Introduction to crystal elasticity and crystal plasticity
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Week-06
Lecture-13

So this time we will try to consider the few examples, so far we have discussed the theory related to the crystal plasticity or maybe that is the crystal plasticity part 1. So here we will focus some of the associated numerical problems with the theory.

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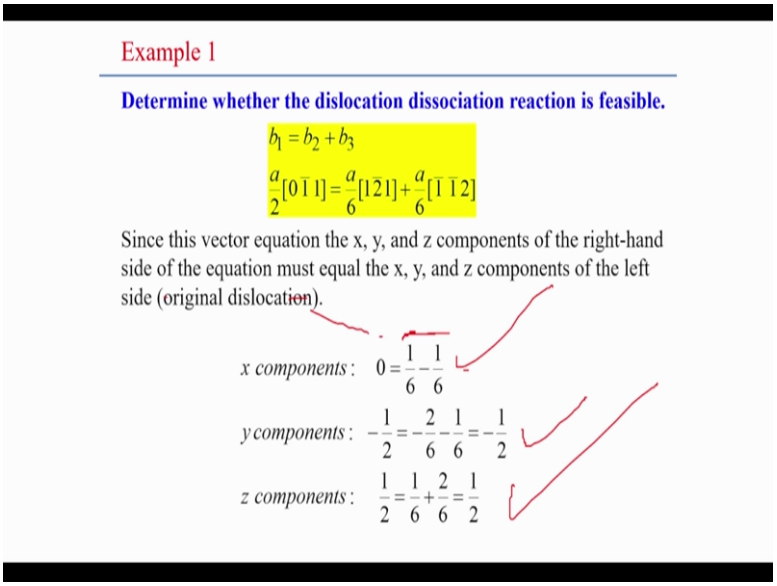

Let us look into this thing one by one, and first to the example 1, here we can see that determine whether the dislocation reaction is feasible or not. So here the dislocation reaction is given b1 equal to b2 plus b3 now we can see that magnitude of the Burgers vector also given. And here from this reaction we will try to investigate the feasibility of this reaction of dislocation. So to do that since b1 b2 represented in terms of vector, first we will try to consider the components of the this vector x, y, z coordinates and we will try to make them balance, if we try to make it balance, the component in the left hand side and right hand side individual x, y, and z axis.

And then if it matches with then we can say that the reaction is feasible, so this is the very thumb rule to do, first checking to whether b1 equal to b2 plus b3 that means whether this equation is valid or not. This is the first checking of the feasibility of the reaction. So here we see the x component left hand side that is the 0, but right hand side if you see the component, you see the right hand side this component and this two components, and here a by 6 and

minus a by 6, because from Millar index it is given minus 1and the right hand side of the second term.

So 1by 6 minus 1 by 6, so a is the lattice parameter is common from both the sides, so we can consider 1 by 6 minus 1 by 6 that is 0 that means nit is satisfied. Let us look into the y components here, from this vector left hand side and right hand side, so left hand side the vector actually becomes minus half and right hand side if you look into that it is the from the first component it becomes minus 2 by 6 and from the second component it becomes minus 1 by 6 and it becomes minus half so that means it is also satisfying. This is satisfying and second component it is also satisfying.

Now if you look into that z component, z component if you see the left hand side it is the plus half and 2 component from the right hand side it comes 1 by 6 plus 2 by 6 that it becomes half that means z component it is also satisfying. So this is the first checking for the feasibility of the reaction.

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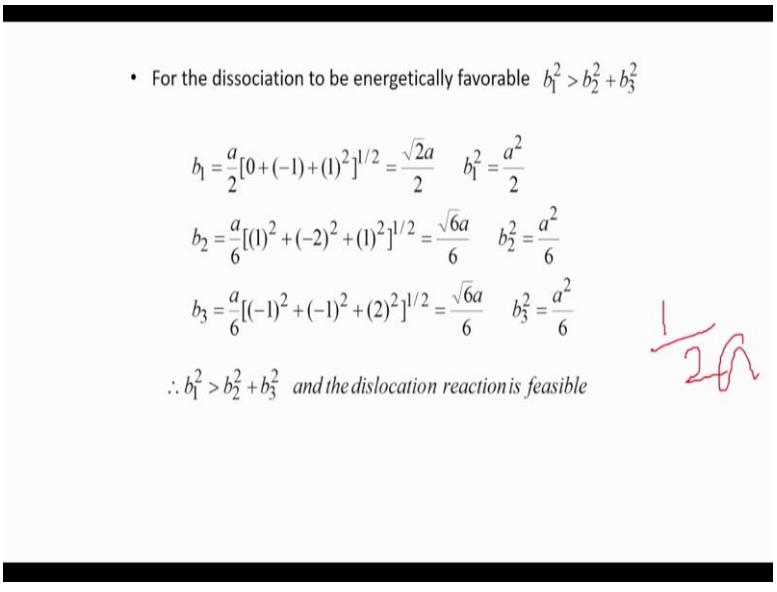

Now we will look into checking on that for the dissociation to be feasible to form the reaction, in this case we need to satisfy b1 square greater than b2 square plus b3 square and that b1 corresponding to this actually there required square terms comes from the amount of the estimated energy and that actually this term comes from that dislocation energy roughly half of Gb square. So half of Gb square and from that b square actually comes so first we see that what is the energy for left hand side so we will try to find out the magnitude of the Burgers vector, it is b1 equal to a by 2 root to the power of the component is given 0 minus 1

and 1 square, so from here we can find out that root 2 a by 2 is the magnitude of the Burgers vector and square terms of this is square by 2.

