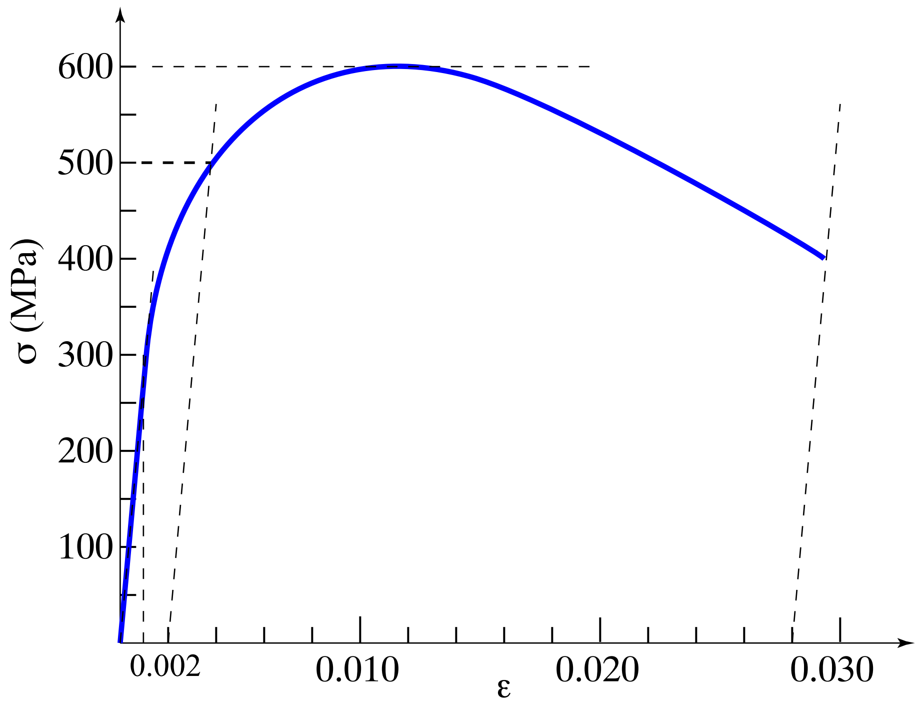
1. Mechanical Properties (20 points)

Refer to the following stress-strain plot derived from a standard uniaxial tensile test of a high performance titanium alloy to answer the following questions. Show all work.



a. What is the yield strength of this alloy?

By the 0.2% offset method (shown on plot), **YS = 500 MPa**

b. What is its ultimate tensile strength?

The maximum in the stress-strain curve determines this (see plot), **UTS = 600 MPa**.

c. What is the elastic modulus of this alloy?

$$E = \frac{\Delta\sigma}{\Delta\epsilon} = \frac{(250-0)\ \mathrm{MPa}}{(10^{-3}-0)}$$

E = **250 GPa**

d. What is its ductility (% elongation at failure)?

By the construction shown on the plot, % elongation at failure = 100 x 0.028 = **2.8%**

2. Bonding (20 points)

a. In problem 1 above, the titanium alloy is described as having metallic bonding. How does the nature of the metallic bond explain *both* elastic behavior in the initial stages of deformation, *and* plastic behavior during the continued deformation of this material?

