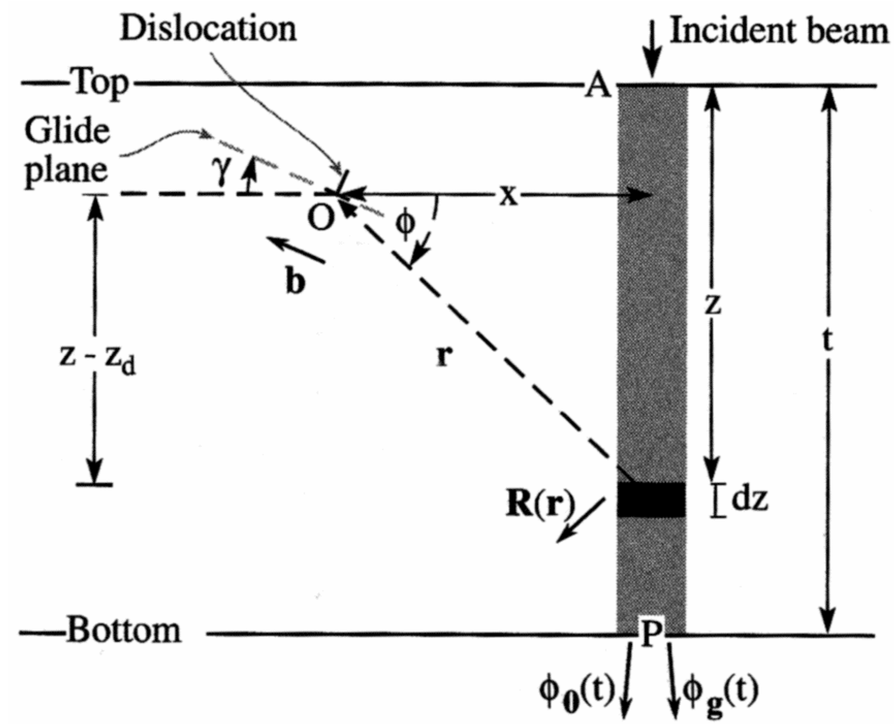
Calculate the amplitude of ϕ_o and ϕ_g for each column

What is R?

- Need to go to elasticity theory
- Find:

$$\vec{R} = \frac{1}{2\pi}\left\{\vec{b}\phi + \frac{1}{4(1-\nu)}\left[\vec{b}_e + \vec{b}\times\vec{u}\left(2(1-2\nu)\ln r + \cos 2\phi\right)\right]\right\}$$

- Or if doing computationally, use anisotropic elasticity theory, or simulation output



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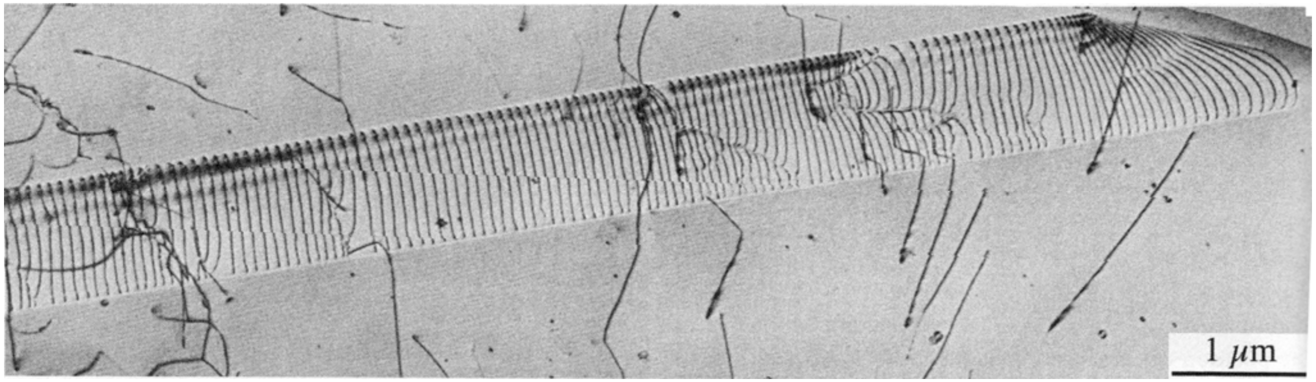
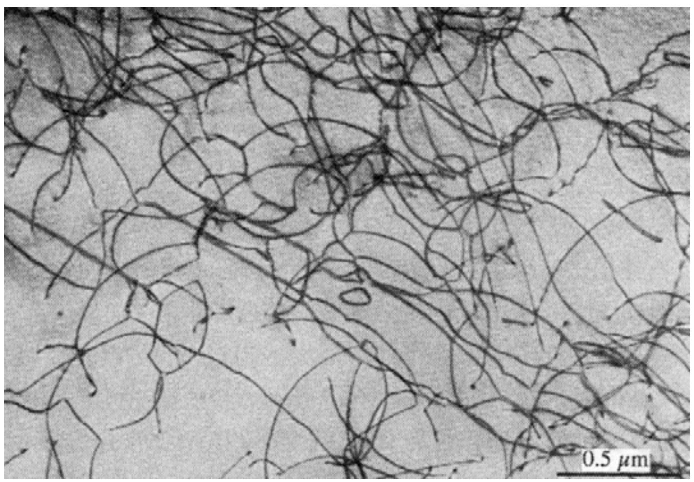
Dislocations interactions & tangles



HVEM Image of slip along an inclined plane



A complex dislocation tangle

Cold rolled alloy

Calculating dislocation contrast

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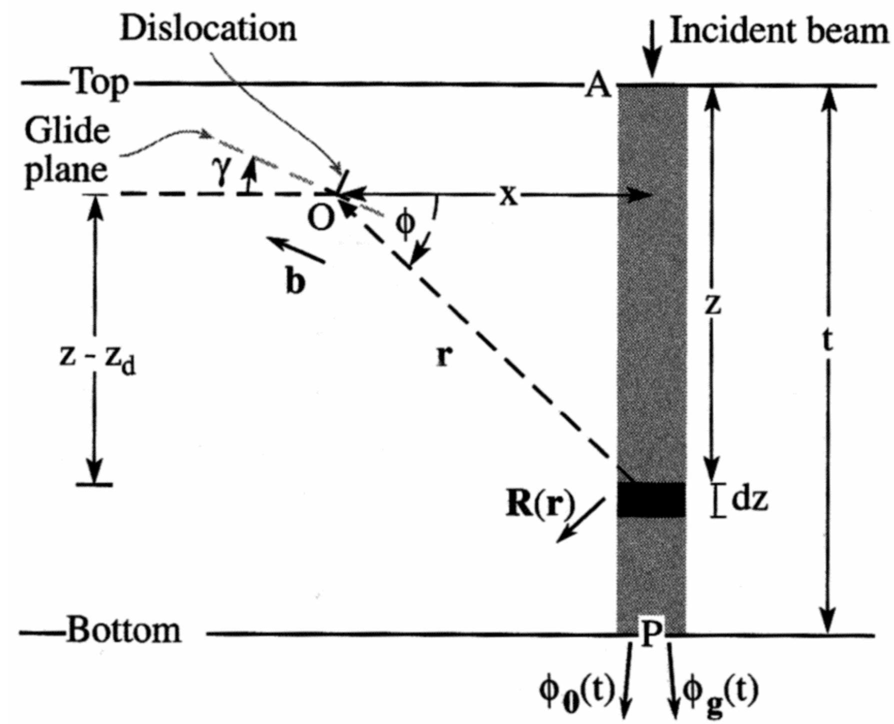

Dislocation contrast

Consider a pure screw dislocation:

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$$\vec{R} = \vec{b}\frac{\phi}{2\pi} = \frac{\vec{b}}{2\pi}\tan\left(\frac{z - z_d}{x}\right)$$

So: $\vec{R} \propto \vec{b}$

Thus: $\vec{g} \cdot \vec{R} \propto \vec{g} \cdot \vec{b}$

"g dot b" contrast

Table 25.1. Different Burgers Vectors and Different Reflections Give Different g·b = *n* Values[a]

g \ b	$\frac{1}{6}[11\bar{2}]$	$\frac{1}{6}[1\bar{2}1]$	$\frac{1}{6}[\bar{2}11]$	$\frac{1}{3}[111]$
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±(200)	± 1/3	± 1/3	± 2/3	± 2/3
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[a]The dislocations all lie on a (111) plane in an fcc material; the beam direction is [011].

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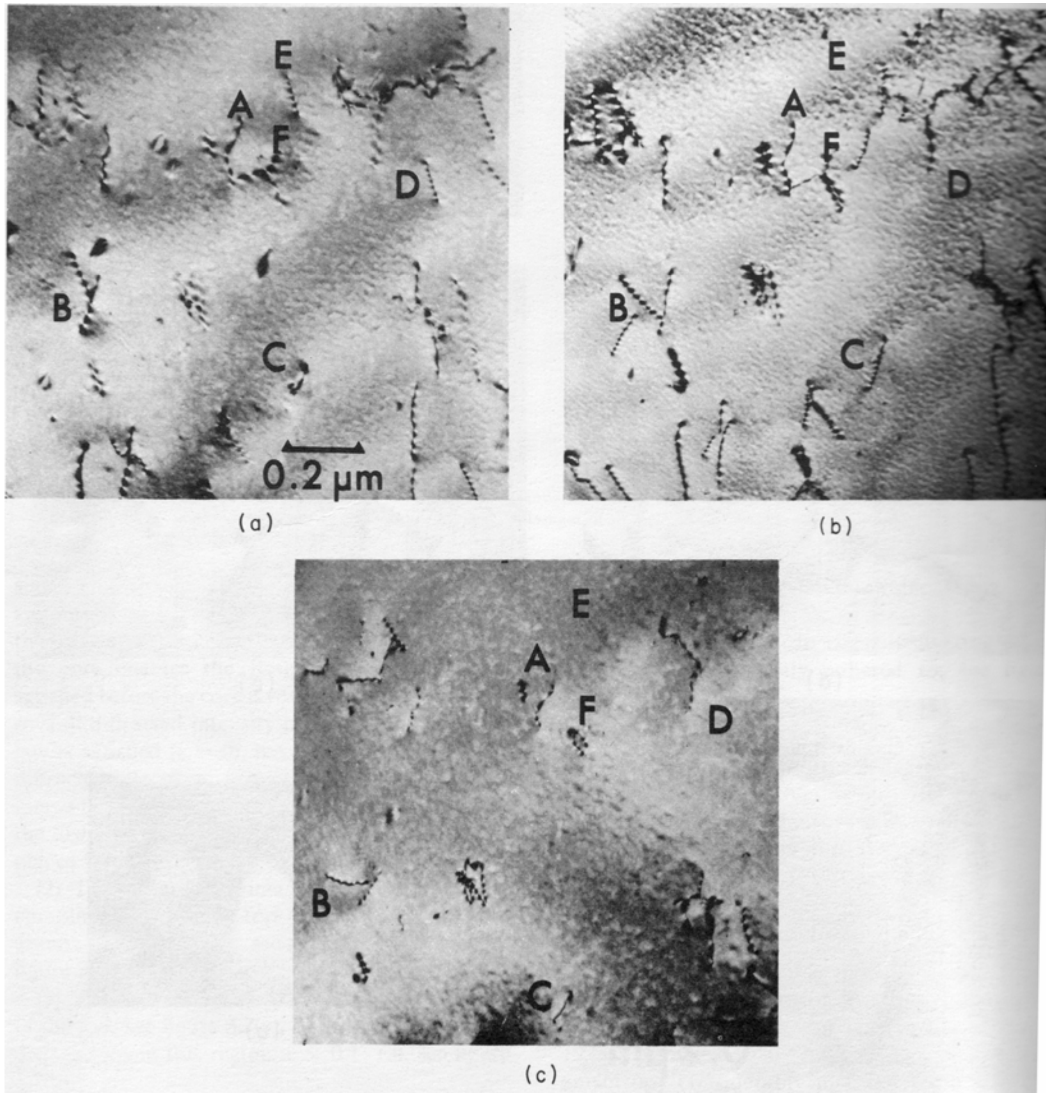