Now similarly we can find out the magnitude of the Burgers vector b2 and b3 in similar way or maybe we can say the magnitude of this vector and from there we can find out b2 square and b3 square and if we check it, we see we find out the b1 square is actually greater than of the summation of b2 square and b3 square. So this indicates that two checking satisfied here so we can say that the dislocation reaction is feasible in this case.

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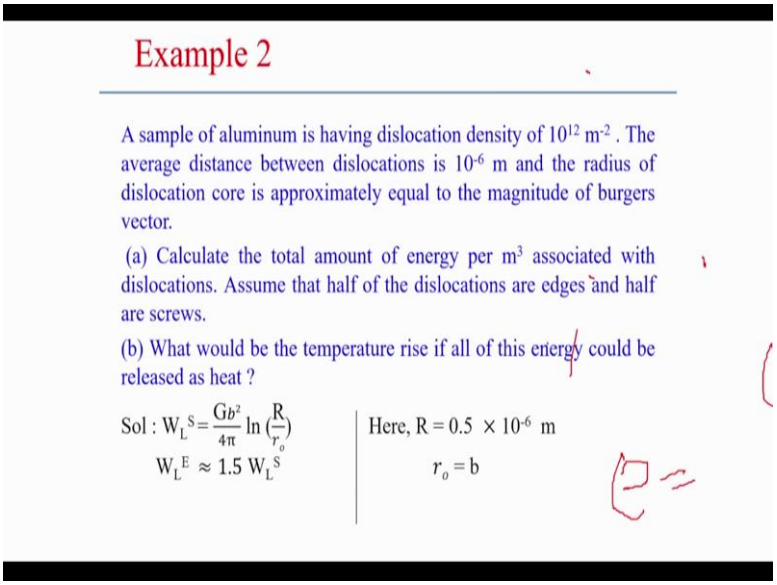

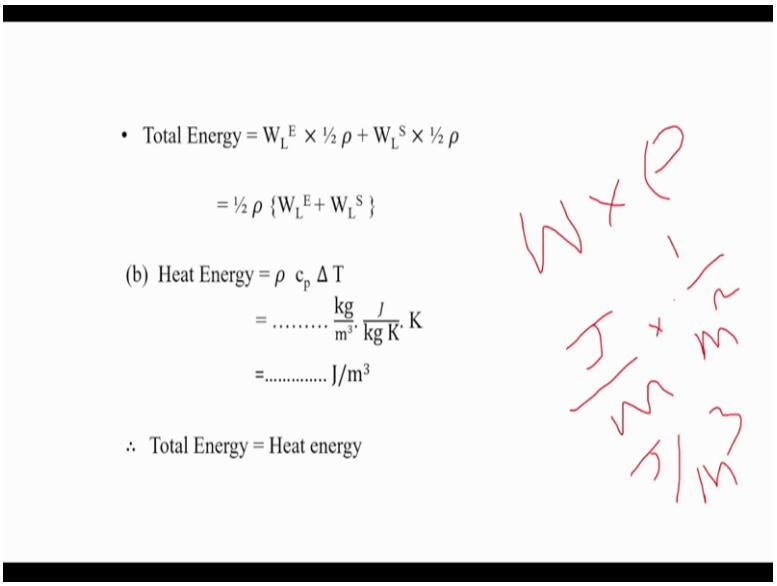

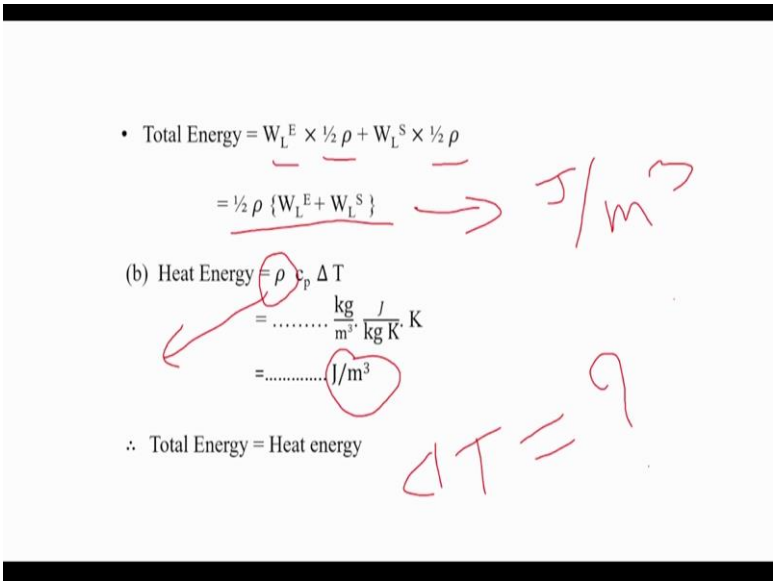

Now we shift to the next problem, here if we see, if we look into that problem, it is explained that a sample of aluminum is having dislocation density equal to 10 to the power 12 1 by meter square. The average dislocation between dislocation is 10 to power minus 6 meter and the radius of dislocation core is approximately equal to the magnitude of Burgers vector. So we have to estimate the total amount of the energy per meter cube associated with dislocation. Assume that with a sample that half of the dislocation are edge dislocation and half 50 percent is the screw dislocation.