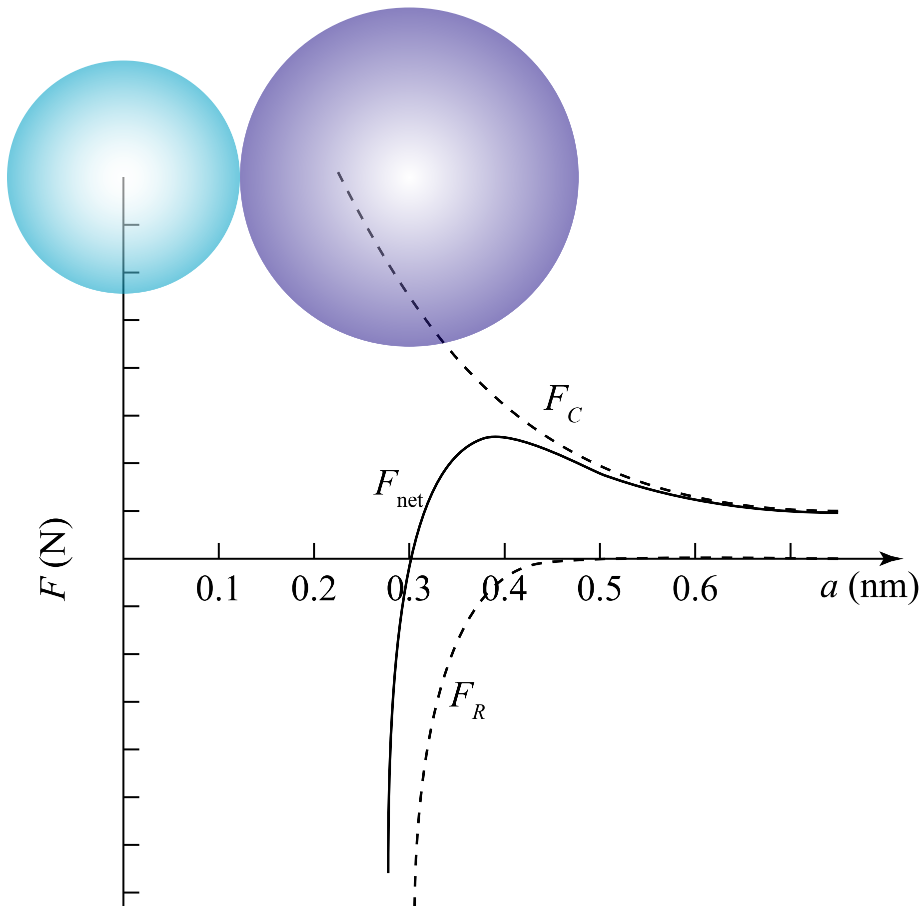
In the initial stages of deformation, atomic bonds are being *stretched* under the applied load, known as elastic behavior. The nature of the metallic bond is a *mutual sharing of electrons*, and because titanium has many electrons to share, the bond is a strong one, resulting in a high elastic modulus.
During continued deformation the stress-strain curve departs from linearity when atomic bonds are *broken* due to dislocation nucleation and propagation. Here the *non-directional* character of metallic bonding provides a benefit, because bonds can be retained even *under severe shape change*. This accounts for the *malleable* response of most metals under deformation.

b. Covalent bonding is described as "directional." What does this mean, and what determines the direction associated with the bond?

Covalent bonds form by the *overlap of electron orbitals* between adjacent atoms. The *direction along which overlap occurs* determines the direction of bond formation. This direction is established by the tendency of covalently bonded atoms to *maximize* the amount of orbital overlap.

2. Bonding (20 points)

c. Refer to the force diagram below describing the contributions of the Coulombic interaction and repulsive interaction between a cation at the origin and an anion at its "equilibrium" separation distance of 0.3 nm. Show directly on the plot why this is the equilibrium spacing.



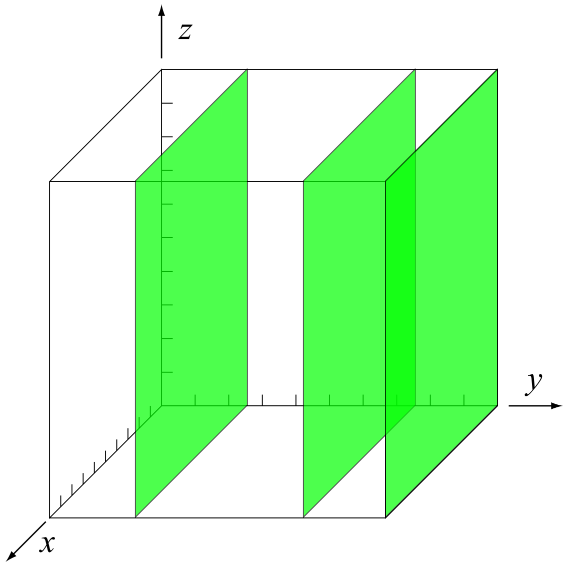
ANALYSIS:
As shown, the spacing is the equilibrium distance because the net force is **zero**.

d. Why is the bond energy associated with secondary bonds no greater than 25% of the bond energy associated with primary bonds?