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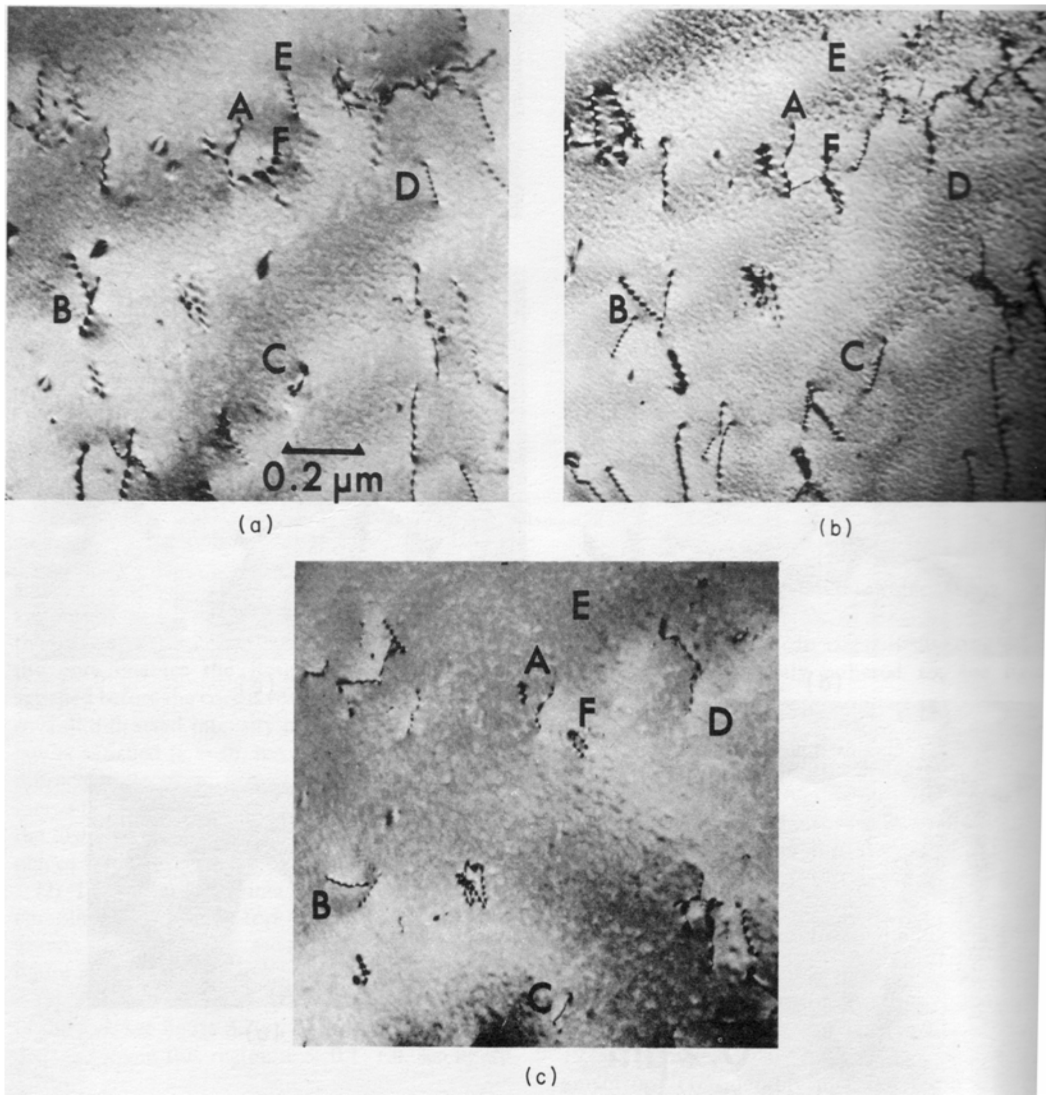


Dislocation contrast

Now for pure edge

$$\vec{b} = \vec{b}_e \;;\; \vec{b}_e \times \vec{u} \neq 0$$

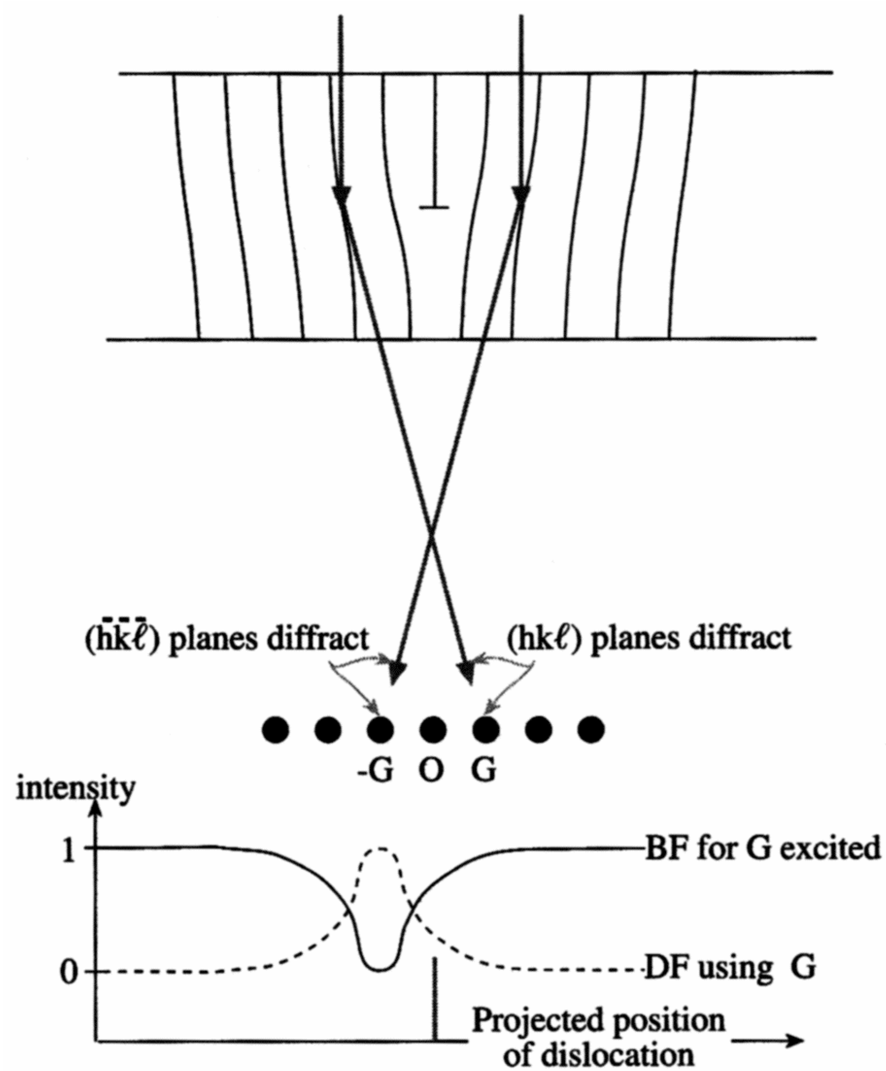
So R has both a $\vec{g} \cdot \vec{b}$ & a $\vec{g} \cdot \vec{b} \times \vec{u}$ term

More on 'g dot b' contrast

Often said that when $\vec{g} \cdot \vec{b} = 0$ the dislocation is 'invisible'

This is because the lattice distortion is on diffracting planes parallel to R

– You won't see it's effect



Dislocation contrast

More to it (unfortunately)

Firstly, what is 'invisible'?

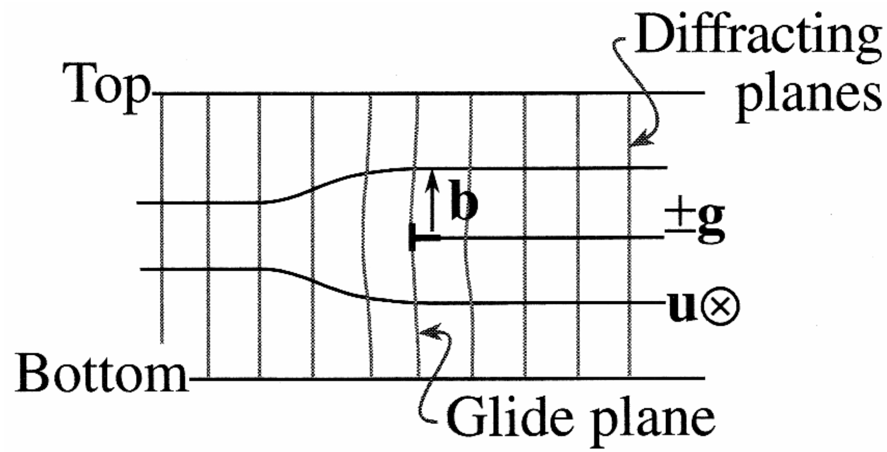
Generally if $\vec{g}\cdot\vec{b} < \frac{1}{3}$ the contrast is faint

More importantly, even if

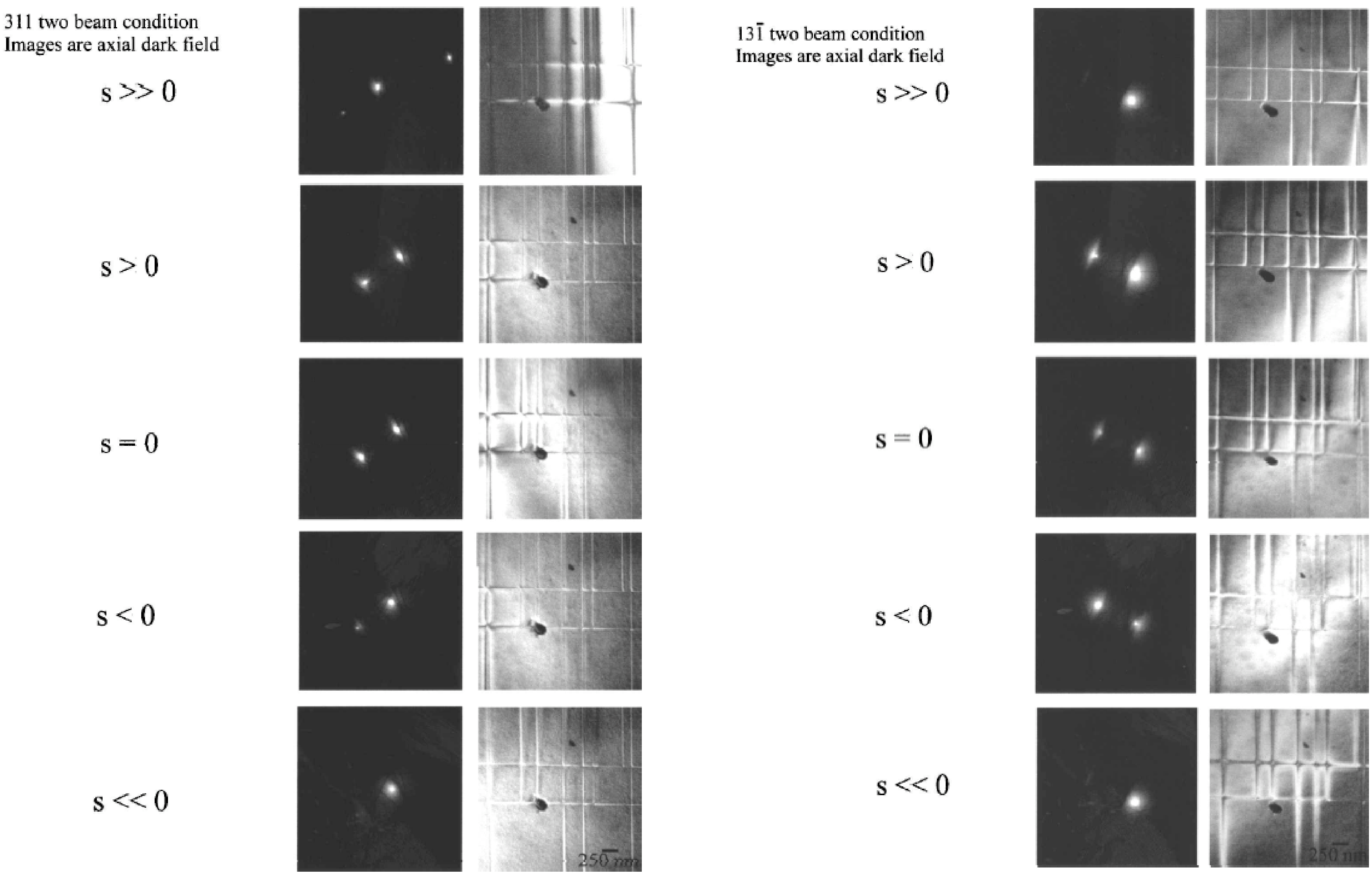
$\vec{g}\cdot\vec{b} = 0$ can have $\vec{g}\cdot\vec{b}\times\vec{u} \neq 0$

So, really need to find conditions where both $\vec{g}\cdot\vec{b} = 0$ & $\vec{g}\cdot\vec{b}\times\vec{u} = 0$ if possible

May have to settle for $\vec{g}\cdot\vec{b} = 0$ & $\vec{g}\cdot\vec{b}\times\vec{u} \leq 0.64$