And second we have to find out that what would be the temperature rise if we consider of all these energy associated with dislocation can be released as heat. To do that first here we can look into that, so dislocation density is basically the unit of the dislocation density here 1 by meter square, that how it comes. Dislocation density means we can find out that dislocation is measures actually in terms of the length so that density means the total dislocation the length divided by the volume. So when you divide the length divided by the volume then the unit becomes 1 by meter square.

Now here the size of the core is given, it is given that R0 equal to the magnitude of the Burgers vector, that means R0 equal to b, it is given that R0 equal to b here and capital R is given but point is that how we can estimate capital R, that can be estimated like that the average dislocation between, average dislocation between two dislocation is given so then effect of the one dislocation can be assumed that the existence of the, the meet point between the two dislocations so that is why capital R, that means upper limit of the dislocation

dislocation energy is limited to the capital R that is half of the distance between the two dislocation, that means 0.5 into 10 to the power minus 6 meter in this case.

So once we define capital R, size of the core then we can easily estimate the what is the amount of the energy associated with the screw dislocation and edge dislocation in this case. So once we estimate because other parameter are given then associated energy with the screw and edge dislocation then…

We can find out that what may be the total energy. Now here when we use this formula of the energy associated with the dislocation we can see that this formula actually given the energy per unit length so when we multiply by the dislocation density then the units becomes for example SI into dislocation, density is having the unit 1 by meter square, so basically the Joule per meter cube, that means the total energy when we multiply the dislocation density within the sample itself then it represents that the amount of energy per unit volume. So to do that we can see that within the sample itself the existence of the dislocation is like that, 50% of the dislocation is edge dislocation and 50% of the screw dislocation.

So that is why the WEL is the amount of the energy calculated for the edge dislocation and 50% we consider we multiply by the half of the density that is the 50% of the dislocation is associated with the edge dislocation and another 50% is associated with the screw dislocation. So finally we can find out the half of dow into the energy associated with the screw and edge and that is the neutral. So this amount of energy actually represents the amount of energy per unit volume, this is the first answer of the first question. Second question is that if all the dislocation energy converted to the heat energy then how we can solve this problem, what maybe the temperature rise in this case.

Now if suppose there is a transformation of the one dislocation energy to the heat energy, in this case the amount of the heat energy is estimated is the rho cp delta t. This rho is actually not the dislocation density, this rho is actually the density of the specific material and this is the material property of it and cp is the specific heat and delta t is the temperature rise. So we can check the units also whether the units constructively is there then we can find out easily the temperature rise, so you see the density of the material is the SI unit is kg per meter cube and specific heat is the Joule per kg Kelvin and suppose increment of the temperature is in Kelvin so that actually represents Joule meter cube, so in that sense this actually represent the amount of the heat energy for unit volume, so once this also represents the amount of energy per unit volume. So in this case maybe we can make it equal total energy and the heat energy

and from there we can find out what is the increment of the temperature if others data are available for this problem.

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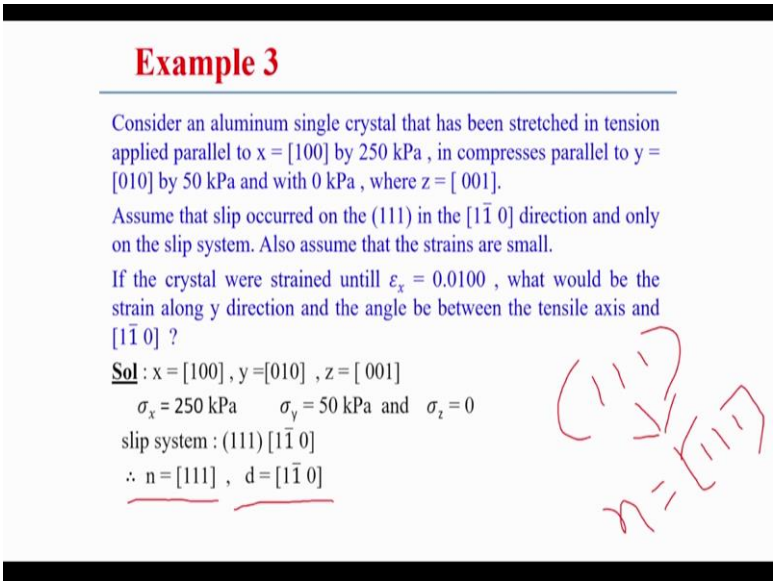

Now we shift to the third problem. Here if we consider a aluminum single crystal that has been stretched in tension applied to the axis x by 250 kiloPascal in compression parallel to the y axis that is 010 and by 50 kiloPascal and with 0 kiloPascal in the z direction. Basically z direction there is no load, there is no stress. Now assume that slip occurred on the 111 plane in the 1 minus 1 0 direction and only on the slip system. Also assume that the strains are very small so basically it is a small strain problem. And if the crystal per strain until some specified normal strain along x direction is 0.01 then what could be the strain along y direction and angle between the tensile axis and 1 minus 10 direction.

So to solve that first we can define the x, y, and z axis of the unit cell, so x direction represents 100 that is Millar index x, y direction 010 and z also 001. So define that x, y, z axis. Now the stress state is like that sigma x is equal to 250 kiloPascal, sigma y equal to 50 kiloPascal and sigma z equal to 0. And slip system is define as 111 plane and 1 minus 10 direction, so when you try to estimate the resolved shear stress in a single crystal structure we define the slip plane is the one specific plane and the slip direction we define as a d here, and normal to the slip plane direction actually represents the 111. If we know that 111 is the slip plane so that normal to that slip plane is the direction of basically 111 same index bar it indicates the direction.

