Fundamentals of Materials Science
Homework 13, SS 2017

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This homework assignment provides a practice on your comprehension of dislocation basics. Please review the lecture notes and textbook chapters before working on the following problems.

1. For both FCC and BCC crystal structures, the Burgers vector $\vec{b}$ maybe expressed as

$$\vec{b} = \frac{a}{2}[h \quad k \quad l]$$

where a is the unit cell edge length and $[h \quad k \quad l]$ is the crystallographic direction having the greatest linear atomic density.

(a) What are the Burgers vector representations for FCC, BCC, and simple cubic crystal structures?

(b) If the magnitude of the Burgers vectors $|\vec{b}|$ is

$$|\vec{b}| = \frac{a}{2}(h^2 + k^2 + l^2)^{1/2}$$

determine the values of $|\vec{b}|$ for aluminum and tungsten. You may want to consult your textbook for lattice parameter data.

Solution

(a)

For FCC crystal structure, the greatest linear atomic density direction is [110], so

$$\vec{b} = \frac{a}{2}[110]$$

For BCC crystal structure, the greatest linear atomic density direction is [111], so

$$\vec{b} = \frac{a}{2}[111]$$

For SC crystal structure, the greatest linear atomic density direction is [100], so

$$\vec{b} = \frac{a}{2}[100]$$

(b) *Known numbers*

Atomic radius of Al: 0.143nm

Crystal structure of Al: FCC

Atomic radius of W: 0.137nm

Crystal structure of W: BCC

For aluminum, ***a*** is equal to $2\sqrt{2}$R , thus, $|\vec{b}| = \frac{a}{2}(h^2 + k^2 + l^2)^{1/2}$=2R=0.286nm;

For tungsten, ***a*** is equal to $\frac{4\sqrt{3}}{3}$R , thus, $|\vec{b}| = \frac{a}{2}(h^2 + k^2 + l^2)^{1/2}$=2R=0.274nm.

2. Calculate the length of the Burgers vector in copper.

Solution

Known numbers

Atomic radius of copper: 0.128nm

Crystal structure of copper: FCC

For copper, ***a*** is equal to $2\sqrt{2}$R , thus, $|\vec{b}| = \frac{a}{2}(h^2 + k^2 + l^2)^{1/2}$=2R=0.256nm.

3. Construct a two-dimensional drawing of the (110) plane of a bcc lattice. By means of vector addition show that $(a/2)[\bar{1}\,\bar{1}\,1] + (a/2)[111] \rightarrow a[001]$ and $(a/2)[\bar{1}\,\bar{1}\,1] + (a/2)[\bar{1}\,\bar{1}\,\bar{1}] \rightarrow a[\bar{1}\,\bar{1}\,0]$. Show that the last reaction is not energetically favorable. (You need to read the George Dieter's chapter to complete this problem.)

Solution

Assume $\vec{b1} = \frac{a}{2}[\bar{1}\bar{1}\,1]$, $\vec{b2} = \frac{a}{2}[\bar{1}\bar{1}\bar{1}]$, thus, $\vec{b1} + \vec{b2} = \vec{b3} = a[\bar{1}\bar{1}0]$

Using the equation, $|\vec{b}| = \frac{a}{2}(h^2 + k^2 + l^2)^{1/2}$,

$|\vec{b}_1| = \frac{a}{2}[(-1)^2 + (-1)^2 + 1^2]^{1/2} = \frac{\sqrt{3}}{2}a$; $|\vec{b}_2| = \frac{a}{2}[(-1)^2 + (-1)^2 + (-1)^2)]^{1/2} = \frac{\sqrt{3}}{2}a$;

$|\vec{b}_3| = a[(-1)^2 + (-1)^2 + 0^2)]^{1/2} = \sqrt{2}a$.

Since $|\vec{b}_1|^2 + |\vec{b}_2|^2 < |\vec{b}_3|^2$, the last reaction is not energetically favorable.

4. There is experimental evidence that [100] dislocations can form in alpha iron by the reaction $a/2[11\bar{1}]+a/2[1\bar{1}1]\rightarrow a[100]$. Show this reaction on a sketch of the iron unit cell and determine that the reaction is energetically favorable. (You need to read the George Dieter's chapter to complete this problem.)

Solution

Assume $\vec{b1}=\frac{a}{2}[1\,1\bar{1}]$, $\vec{b2}=\frac{a}{2}[1\bar{1}1]$, thus, $\vec{b1}+\vec{b2}=\vec{b3}=a[100]$

Using the equation, $\left|\vec{b}\right|=\frac{a}{2}(h^2+k^2+l^2)^{1/2}$,

$\left|\vec{b}_1\right|=\frac{a}{2}[1^2+1^2+(-1)^2]^{1/2}=\frac{\sqrt{3}}{2}a$, $\left|\vec{b}_2\right|=\frac{a}{2}[1^2+(-1)^2+1^2]^{1/2}=\frac{\sqrt{3}}{2}a$;

$\left|\vec{b}_3\right|=a[1^2+0^2+0^2]^{1/2}=a$.

Since $\left|\vec{b}_1\right|^2+\left|\vec{b}_2\right|^2>\left|\vec{b}_3\right|^2$, the last reaction is not energetically favorable.