Secondary bonds are formed between *groups or clusters of atoms* due to *dipole-dipole* interactions, a much weaker interaction than the *sharing or transfer of electrons* between *individual atoms or ions* associated with the primary bonds.

3. Lattice Geometry (20 points)

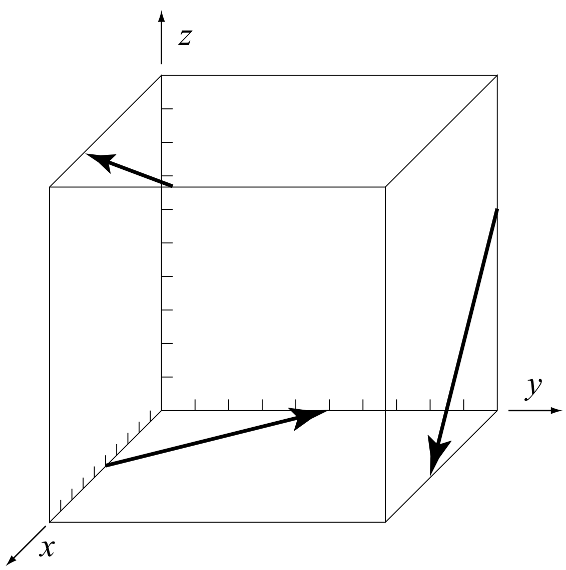
a. Identify the family to which the following three planes in a cubic lattice belong. Use Miller index notation.



Answer

(040)

b. What symmetry-related directions through the same cubic lattice are indicated below? Use Miller index notation.

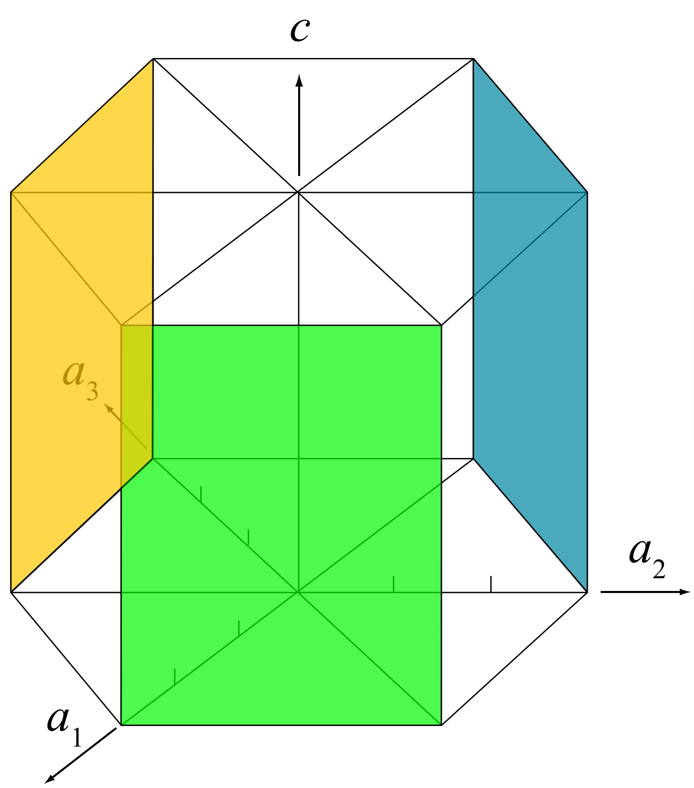


Answer

$< 110 >$

3. Lattice Geometry (20 points)

c. Identify the symmetry-related families to which the following three planes in a hexagonal lattice belong.
Use Miller-Bravais notation.