So once end to the normal slip plane direction define d alone direction in which direction the slip occurs and we define the x, y and z direction and x, y, and z direction is subjected to the amount, this is the, there maybe subjected to the different type of stress state along x direction sigma x, along y direction sigma y and along z direction sigma z.

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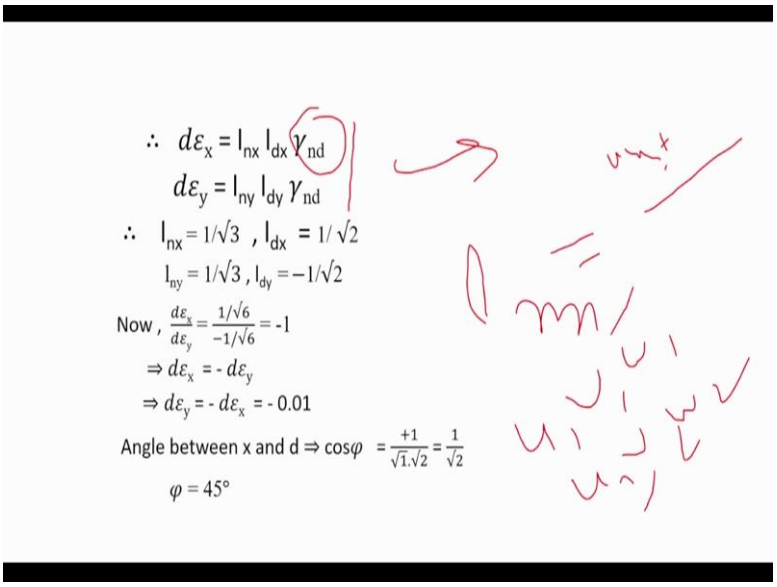

Now once we can estimate this thing, now we can estimate the incremental strength there is small strain along x direction is basically we need to consider the direction cosines lnx and ldc, here and this is the gamma nd is basically the amount of the shear strain on that slip plane. Actually the shear strain on the slip plane is basically independent of the amount of the external stress of strain. Similarly this we can found out that the increment of the strain along y direction also by looking into the direction cosine and we can link into the strain on the slip plane but this actually estimation comes from the very first module where we can estimate the transform of the axis and we can represent the relation between the stress, strain state between the two axis in terms of the direction cosines.

Now how to define the direction, how to estimate mathematically the direction cosine lnx is simply the x direction and n direction have already defined and then from this vectors maybe we can estimate that direction cosines is like that suppose u1, v1 and w1 and u2, v2 and w2 is the two direction, and we can find out that u1 u2 plus v1 v2 plus w1 w2 by root the power of b1 square plus w1 square into u2 square v2 square plus… This formula we have already derived, we have already shown that how we can estimate this amount of the direction

cosines. So once we can estimate the direction cosine it can be like that lnx equal to 1 by root 3, ldx, lny and ldy so that means direction cosines d and y that is define by ldy in this case.

Now once we define the direction cosines we put it here and we can find out that amount of the increment of the strain along x and y direction and we found out that the ratio is coming minus 1 so that d Epsilon y is same as the d Epsilon we plot in the negative magnitude and this is the way the answer of the first question that if the crystal strain limit is until 0.1, 0.01, then what maybe the strain along y direction, so strain along y direction is this one. Now second question is that what the angle be between the tensile axis and 1 minus 10 in this two direction, how we can estimate the angle.

So tensile axis in this case if you see the problem that already define that kiloPascal is applied in the x direction and that is in tensile load, so that means we have to find out that angle between the x axis and 1 minus 1 0.

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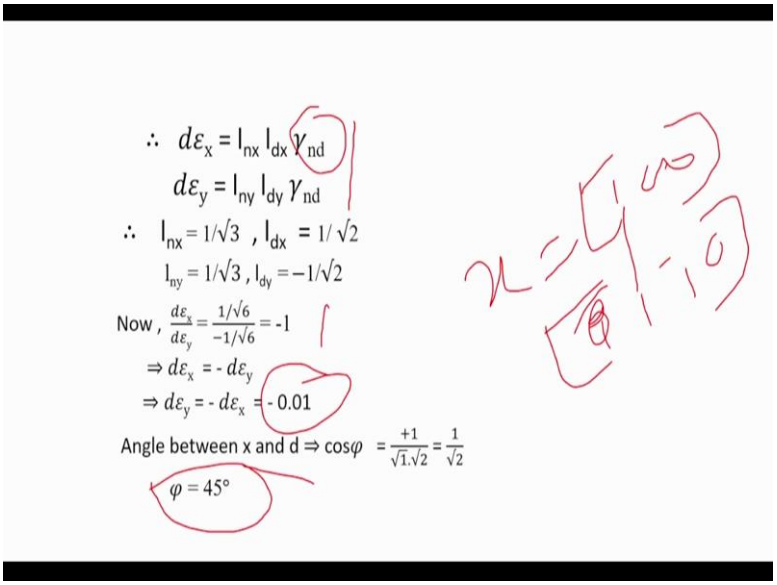

So x axis that is define 100 and minus 1, sorry 1 minus 10, this two direction you can find out easily, so you can find out that cos phi between x and d are multiplying by this component 111 and other component is 0 upper side and lower side, root the power of 1plus 1, another case is root the power of 2, so it becomes 1 by 2 so phi becomes 45 degree.