Surface effects & interfaces



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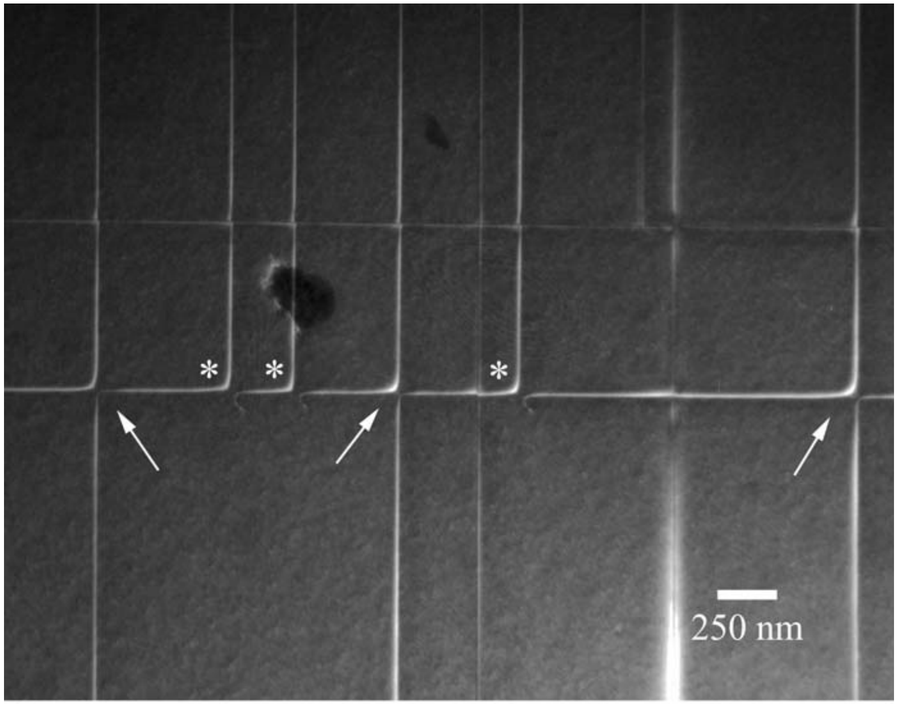
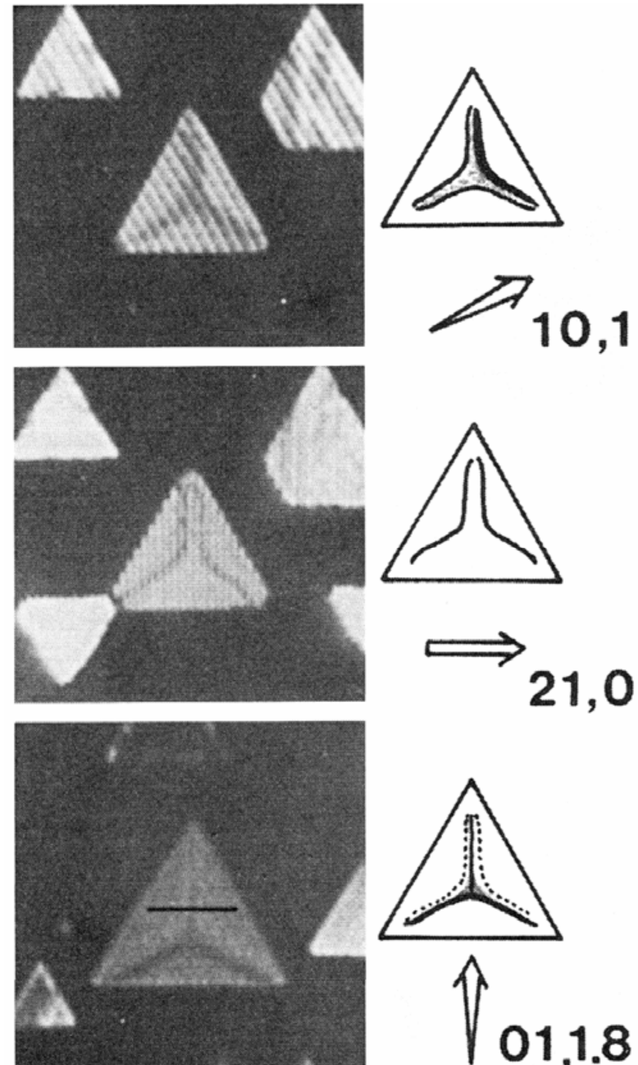
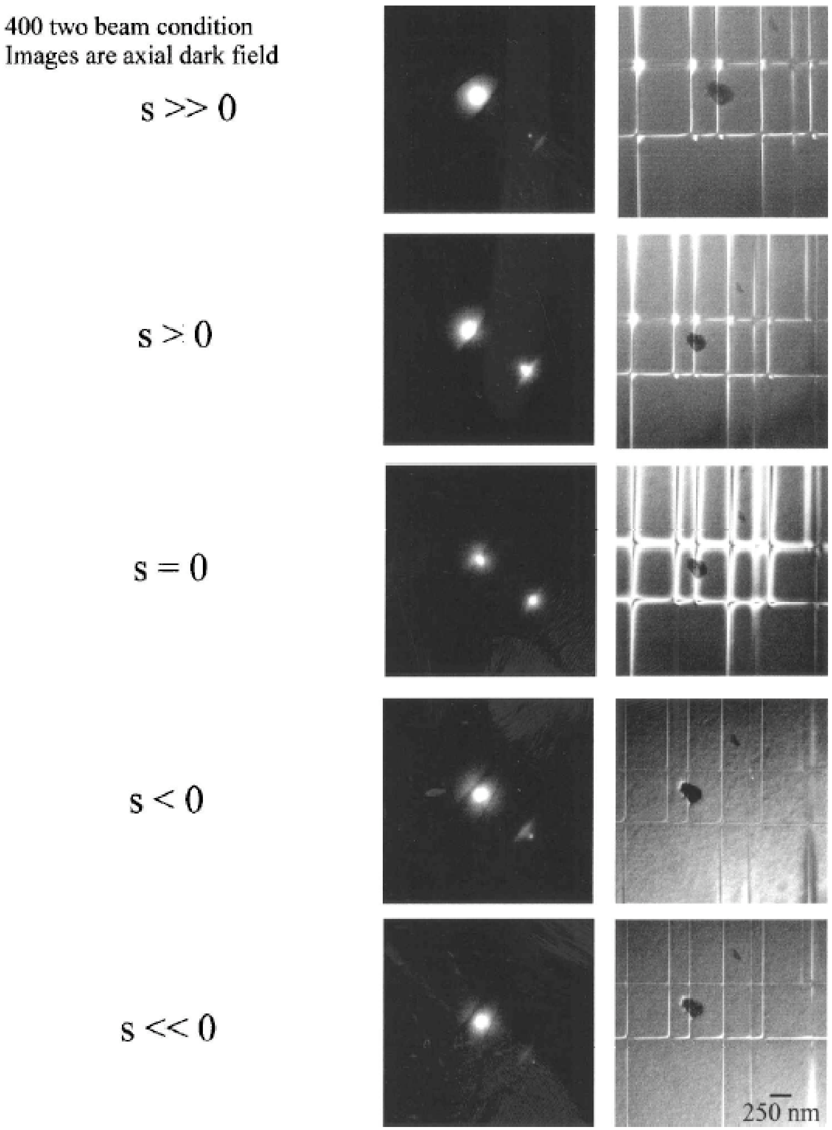


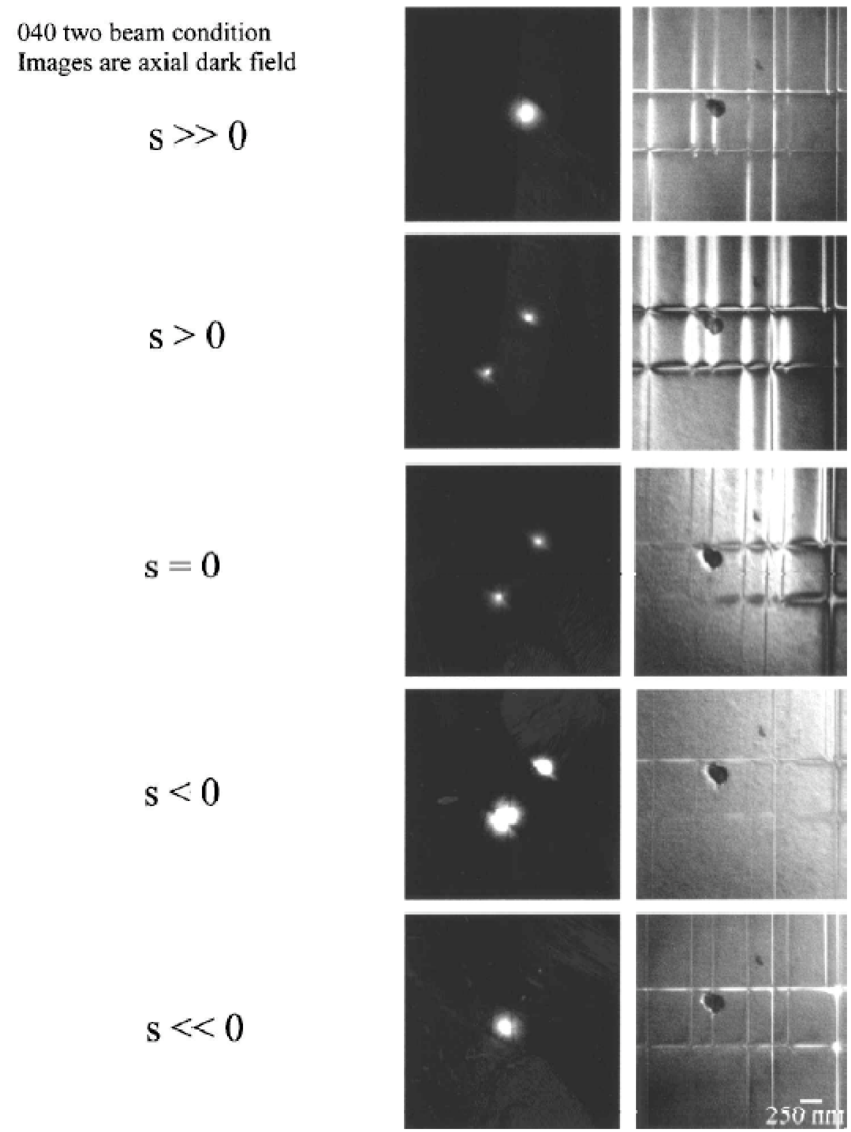


Interface misfit dislocations are a common class of defects to image

Be aware of surface relaxation effects (i.e $\vec{g} \cdot \vec{b} \times \vec{u} \neq 0$)

Surface effects & interfaces





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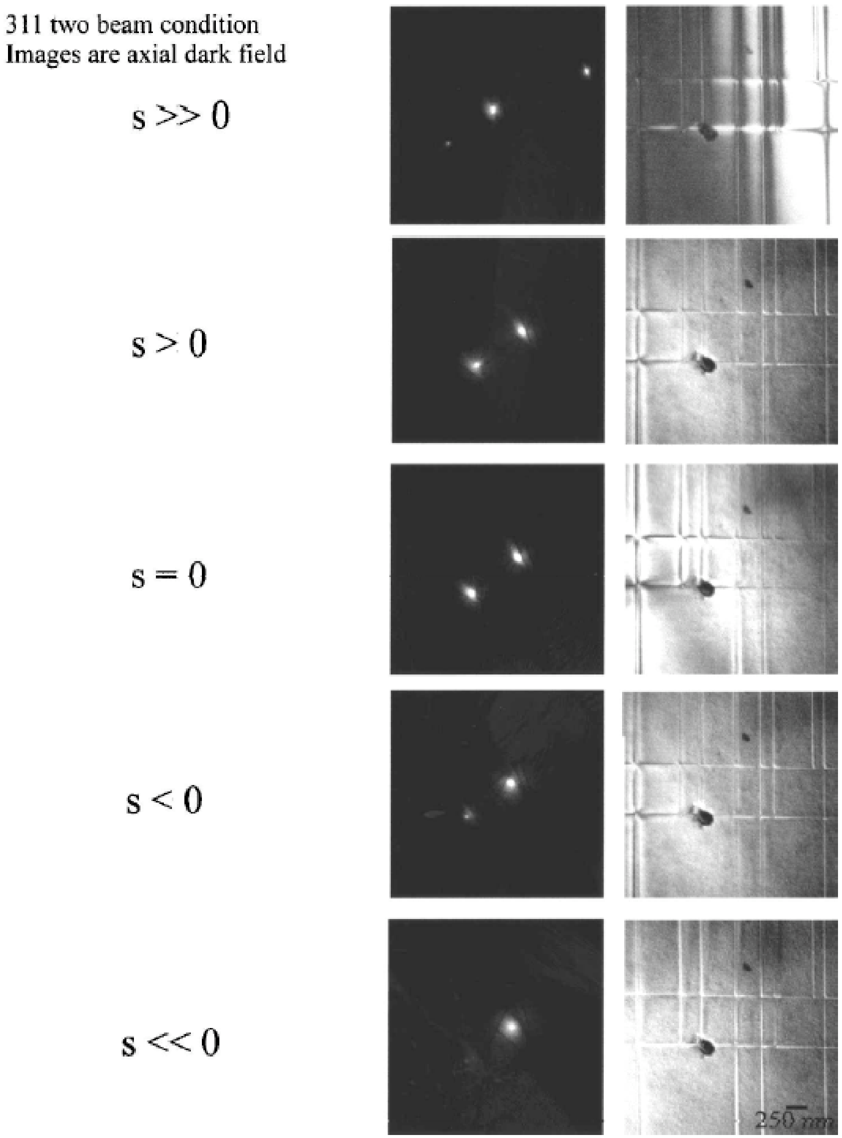