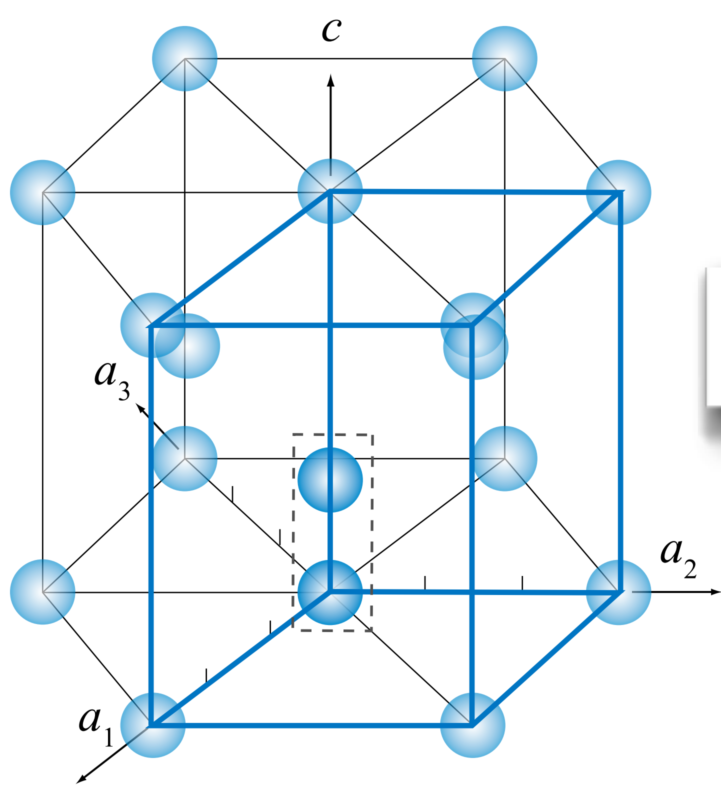


Answer

$\{10\bar{1}0\}$

3. Lattice Geometry (20 points)

d. The hexagonal close packed (HCP) structure is illustrated below. Its Bravais lattice is simple hexagonal, adorned with a two-atom motif, one atom at 0,0,0, and a second atom at ⅔, ⅓, ½ relative to the simple hexagonal unit cell outlined below. All of the (0002) planes are closest-packed (see problem 5 below), consequently the second atom of the motif rests on a triangular bed of three atoms in the basal plane, one of which is the 0,0,0 atom. The motif is outlined (dashed line) in the sketch below. Identify the lattice direction connecting the two atoms comprising the motif in the HCP structure.
Use Miller-Bravais notation.



Answer

$[20\bar{2}3]$

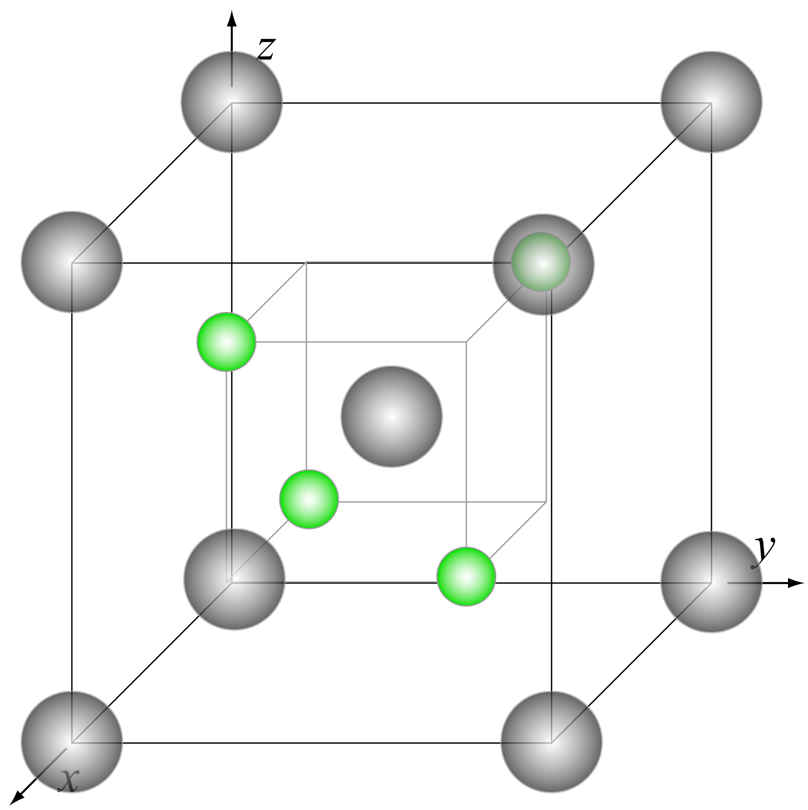
ANALYSIS:
In Miller-Bravais notation, the location of the first atom in the motif is 0,0,0,0. The location of the second atom is ⅓, 0, –⅓, ½. Clearing fractions, the direction is obtained. Note that this is a "direction" and as such, can have arbitrary magnitude.