So these are the way we can estimate the angles between the two axis and if there exist some slip system and which direction slip occurs and how to know the normal to the slip plane and which direction the slip will occurs so these kind of problem, when we will try to solve this

thing first we need to define completely what are the different axis x, y, z axis then we need to define the slip direction d axis and then we need to define the normal to the slip plane x axis. So once we define all this axis system then systematically we can estimate the different direction cosines and in terms of the direction cosines we can correlate the amount of the stress or strain and finally we can solve this problem.

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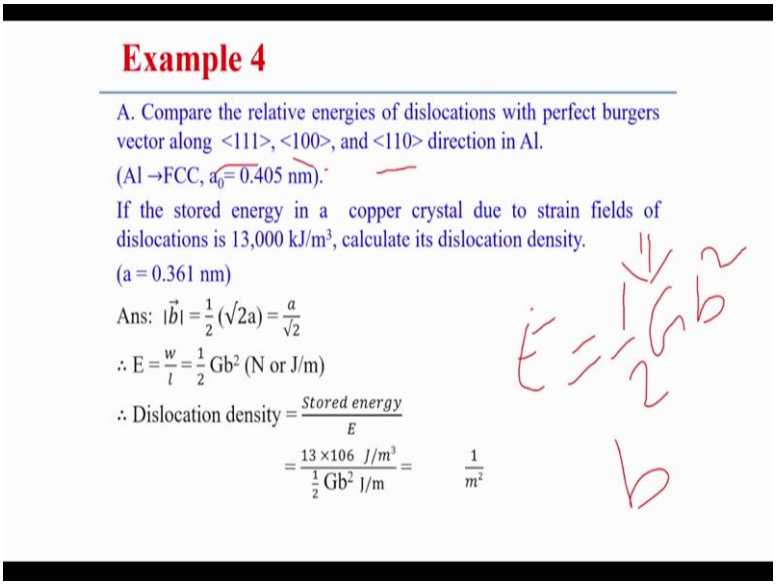

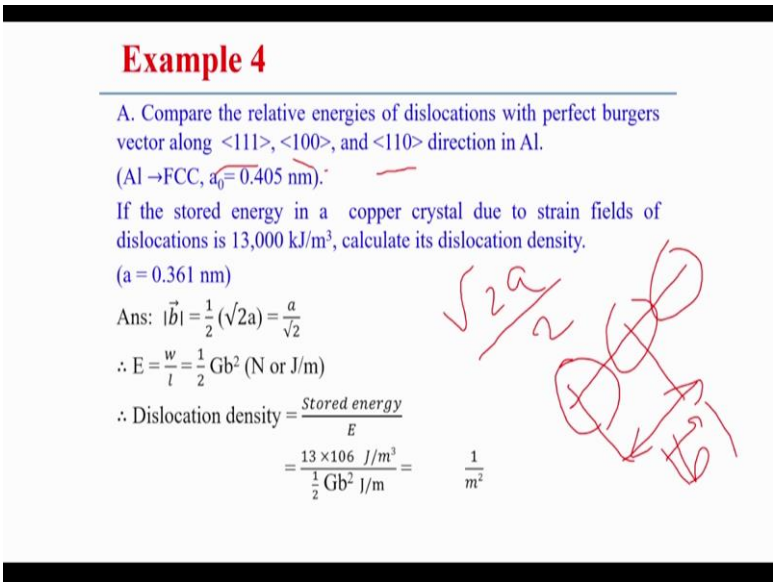

Now we try to, next problem is that here compare the relative energies of dislocation with perfect Burgers vector. Burgers vector in the sense that dislocation of the unit strength actually represented by the perfect Burgers vector and that Burgers vector actually represented in the shortest repeat dislocation in case of the simple cubic structure. So with

perfect Burgers vector along 111, 100 and 110 direction in case of aluminum. We know that aluminum is having FCC crystal structure and the lattice parameter of the aluminum is also given here. If the stored in a copper crystal due to strain fields of dislocation is this one then calculate its dislocation density.

So first thing is that first problem how we can solve it that compare the relative energies of dislocation with perfect Burgers vector so that since here to solve this problem we know that amount of the energy is basically half of Gb square, but remember here this problem we are not explicitly define what is the size of the core, when that data not available we can assume that the amount of the energy associated with a dislocation is simply representation e equal to half of Gb square. So that energy is per unit length, but in this case G is the shear modulus symmetrical property we can easily define or it is or it can be defined, it should be given here or it should be known.

And second is the Burgers vector but we need to estimate the Burgers vector for aluminum in this case, aluminum is having FCC crystal structure and lattice parameter also given. So perfect Burgers vector in this case can be consider as the shortest repeat dislocation that means along the phase diagonal, the half of the phase diagonal that is the shortest repeat distance here represents the Burgers vector. So that Burgers vector is specifically root to a 0 a by 2 half of that, this is the perfect Burgers vector and a is given here and from here we can find out the Burgers vector.

So once we estimate the Burgers vector we can estimate the amount of the energy associate at the perfect Burgers vector in different direction, but point is here that we can easily find out the perfect Burgers vector along 111 direction, but may be the perfect Burgers vector if we consider that there existence of the perfect Burgers vector along 100 direction in this case we need to find out what is the shortest repeat distance along 110 direction then we can estimate the Burgers vector in all the in case of FCC structure. And once we estimate the Burgers vector then we can find out the amount of the strain energy.

Now second part of this thing if the stored energy in the copper crystal due to strain field of the dislocation is given a sum kiloJoules pre unit volume is given calculate its dislocation density.