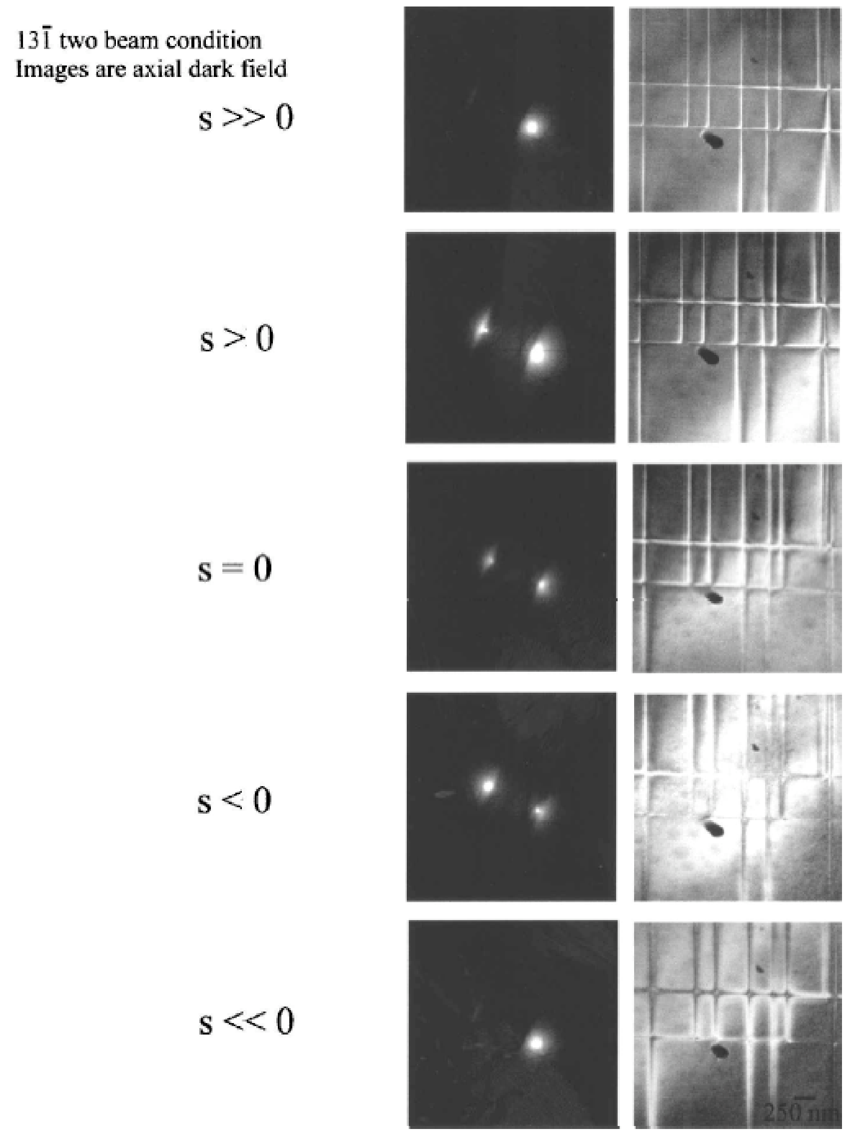

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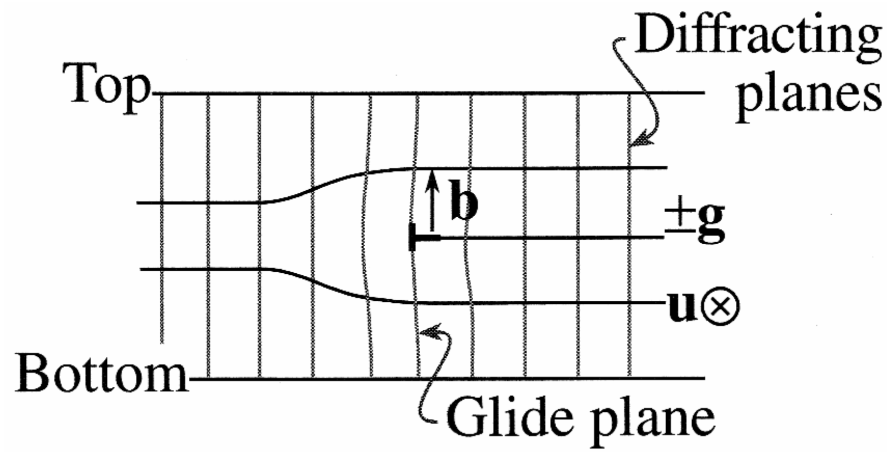

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Surface effects & interfaces

400 two beam condition
Images are axial dark field

s >> 0

s > 0

s = 0

s < 0

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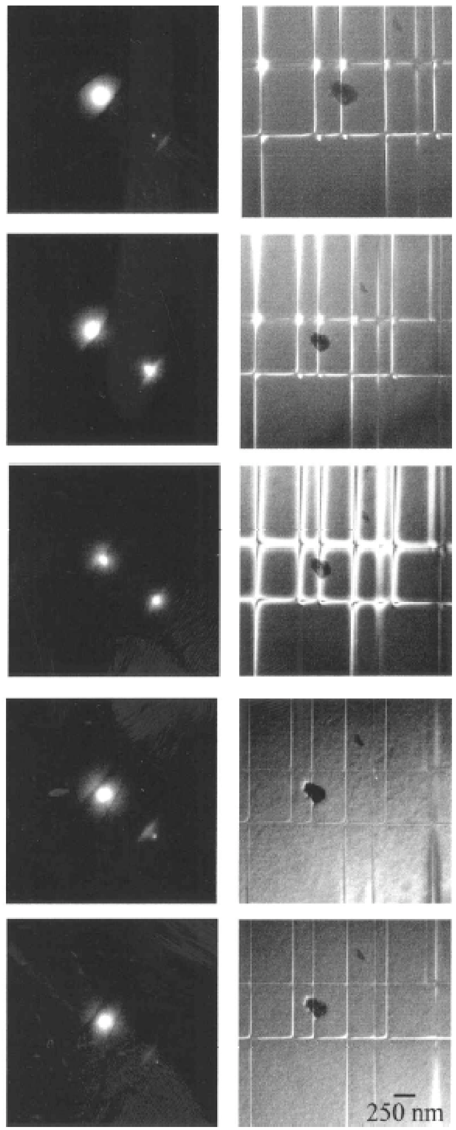

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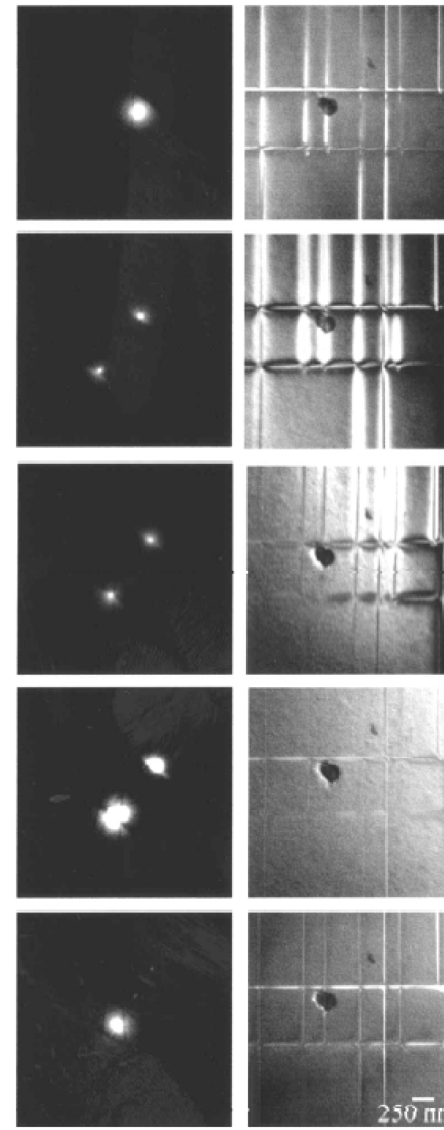
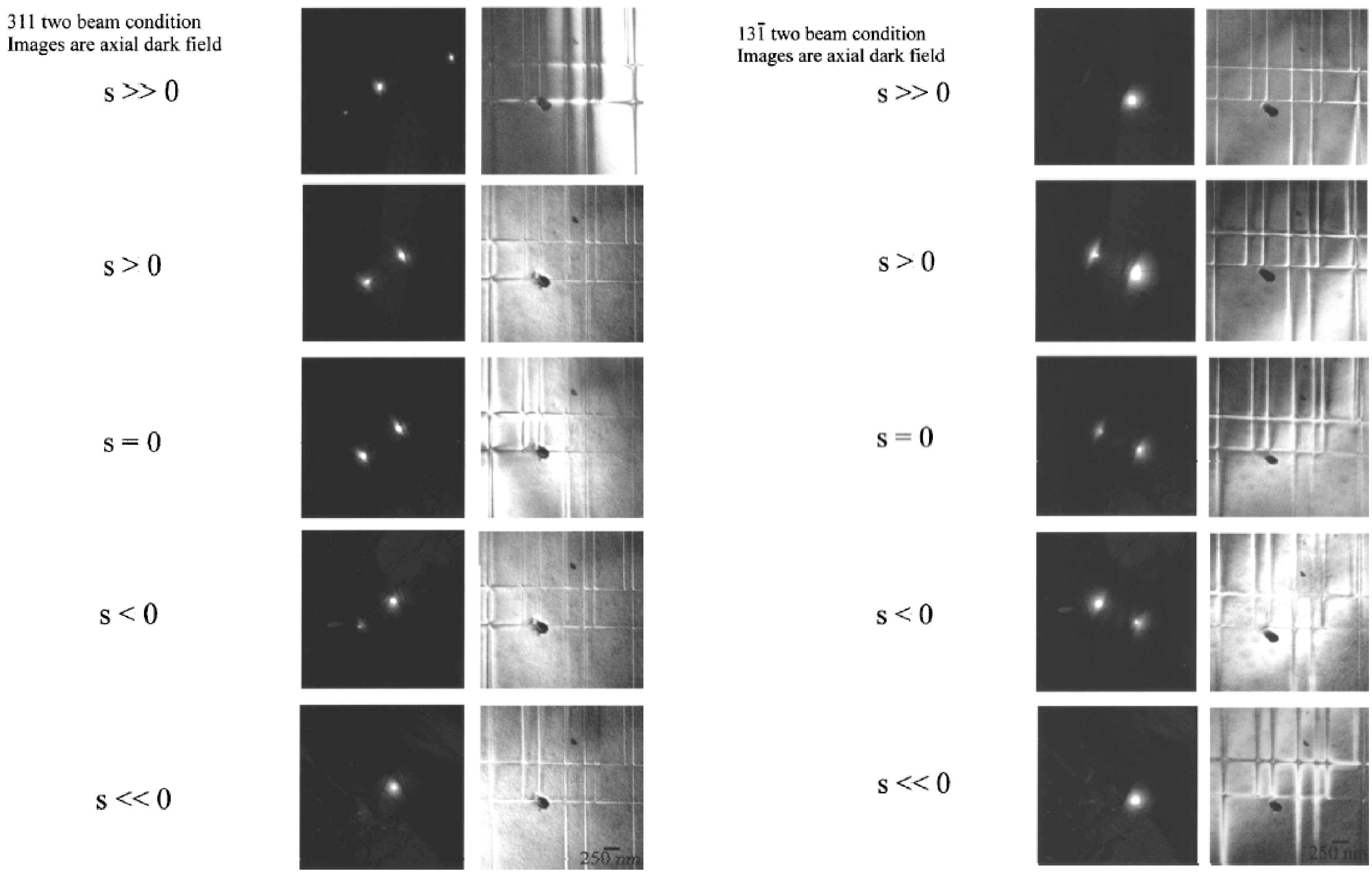


Surface effects & interfaces



Surface effects & interfaces

An example: Interfacial misfit dislocations in SiGe

For details, see Stach, et al, Phil Mag <u>80</u>, 2000.