Alternative location of second atom: ⅔ [⅔, –⅓, –⅓, 0] + ⅓ [–⅓, ⅔, –⅓, 0] + ½ [0,0,0,1]. Summing and clearing fraction, the same direction is obtained (reduced to smallest integers because magnitude is arbitrary).

4. Crystal Structure (20 points)

One form of copper oxide has a cubic structure with copper atoms at locations ¼, ¼, ¼; ¼, ¾, ¾; ¾, ¼, ¾; and ¾, ¾, ¼. The oxygen atoms are at 0,0,0 and ½, ½, ½. These are confirmed by a diffraction experiment, where Bragg's Law is the operating equation, $n\lambda = 2d \sin\theta$. The structure factor rules for cubic structures allow all *hkl* reflections for a simple cubic lattice. For a body-centered cubic lattice, $h+k+l$ must sum to an even number, and for a face-centered cubic lattice, h,k,and l must be "unmixed," all even or all odd.

a. On the following template showing an inner cube with the locations of all tetrahedral interstices at its corners, populate a unit cell with Cu and O atoms in their appropriate locations to generate this copper oxide structure.



b. What is the chemical formula of this structure?

The chemical formula is reflected in the contents of the unit cell, four (4) copper atoms and two (2) oxygen atoms, making the formula $\mathbf{Cu_2O}$.

c. Specify a lattice and motif that defines this structure?

Although the oxygens sit at positions normally associated with a body-centered cubic Bravais lattice, they have different environments. Compare the oxygen at the 0,0,0 location with it closest copper at ¼, ¼, ¼, to the oxygen at the body center, with its copper at relative position –¼, ¼, ¼.
Consequently the lattice must be **simple cubic**.

The motif must also reflect the chemical formula, and in this case, it is identical to the specification in the problem statement. The motif consists of **four (4) Cu atoms** at locations ¼, ¼, ¼; ¼, ¾, ¾; ¾, ¼, ¾; and ¾, ¾, ¼, and **two (2) oxygen atoms** at 0,0,0 and ½, ½, ½.