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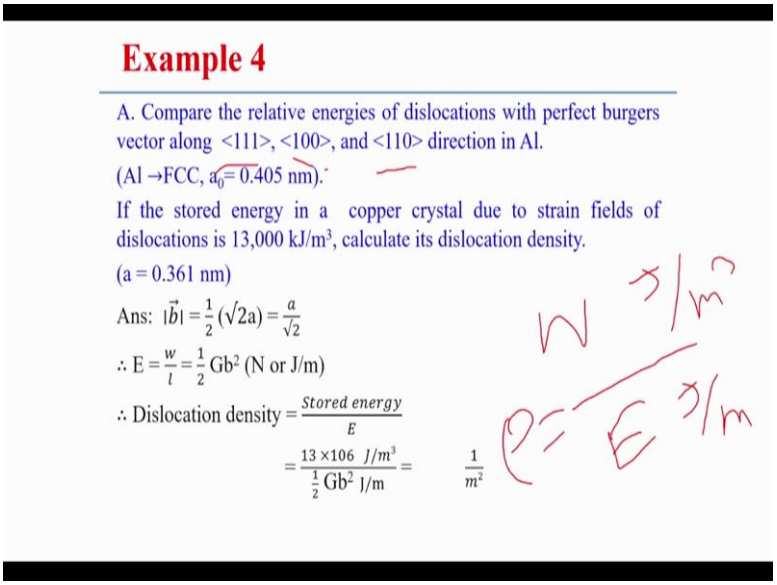

So once that means the amount of the energy actually stored energy is given here so for example, stored energy is w. So that stored energy actually given per unit volume, and we know that is the strain energy per unit volume that is for example E so in this case it is Joule per meter. That actually ratio represents the dislocation density, so with this relation we can find out that what is the, sorry in this case we can find out what is the dislocation density in this case we are just simply tracking the unit consistency to solve to this kind of problem. So it is like that only, physically if we consider there is a small sample of the materials and within that sample of the materials there exist several dislocations.

So when there existence of the several dislocations and we try to estimate the amount of the energy associated with the dislocation then we need to consider what is the dislocation density with that sample. So that can be linked and then we have already estimated the amount of the energy associated with the single dislocation. So once the single dislocation energy is associated and the total, so for a sample what is the amount of the total energy then we have to link with the dislocation density to find out the amount of the energy associated with the whole sample. So that's why it is simple looking into the unique consistency the relation between the dislocation density and the amount of the energy associated with the single dislocation and amount of the energy measured as a bar from the whole sample.

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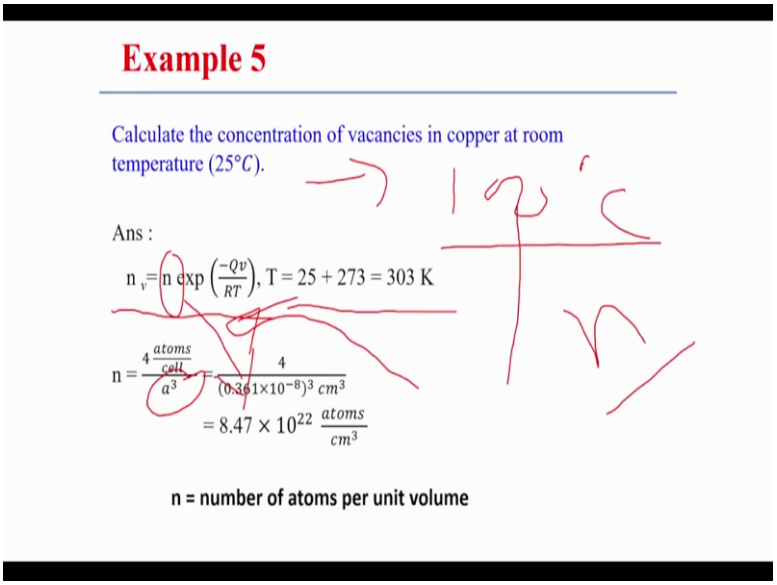

Second problem, next problem we will try to look into that calculate the concentration of the vacancies at room temperature basically here we are going back to the problem related to the crystal imperfections and crystal defect. So that how we can solve this problem that the concentration of the vacancies in the copper at a room temperature as a (())(28:28). So here you see we have already know, we have already explained that the amount of the vacancy in case of crystal structure can be represented by this type of equation where nv equal to n exponential minus Qv by RT. So basically the Qv is the activation energy to create the defect like vacancy.

R is the characteristic gas constant, t is the temperature and but what is the n here. In what way you can represent the n here. Now here the temperature is given is the room 25 degree so when you try to solve this problem and it is better to use the temperature unit in terms of the Kelvin and not in degree centigrade. So we are converting the temperature unit in terms of the Kelvin, then we can found out what is the number of atoms per unit volume, so the calculate the concentration of the vacancies in copper so that n in this cases the n actually represents the vacancies, number of vacancies or number of concentration vacancies that can be considered as the defect per unit volume.

So when you try to represents on this per unit volume how we can do that in case of copper having FCC structure, so in FCC structure what is the total number of atoms per unit cell. We know that there are 4 atoms per unit cell, now what is the volume of the unit cell, so volume of the unit cell is basically the a cube, a cube is the lattice parameter so edge, edge of the

volume of the cube basically. So then when 4 divided by the a cube so that actually represents the number of the atoms exist per unit volume, once you convert the number of atoms exist unit volume and we apply the available data activation energy, what is the temperature is given R it is known then we can find out that number of vacancies of copper at a room temperature.