Table A 1. Diffraction conditions for which $\mathbf{g}\cdot\mathbf{b} = 0$ is true for at least one Burgers vector.

g	$\mathbf{b} = \frac{a}{2}[0\bar{1}1]$	$\mathbf{b} = \frac{a}{2}[\bar{1}01]$	$\mathbf{b} = \frac{a}{2}[011]$	$\mathbf{b} = \frac{a}{2}[101]$
400	0	2	0	2
040	2	0	2	0
311	0	1	1	2
$13\bar{1}$	2	1	1	0

Table A 2. List of $|\mathbf{g}\cdot\mathbf{b}|$, $|\mathbf{g}\cdot\mathbf{b}\times\mathbf{u}|$ and m for each of the slip systems for the four diffraction conditions shown in Table A 1.

g	$\lvert\mathbf{g}\cdot\mathbf{b}\rvert$	$\lvert\mathbf{g}\cdot\mathbf{b}\times\mathbf{u}\rvert$	$m = \frac{1}{8}\lvert\mathbf{g}\cdot\mathbf{b}\times\mathbf{u}\rvert$
		$\mathbf{b},(a/2)[0\bar{1}1]; \mathbf{u},[\bar{1}10]$	
400	0	$\sqrt{2}$	0.18
040	2	$\sqrt{2}$	0.18
311	0	$5/2\sqrt{2}$	0.22
$13\bar{1}$	1	$3/2\sqrt{2}$	0.13
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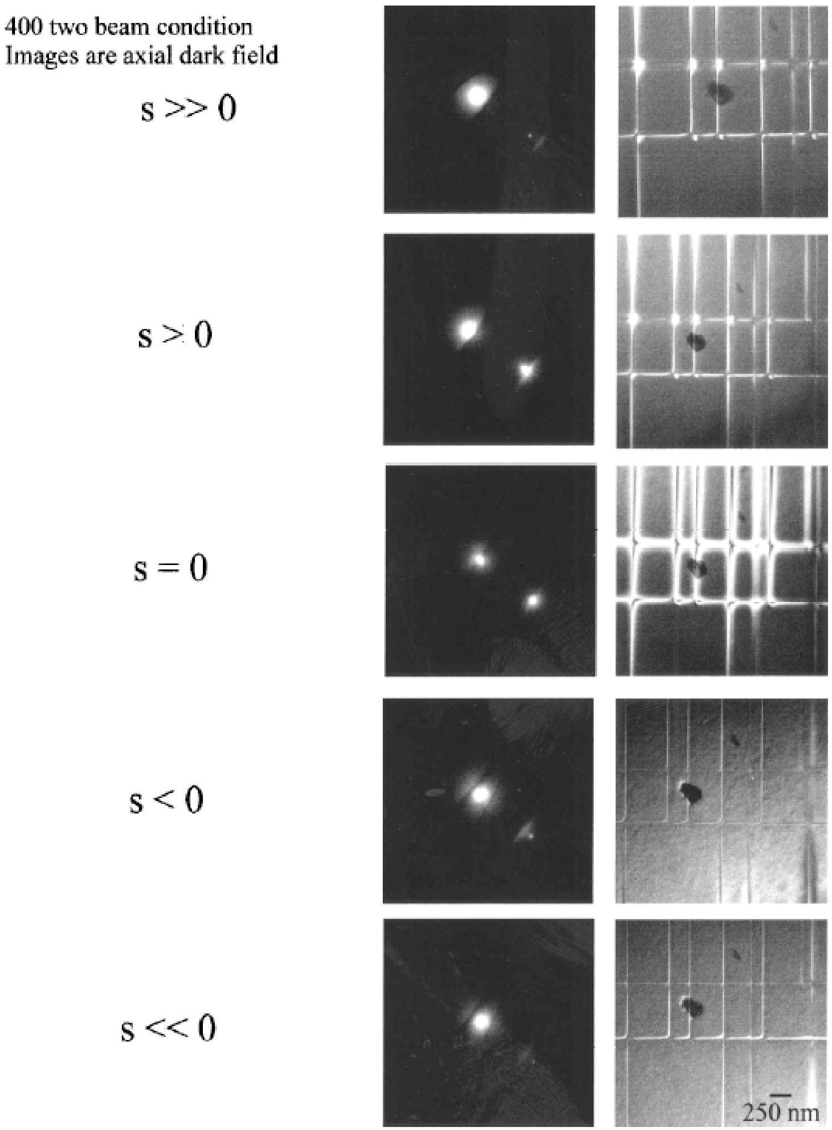

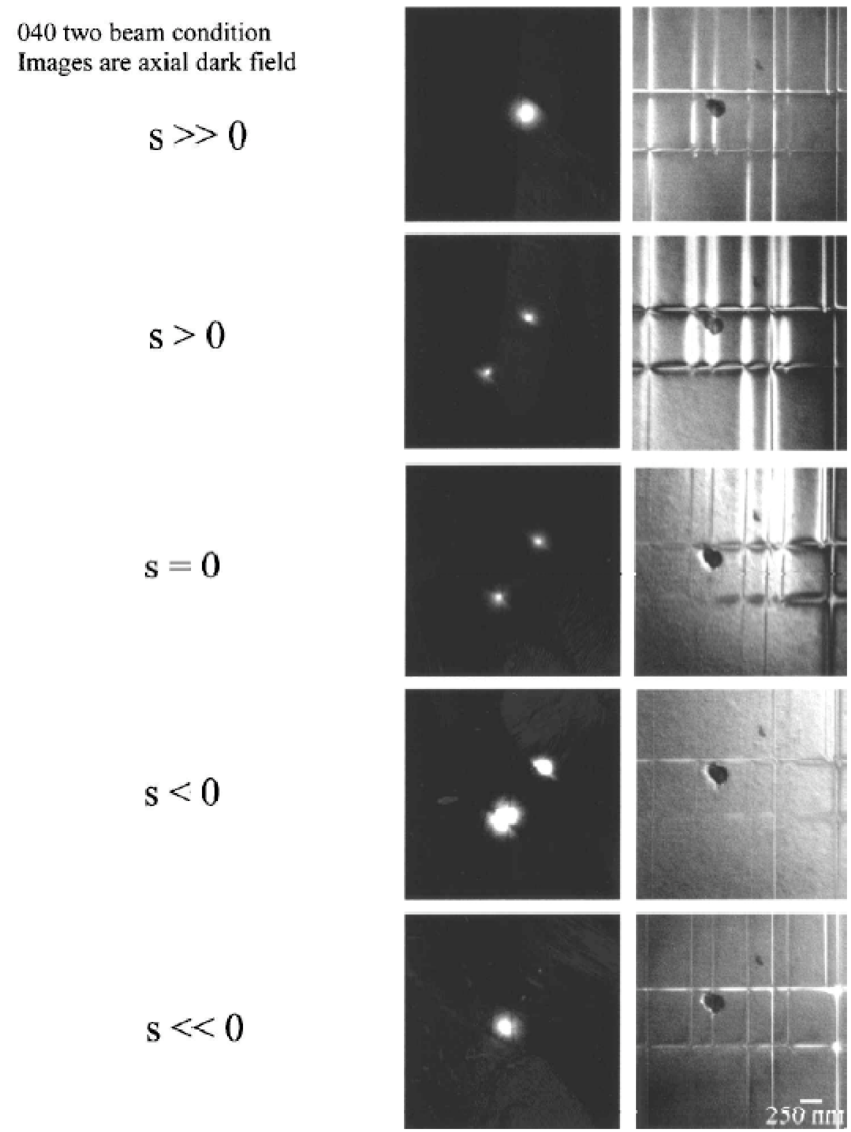

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040	2	$\sqrt{2}$	0.18
311	0	$1/2\sqrt{2}$	0.05
$13\bar{1}$	1	$1/2\sqrt{2}$	0.05
		$\mathbf{b},(a/2)[\bar{1}01]$; $\mathbf{u},[110]$	
400	2	$\sqrt{2}$	0.18
040	0	$\sqrt{2}$	0.18
311	1	$3/2\sqrt{2}$	0.13
$13\bar{1}$	1	$3/2\sqrt{2}$	0.13
		$\mathbf{b},(a/2)[011]$; $\mathbf{u},[110]$	
400	0	$\sqrt{2}$	0.18
040	2	$\sqrt{2}$	0.18
311	1	$3/2\sqrt{2}$	0.13
$13\bar{1}$	1	$3/2\sqrt{2}$	0.13
		$\mathbf{b},(a/2)[101]$; $\mathbf{u},[110]$	
400	2	$\sqrt{2}$	0.18
040	0	$\sqrt{2}$	0.18
311	2	$1/2\sqrt{2}$	0.05
$13\bar{1}$	0	$1/2\sqrt{2}$	0.05

Dislocation contrast

Consider a pure screw dislocation:

$$\vec{b}_e = 0 \;\; ; \;\; \vec{b} \times \vec{u} = 0$$

$$\vec{R} = \vec{b}\frac{\phi}{2\pi} = \frac{\vec{b}}{2\pi}\tan\left(\frac{z - z_d}{x}\right)$$

So: $\vec{R} \propto \vec{b}$

Thus: $\vec{g}\cdot\vec{R} \propto \vec{g}\cdot\vec{b}$

"g dot b" contrast

Table 25.1. Different Burgers Vectors and Different Reflections Give Different g·b = *n* Values[a]

g \ b	$\frac{1}{6}[11\bar{2}]$	$\frac{1}{6}[1\bar{2}1]$	$\frac{1}{6}[\bar{2}11]$	$\frac{1}{3}[111]$
$\pm(1\bar{1}1)$	± 1/3	± 2/3	± 1/3	± 1/3
$\pm(\bar{1}\bar{1}1)$	± 2/3	± 1/3	± 1/3	± 1/3
$\pm(0\bar{2}2)$	± 1	± 1	0	0
$\pm(200)$	± 1/3	± 1/3	± 2/3	± 2/3
$\pm(3\bar{1}1)$	0	± 1	± 1	± 1
$\pm(\bar{3}\bar{1}1)$	± 1	0	± 1	± 1

[a]The dislocations all lie on a (111) plane in an fcc material; the beam direction is [011].

Surface effects & interfaces

An example: Interfacial misfit dislocations in SiGe

For details, see Stach, et al, Phil Mag <u>80</u>, 2000.

Table A 2. List of $|\mathbf{g}\cdot\mathbf{b}|$, $|\mathbf{g}\cdot\mathbf{b}\times\mathbf{u}|$ and m for each of the slip systems for the four diffraction conditions shown in Table A 1.