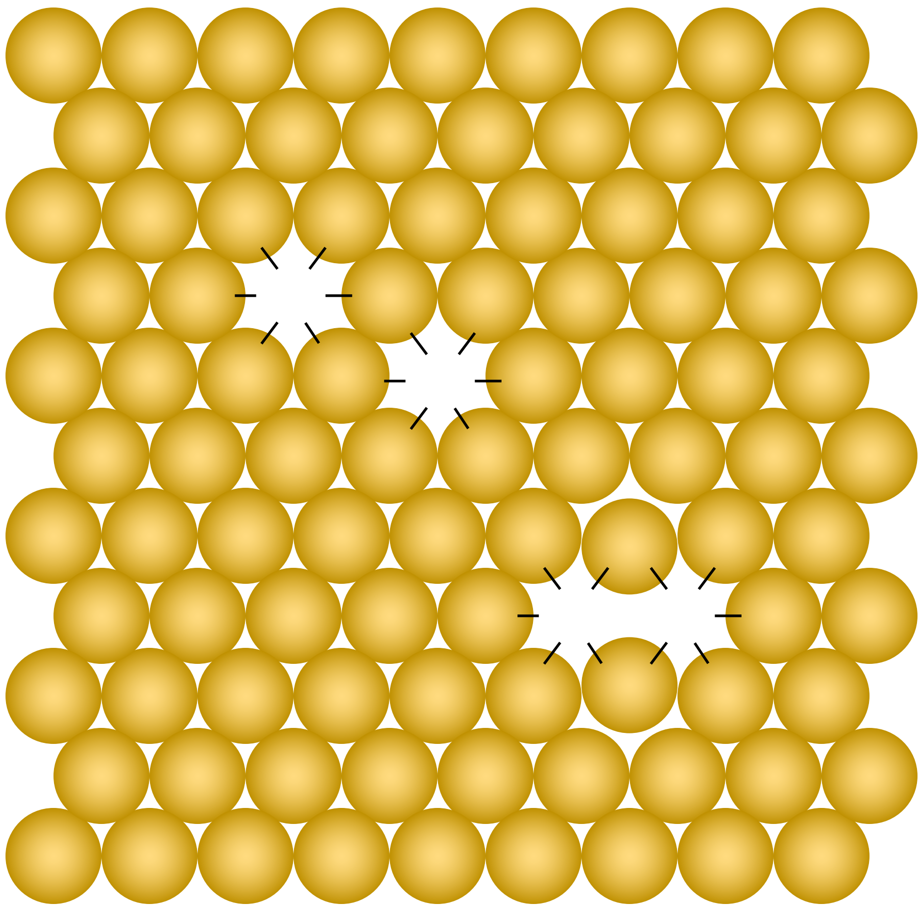
d. In a diffraction experiment with this structure as the sample, what are the indices of the first three diffraction peaks? Recall that for cubic structures,

$$d_{hkl} = \frac{a_0}{\sqrt{h^2 + k^2 + l^2}}$$

For a simple cubic lattice, all reflections are allowed, so the first three peaks are indexed **001**, **011**, and **111**.
(Note that 100, 010, and 001 are equivalent, as are 011, 101, and 110).

5. Crystalline Defects (20 points)

a. Refer to the following illustration of the atomic configuration in the (0002) planes of an HCP structure showing two vacancies in the upper left and a defect called a "divancy" in the lower right. It should be evident that a divacancy is simply a cluster of two vacancies. Explain, using this illustration, why divacancies are energetically favored over two isolated vacancies. In your answer, consider the energy associated with breaking atomic bonds.



The simple explanation here is that the creation of a single vacancy in the (0002) planes requires the breaking of six bonds. Two isolated vacancies therefore have twelve (12) broken bonds, but a single divacancy has only ten (10) broken bonds. The *energy difference associated with these two (2) bonds* makes the divacancy more favorable because it has a lower energy.

b. The concentration of vacancies C_V in a solid is a strong function of temperature, obeying an Arrhenius expression,

$$C_V \;=\; A\,\exp\left(\frac{-E_V}{kT}\right)$$

where A is a constant, E_V is the vacancy formation energy, k is Boltzman's constant, and T is the absolute temperature. Explain why it is customary to plot ln C_V vs. $1/T$ when data is collected on vacancy concentration as a function of temperature. What insight does this provide?