5. 已知单位位错$a/2[\bar{1}01]$能与肖克莱不全位错$a/6[12\bar{1}]$相结合，形成弗兰克不全位错，试说明：（1）新生成的弗兰克不全位错的柏氏矢量是什么；（2）判断此位错反应能否进行；（3）这个位错为什么是固定位错？（2010 年 1 月研究生入学考试题，你需要阅读我发的讲义和中文教材“实际晶体中的位错”后来完成此题。）

Solution

(1) $a/2[\bar{1}01]+a/6[12\bar{1}]$=a/3$[\bar{1}11]$

(2) Assume $\vec{b1}=\frac{a}{2}[\,\bar{1}01]$, $\vec{b2}=\frac{a}{6}[12\bar{1}]$, thus, $\vec{b1}+\vec{b2}=\vec{b3}=a/3[\bar{1}11]$,

Using the equation, $\left|\vec{b}\right|=\frac{a}{2}(h^2+k^2+l^2)^{1/2}$,

$\left|\vec{b}_1\right|=\frac{a}{2}[(-1)^2+0^2+1^2]^{1/2}=\frac{\sqrt{2}}{2}a$;

$\left|\vec{b}_2\right|=\frac{a}{6}[1^2+2^2+(-1)^2]^{1/2}=\frac{\sqrt{6}}{6}a$;

$$\left|\vec{b}_3\right| = \frac{a}{3}[(-1)^2 + 1^2 + 1^2]^{1/2} = \frac{\sqrt{3}}{3}a$$;

Since $\left|\vec{b}_1\right|^2 + \left|\vec{b}_2\right|^2 > \left|\vec{b}_3\right|^2$, the last reaction is not energetically favorable.

(3) Since the Frank partial dislocation's Burgers vector is perpendicular to the central stacking fault, and the glide must be restricted to the plane of the stacking fault and the Burgers vector is normal to this plane, the Frank partial dislocation cannot move by glide, so it is a sessile dislocation.

6. Dislocations must have a Burgers vector that connects one crystal lattice site to another. There are therefore many possible magnitudes and directions for b. However, it has been experimentally observed that b always corresponds in direction to a close packed row of atoms and in magnitude to the distance between lattice sites (atoms) along such a close packed row. Figure 5.9 shows the Burgers vector around an edge dislocation in a cubic cell, where the close-packed direction is along [1 0 0].

(a) In what direction will $\vec{b}$ point for the BCC crystal of iron?

(b) What will be the magnitude of $\vec{b}$ in iron?

We will return to Burgers vectors in the next Chapter, in the context of deformations of materials, and such exercises could be very good preparations.

Solution

(a) According to the question, BCC crystals have Burgers vectors along the closest packed directions, they are family<111>, which are the body diagonals of the unit cell.

(b) Since the atoms along <111> directions are touching, the smallest Burgers vector possible is equal to 2R, so the magnitude of Burgers vector in iron is 0.248nm.

7. Mini Lab

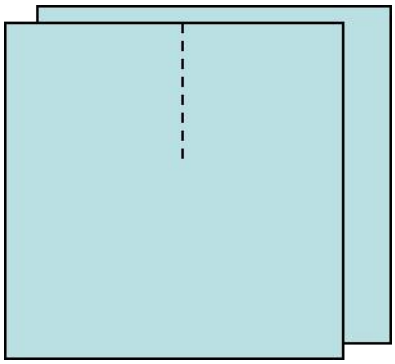
Make photographs for each part, or a movie of all the process, and hand in electronically; you do not need to show these during office hours, although you are welcome to do so if you like or if you wish to discuss the result. Also prepare a short text document answering the questions below.

You will need 4 sheets of paper (of any size), something to cut or punch with, and tape.

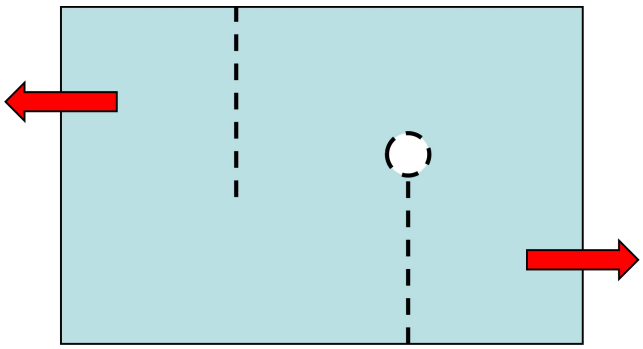
a) Cut one of the sheets of paper in half. Stack two pages and add the half a page between them. What do you observe? Compare with Figure 6.9.

b) Cut three pages as shown in the figure, in a straight line from the center top to the middle. Now attach the left half of the top page to the right half of the page

underneath, for each layer in the stack. What do you observe? Compare with Figure 6.10.



c) Take a piece of paper and cut it into a rectangle on the order of 2-2.5 x 3.5 inches OR use a small piece of cardstock, like a business card. Then cut this along the lines indicated in the figure: about a third of the way in from the left edge, cut down to a bit more than halfway, then from a third of the way from the right edge, cut up from the bottom to a bit more than halfway. The lines should overlap a bit. At the top of one of these cuts, cut or punch a circle.



Finally, grab the edges of the card and pull, as indicated by the red arrows. What happens? Why? Does this happen every time you do the experiment?