$\mathbf{g}$	$\lvert\mathbf{g}\cdot\mathbf{b}\rvert$	$\lvert\mathbf{g}\cdot\mathbf{b}\times\mathbf{u}\rvert$	$m=\frac{1}{8}\lvert\mathbf{g}\cdot\mathbf{b}\times\mathbf{u}\rvert$	
		$\mathbf{b},(a/2)[0\bar{1}1];\ \mathbf{u},[\bar{1}10]$		
400	0	$\sqrt{2}$	0.18	
040	2	$\sqrt{2}$	0.18	
311	0	$5/2\sqrt{2}$	0.22	
$13\bar{1}$	1	$3/2\sqrt{2}$	0.13	
		$\mathbf{b},(a/2)[\bar{1}01];\ \mathbf{u},[\bar{1}10]$		
400	2	$\sqrt{2}$	0.18	
040	0	$\sqrt{2}$	0.18	
311	1	$5/2\sqrt{2}$	0.22	
$13\bar{1}$	1	$3/2\sqrt{2}$	0.13	
		$\mathbf{b},(a/2)[011];\ \mathbf{u},[\bar{1}10]$		
400	0	$\sqrt{2}$	0.18	
040	2	$\sqrt{2}$	0.18	
311	1	$3/2\sqrt{2}$	0.13	
$13\bar{1}$	1	$5/2\sqrt{2}$	0.22	
		$\mathbf{b},(a/2)[101];\ \mathbf{u},[\bar{1}10]$		
400	2	$\sqrt{2}$	0.18	
040	0	$\sqrt{2}$	0.18	
311	2	$3/2\sqrt{2}$	0.13	
$13\bar{1}$	0	$5/2\sqrt{2}$	0.22	
		$\mathbf{b},(a/2)[0\bar{1}1];\ \mathbf{u},[110]$		
400	0	$\sqrt{2}$	0.18	
040	2	$\sqrt{2}$	0.18	
311	0	$1/2\sqrt{2}$	0.05	←
$13\bar{1}$	1	$1/2\sqrt{2}$	0.05	←
		$\mathbf{b},(a/2)[\bar{1}01];\ \mathbf{u},[110]$		
400	2	$\sqrt{2}$	0.18	
040	0	$\sqrt{2}$	0.18	
311	1	$3/2\sqrt{2}$	0.13	
$13\bar{1}$	1	$3/2\sqrt{2}$	0.13	
		$\mathbf{b},(a/2)[011];\ \mathbf{u},[110]$		
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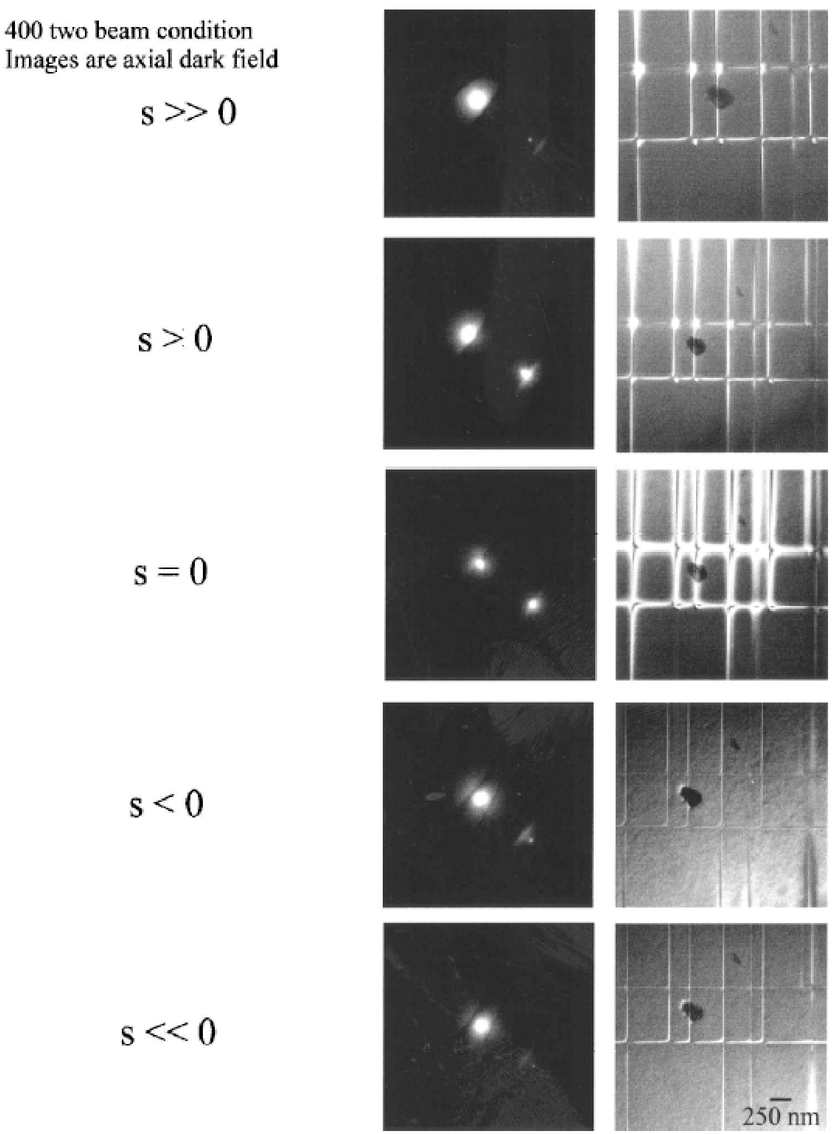
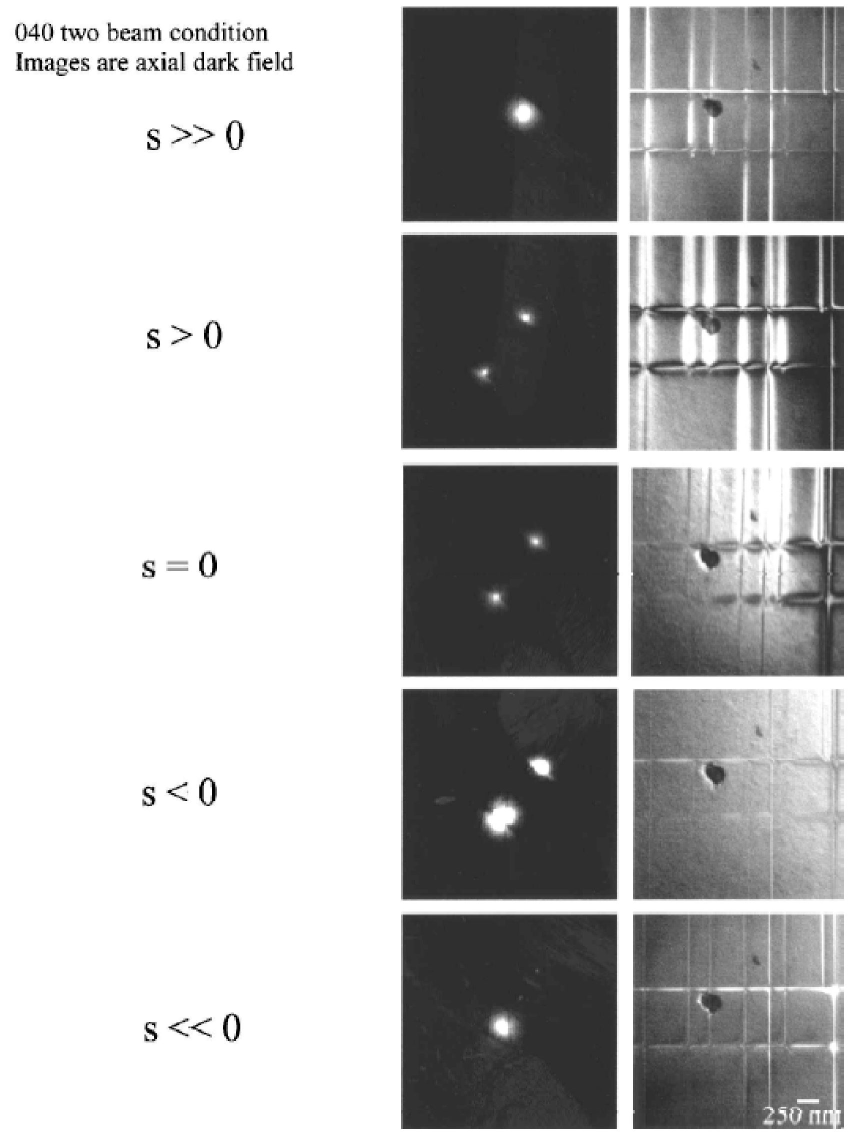
040	2	$\sqrt{2}$	0.18	
311	1	$3/2\sqrt{2}$	0.13	
$13\bar{1}$	1	$3/2\sqrt{2}$	0.13	
		$\mathbf{b},(a/2)[101];\ \mathbf{u},[110]$		
400	2	$\sqrt{2}$	0.18	
040	0	$\sqrt{2}$	0.18	
311	2	$1/2\sqrt{2}$	0.05	←
$13\bar{1}$	0	$1/2\sqrt{2}$	0.05	←

Table A 1. Diffraction conditions for which $\mathbf{g}\cdot\mathbf{b}=0$ is true for at least one Burgers vector.

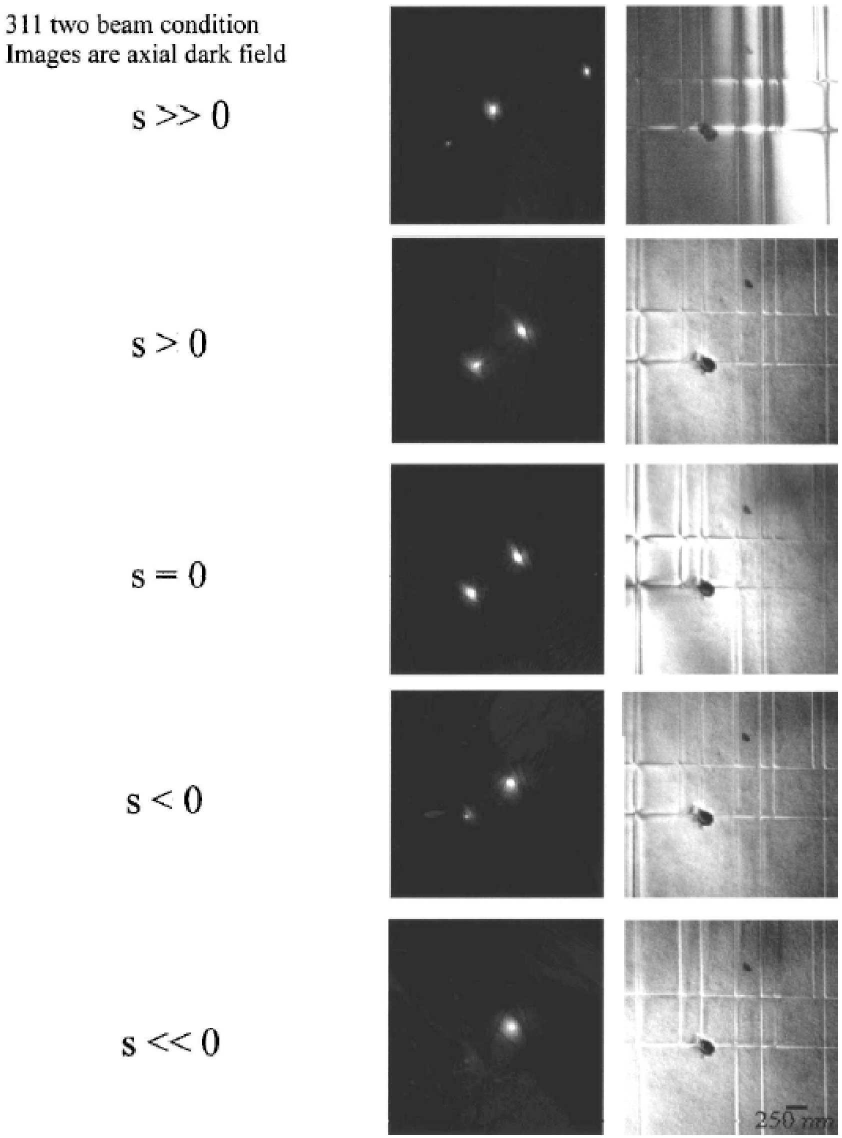
$\mathbf{g}$	$\mathbf{b}=\frac{a}{2}[0\bar{1}1]$	$\mathbf{b}=\frac{a}{2}[\bar{1}01]$	$\mathbf{b}=\frac{a}{2}[011]$	$\mathbf{b}=\frac{a}{2}[101]$
400	0	2	0	2
040	2	0	2	0
311	0	1	1	2
$13\bar{1}$	2	1	1	0

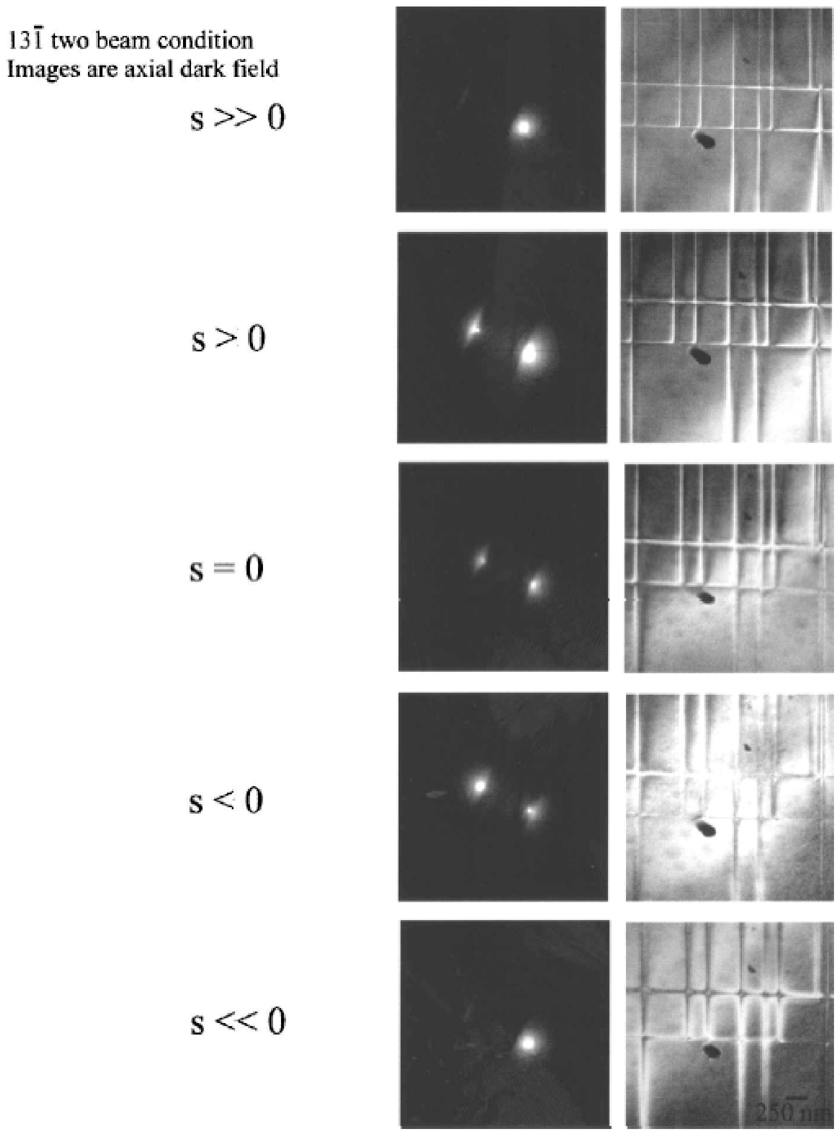
Surface effects & interfaces





Surface effects & interfaces





Dislocation contrast

Consider a pure screw dislocation:

$$\vec{b}_e = 0 \;;\; \vec{b} \times \vec{u} = 0$$

$$\vec{R} = \vec{b}\frac{\phi}{2\pi} = \frac{\vec{b}}{2\pi}\tan\left(\frac{z - z_d}{x}\right)$$