Taking the natural log of both sides of the Arrhenius expression given in the problem statement,

$$\ln C_V \;=\; \ln A \;+\; \left(\frac{-E_V}{k}\right)\left(\frac{1}{T}\right)$$

produces an equation for a straight line ($y = mx + b$). Consequently, by plotting ln C_V *vs*. $1/T$, the result is a straight line with a slope of $-E_V/k$, from which the *vacancy formation energy* can be readily obtained. This offers significant insight into the mechanisms of vacancy formation.

c. Creep is defined as plastic deformation at high temperatures under constant load that occurs over a long period of time. Ceramics are normally used as high temperature materials due to their high melting point, but are also subject to creep, believed to be due to "grain-boundary sliding." Comment on the effect of grain size on creep deformation of ceramics. Is it more desirable to design creep-resistant ceramics with small grains or large grains, and why?

Grain boundary sliding will be aggravated by more grain boundaries, offering a larger interfacial area over which sliding can occur. Since small grained materials have larger grain boundary area, they are more likely to suffer creep. Consequently it is more desirable to design creep-resistant ceramics having **large grains**.

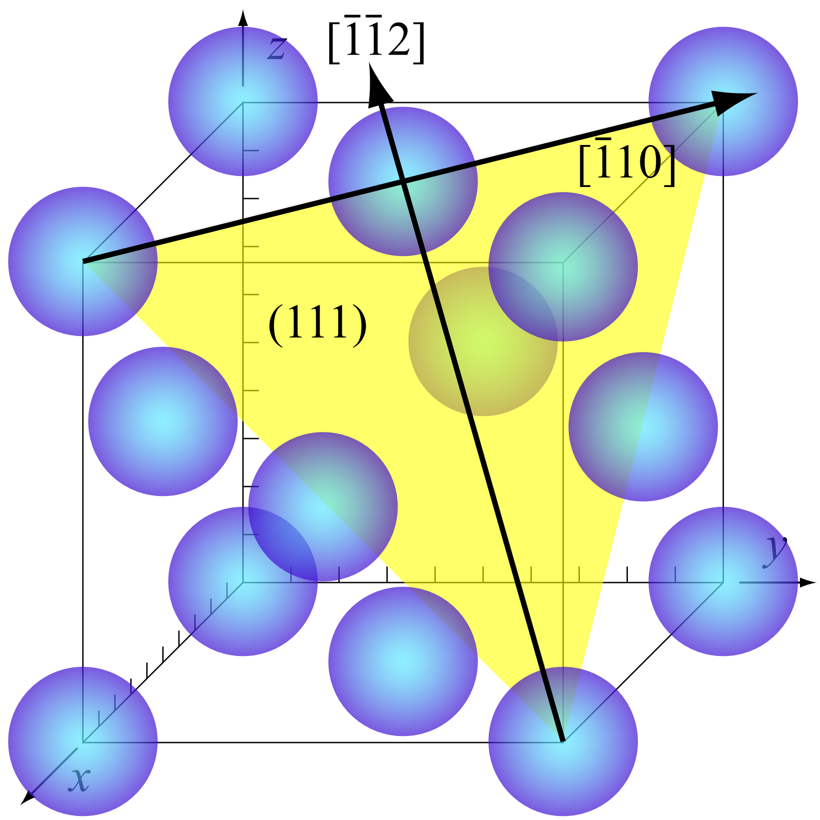
d. In an FCC crystal, active slip systems consist of close-packed {111} planes and the <011> directions in those planes. Following an electron microscopy investigation, it is discovered that a dislocation in a Ni-based superalloy (FCC) has a Burgers vector

$$\vec{b} = \frac{a}{2}[\bar{1}10]$$

and a line direction vector

$$\vec{\xi} = [\bar{1}\bar{1}2]$$

Is this an edge or screw dislocation?
What is its slip plane?



The dot product between ***b*** and *ξ* is zero, so they are perpendicular, meaning that the dislocation is, by definition, a pure **edge dislocation**. The directions of both ***b*** and *ξ* are illustrated on the drawing above.
The *slip plane* is the plane containing both ***b*** and *ξ*, which in this case is **(111)**, as illustrated on the drawing. Its normal can alternatively be *calculated* by simply taking the vector *cross product* of ***b*** and *ξ*, or noting that the dot product between the normal to the slip plane and both ***b*** and *ξ* must be zero.