Actually the number of vacancies it varies depending upon the temp, if there is a variation of the temperature then actually number of vacancies generally increases. So this calculation can be different if for example what is the number of vacancies of copper if it is 100 degree centigrade, definitely the number of vacancies 100 degree centigrade will be different, but n actually given is the n actually we have calculated the number of atoms per unit volume looking into the crystal structure at room temperature.

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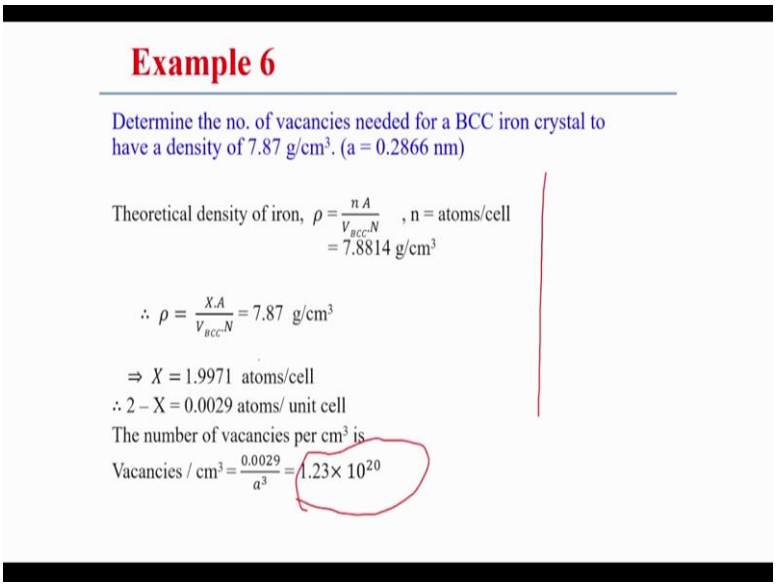

Next problem, it is necessary to found out that determine the number of vacancies needed for a BCC iron crystal to have a density of 7.87 gram per centimeter cube. Remember that when you try to measure the density, for density we measure for a sample 7.87 gram per centimeter cube and lattice parameter is also given. Now looking into the information of this density we can found out what are the number of vacancies actually needed in a BCC crystal structure to maintain this density values of the 7.87 gram per centimeter cube. Here we see rho equal to nA by volume V BCC, n is the Avogadro's number. So n is the, n actually represents the atoms per unit cell.

So this is the simple formula of estimating the theoretical density of the specific crystal structure. Now since if we know for specific crystal structure and n, A, V BCC n the lattice parameter is well defined so we can easily estimate the theoretical density of a material. Once the material is define then crystal structure is also define all are define. But since the this density is actually not exactly the theoretical density of the material is it some deviation of the theoretical density of the metal presence and assuming that presence of vacancies actually there is a change of the density.

So to look into that assuming that there is a x number of atoms exist within the x number of atoms exist per unit cell to compensate the presence of vacancies within the unit cell. So once we do that rho equal to xA by c and everything and C and density is given here, from here we can simply calculate what is the x value here. So once x is estimated the 1.9971 atoms per cell. So that means that 2 minus x because 2 is the perfect crystal structure without any defects, the total number of atoms per unit cell is 2 in case of the BCC structure. So then 2 minus x actually represents that number of atoms per unit cell is basically represent the equivalent to the vacancies presence in that specific circle.

So once per unit cell can know when you multiply that volume of the unit cell can know you multiply that volume of the unit cell then we can the vacancies per unit volume it maybe very high. So in this case typical idea that 1.23 10 to the power number of vacancies exist per 1 centimeter cube volume of incase of BCC structure. So this are the way to find out the different problem associated with the different or maybe vacancies exist within the crystal structure, so due to the presence of the vacancies it may not be exactly equal to the theoretical density of a perfect crystal. So this is the one way to estimate the number of vacancies in case of BCC crystal structure when we as a gross measure the density of the specific metal that is the different from the theoretical density of the specific material.

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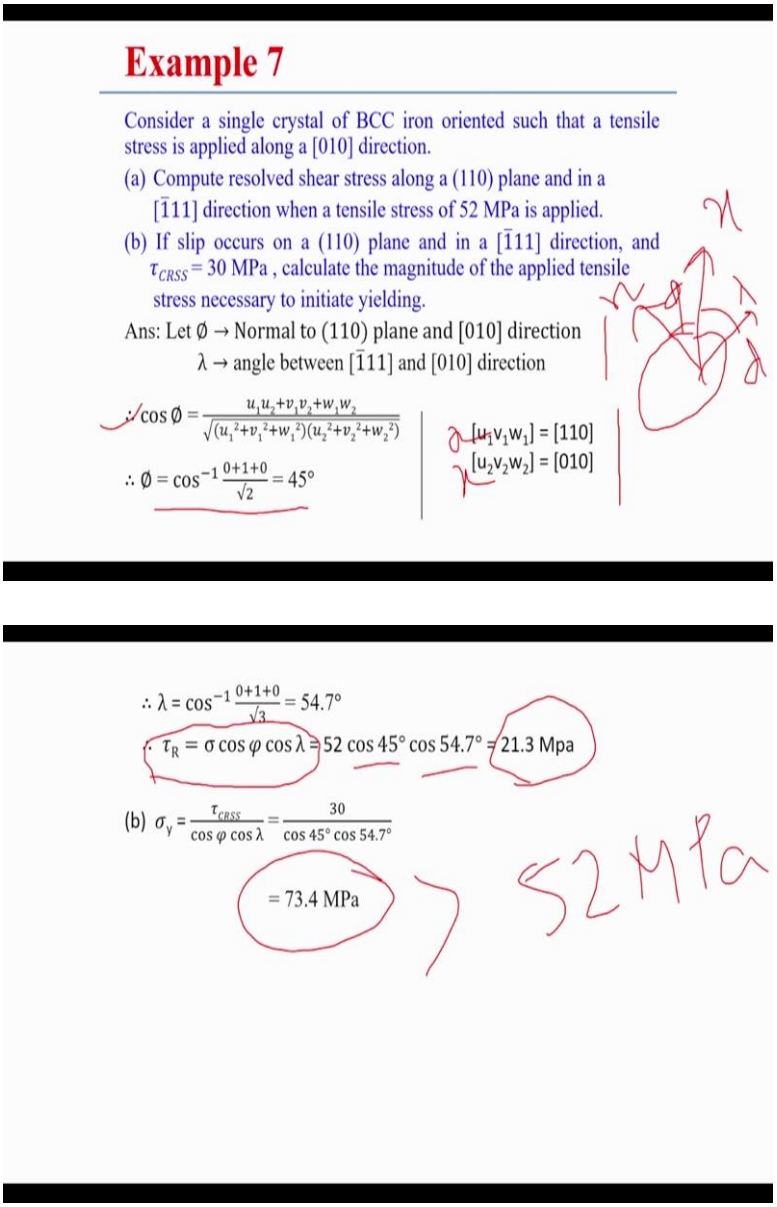