So: $\vec{R} \propto \vec{b}$

Thus: $\vec{g} \cdot \vec{R} \propto \vec{g} \cdot \vec{b}$

"g dot b" contrast

Table 25.1. Different Burgers Vectors and Different Reflections Give Different g·b = *n* Values[a]

g \ b	$\frac{1}{6}[11\bar{2}]$	$\frac{1}{6}[1\bar{2}1]$	$\frac{1}{6}[\bar{2}11]$	$\frac{1}{3}[111]$
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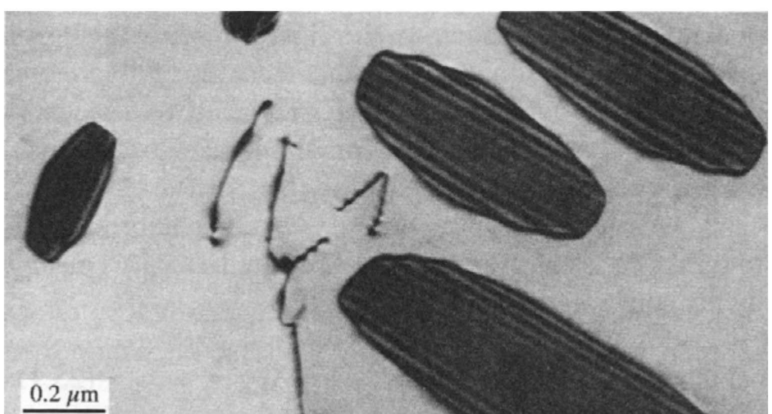
$\pm(\bar{1}\bar{1}1)$	± 2/3	± 1/3	± 1/3	± 1/3
$\pm(0\bar{2}2)$	± 1	± 1	0	0
$\pm(200)$	± 1/3	± 1/3	± 2/3	± 2/3
$\pm(3\bar{1}1)$	0	± 1	± 1	± 1
$\pm(\bar{3}\bar{1}1)$	± 1	0	± 1	± 1

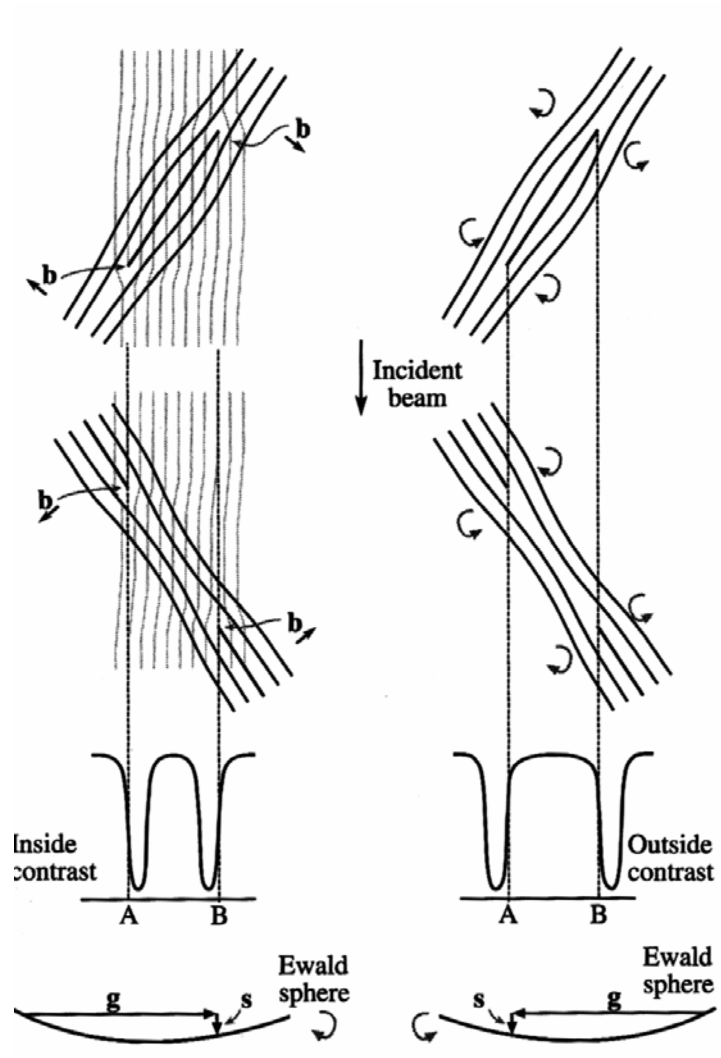
[a]The dislocations all lie on a (111) plane in an fcc material; the beam direction is [011].

Dislocation loops & dipoles

Often dislocation loops formed by collapse of interstitials or vacancies

Can thus enclose intrinsic or extrinsic stacking faults, or may be no fault



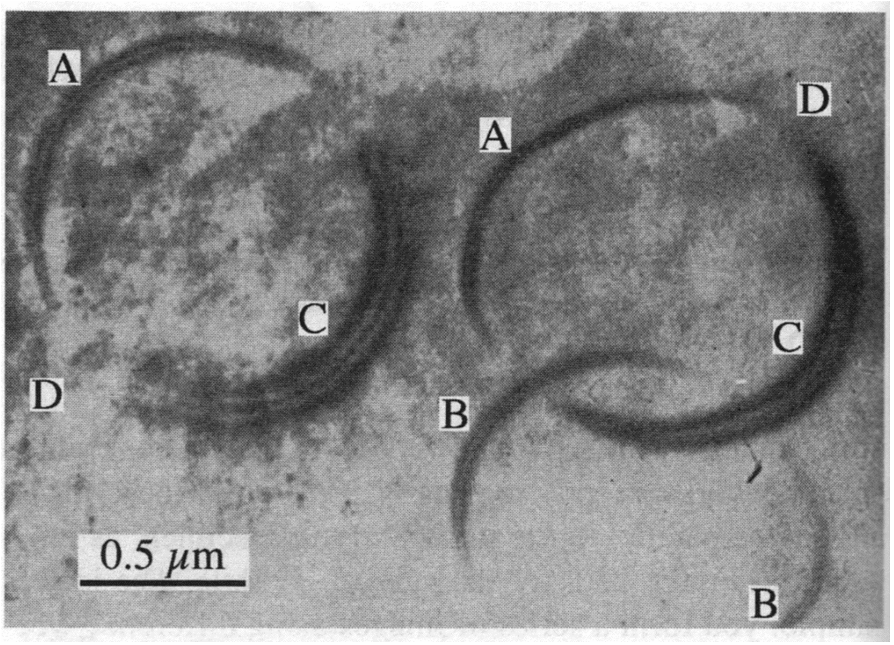


Dislocations loops & dipoles

Prismatic dislocation loops can nicely demonstrate

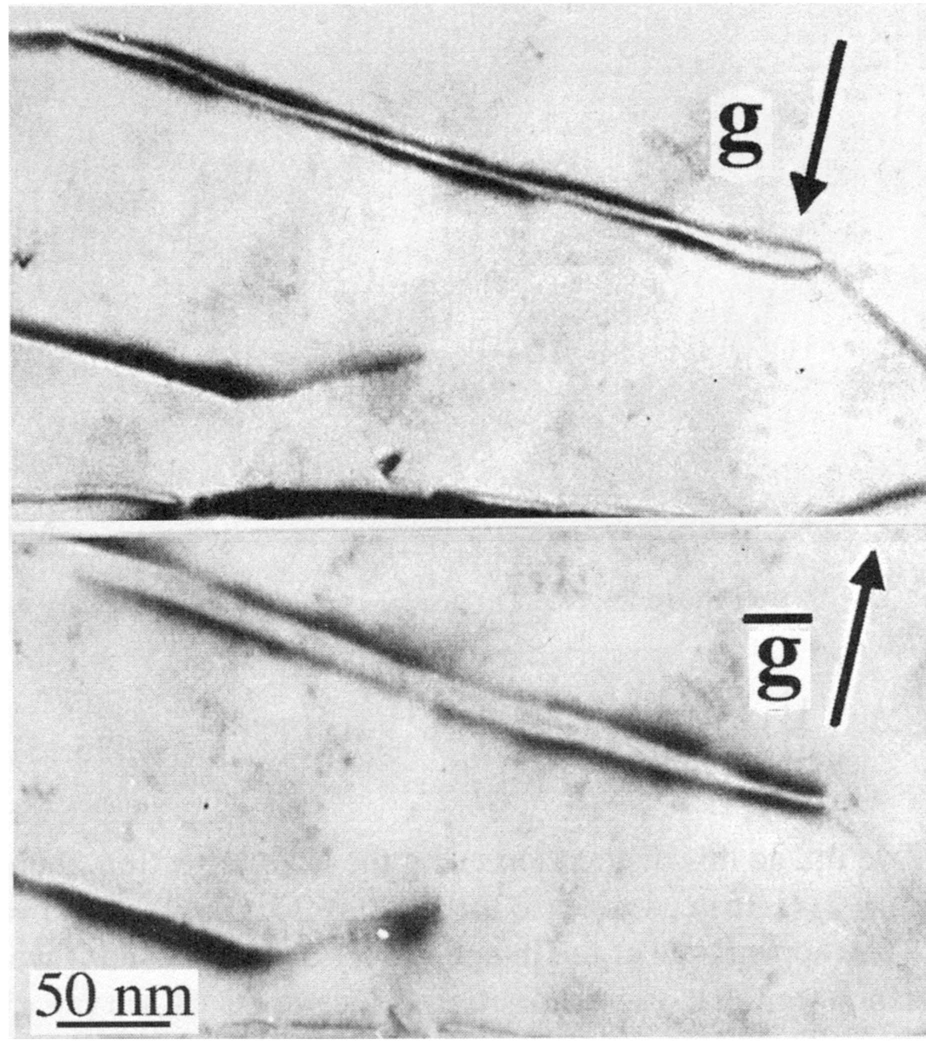
$\vec{g} \cdot \vec{b} = 0$ & $\vec{g} \cdot \vec{b} \times \vec{u} = 0$

effects

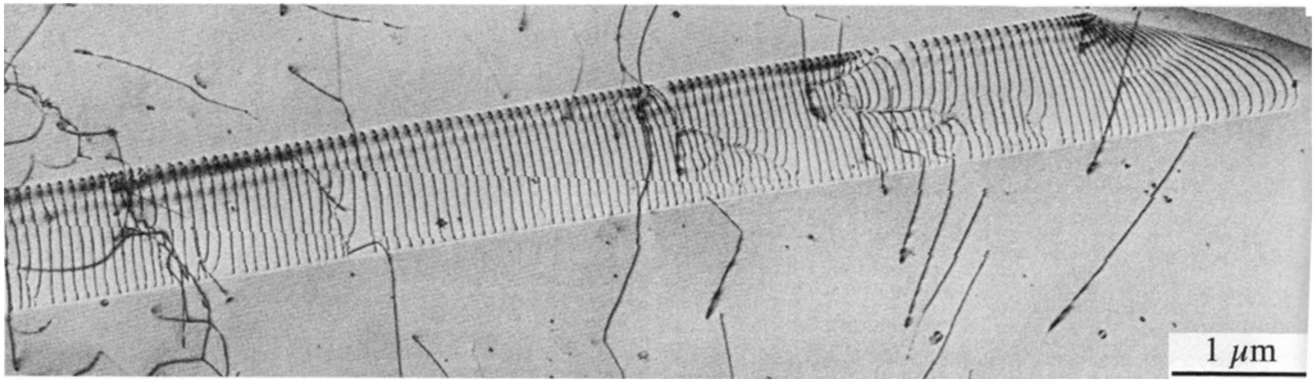


Dislocations loops & dipoles

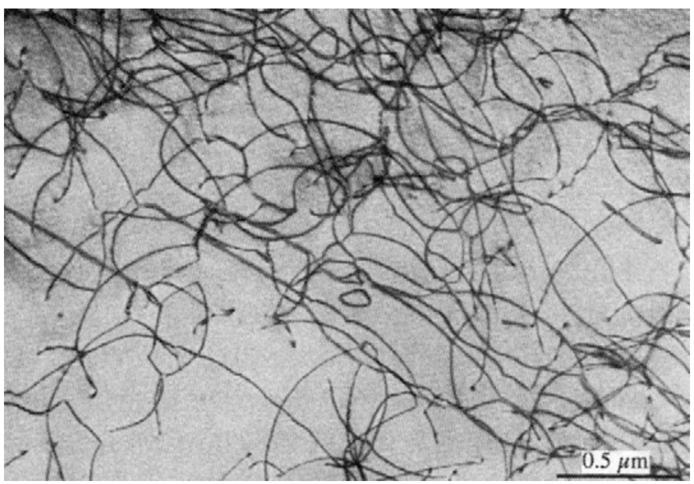
- Dislocation dipoles are essentially elongated loops
- Have no net Burgers vector, and thus no long range stress field
- Exhibit same 'inside / outside' contrast on reverse of s
  - Remember contrast origin tied to $(\vec{g} \cdot \vec{b})s$



Dislocations interactions & tangles

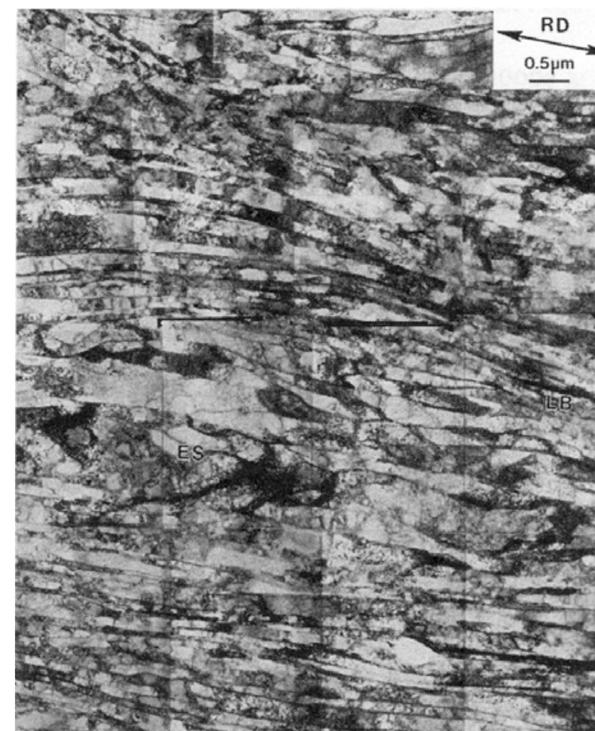


HVEM Image of slip along an inclined plane



A complex dislocation tangle

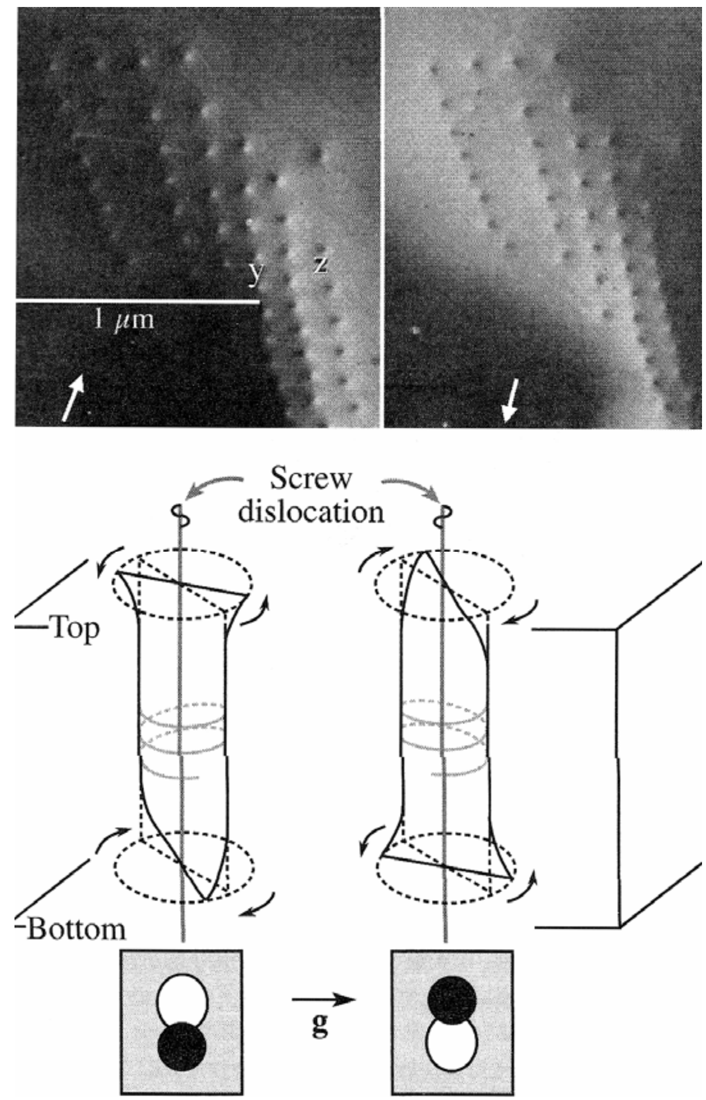
Cold rolled alloy



Surface effects & interfaces

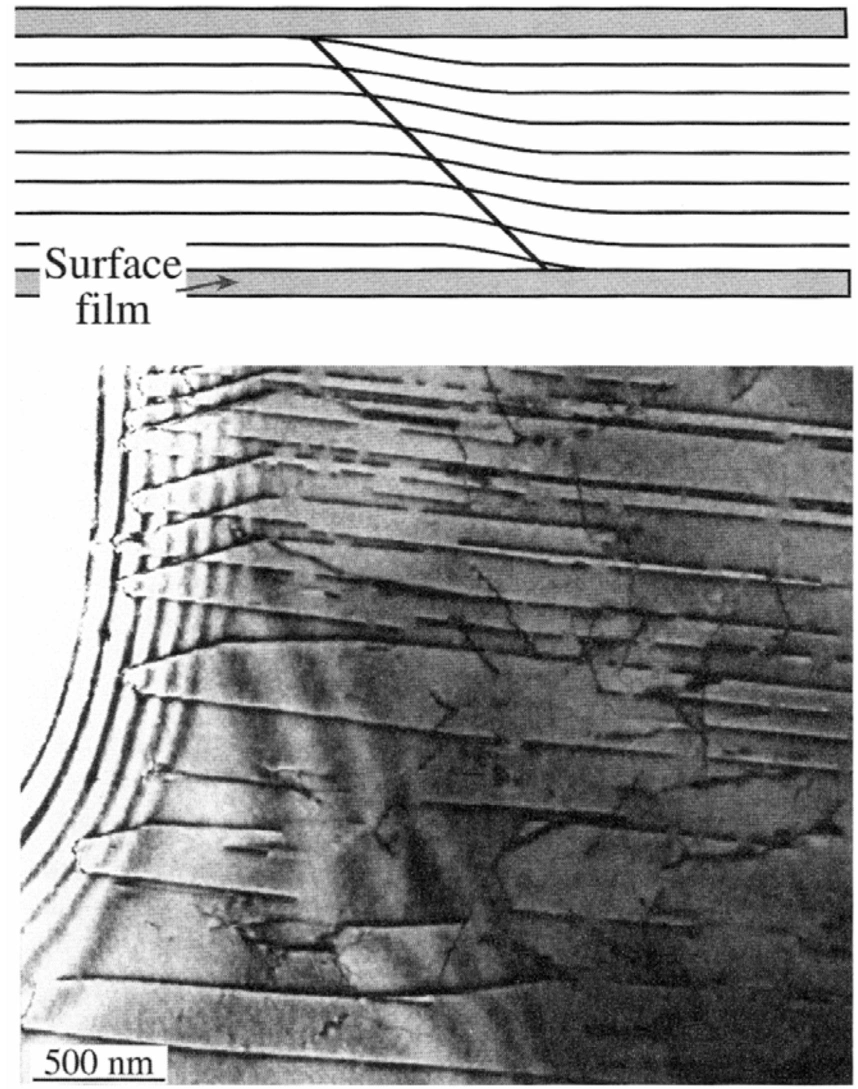
For a screw dislocation, only worry about $\vec{g}\cdot\vec{b}=0$

However, even if $\vec{g}\cdot\vec{b}=0$ can see effects of surface relaxation

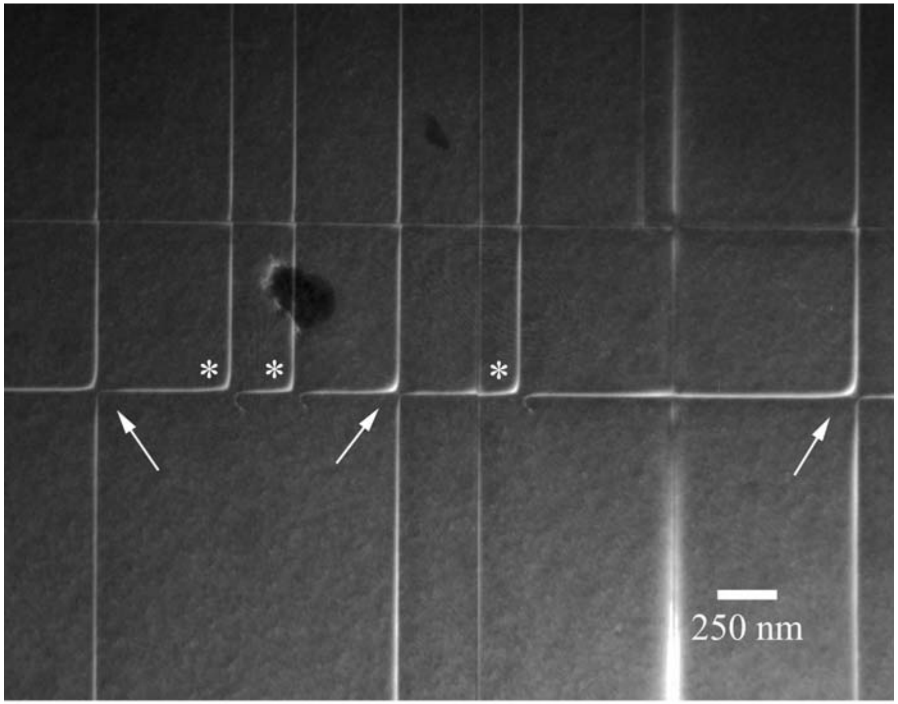


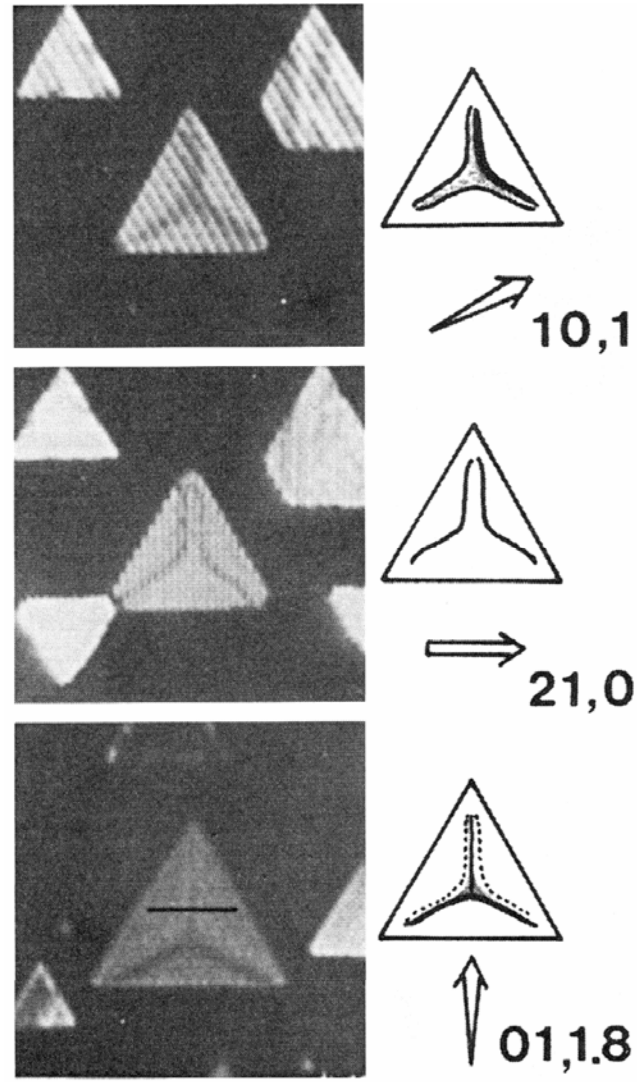
Surface effects & interfaces

Oxides on TEM samples (an artifact) can pin dislocations



Surface effects & interfaces





Interface misfit dislocations are a common class of defects to image

Be aware of surface relaxation effects (i.e $\vec{g} \cdot \vec{b} \times \vec{u} \neq 0$)

Coherent precipitates & islands

Strain field from coherent precipitates also give "g dot b contrast"

A line of zero contrast is observed perpendicular to g