If we look into the next problem here if you see need to consider a single crystal of BCC iron oriented such that a tensile stress is applied along 010 direction, so it is well defines the tensile stress is acting one specific direction among x, y, and z. Compute the resolved shear stress along on 110 plane and in a minus 111 direction when a tensile stress of 52 megaPascal is applied. This is the first problem and second problem if slip occurs on that plane and in that direction and critically resolved shear stress is define then calculate the magnitude of the applied stress necessary to initiate the yielding. So that applied tensile stress should be different from the resolved shear stress and let us look into the first problem, how we can solve this problem.

So first we define that normal to the 111 plane and 010 direction, let us look in define the angle is phi in this case. So that means I can say suppose this is the slip plane and this is the direction d and this is the axis x and we define the normal to the slip plane is n. So phi is normal to the slip plane and between the 010 which direction the load is acting, so this is basically phi. A lambda angle between the slip direction d and the x axis which direction the load is applied, suppose this is the angle lambda. So once we define phi and lambda and then we know the n, x and d direction simply we can find out cos phi looking into the formula and then we found out phi equal to 45 degree and u1 v1 w1, u2 v2 w2 is defined 110 or 010 that means, 110 normal to this plane, this is n and this is x. So here you can find out phi.

Similarly we can find out lambda also and we can found out, once we find out the lambda we can find out the resolved shear stress on the slip plane is this one sigma cos phi cos lambda, cos phi cos lambda sigma is the normal stress is given 52 megaPascal and finally we can found out that 21.3 megaPascal is the resolved shear stress along the direction d. Now on the same slip system if the critically resolved shear stress is 30 megaPascal what maybe the normal stress is required to start the yielding, so what maybe the normal stress acting along the x axis to start the yielding.

Similarly replace the tau r resolved shear stress in terms of critically resolved shear stress so critically resolved shear stress just about to start the slip process, then if we put it and we can found out that sigma y equal to 73.4 megaPascal that means here if you see critically resolved shear stress is more than the resolved shear stress so when critically resolved shear stress we put the limit and we can say just start the yielding of the material on this crystal structure and we can find out which is 73.4 which is more than what was initially it was applied stress on 50 megaPascal it is more than that of the initial stress value. So if we apply the 73.5 megaPascal the load it will just to start the yielding on the slip plane along the slip direction.

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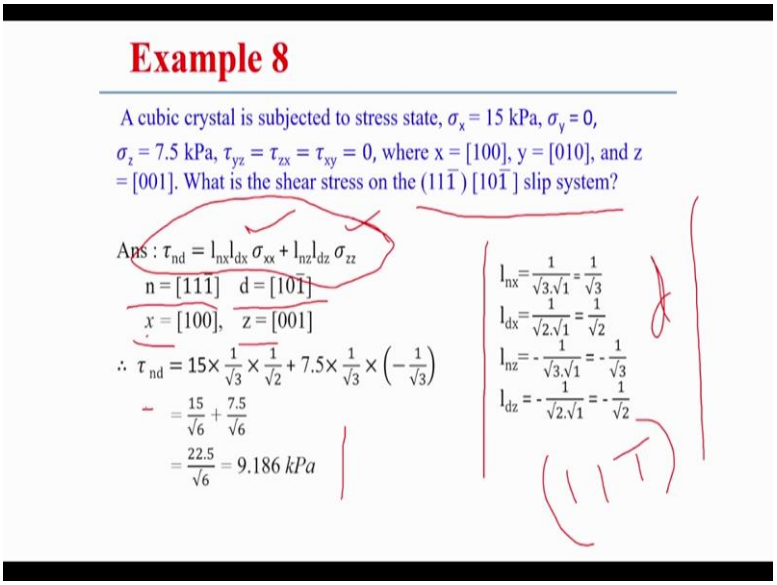

Now look into another problem we say a cubic crystal is subjected to the stress state sigma x equal to 15 kiloPascal, sigma y equal to 0, sigma z equal to 7.5 kiloPascal and the shear stress, all the shear stress component are 0 and we have defined the x, y, and z axis. Now what is the shear stress on the slip system. This type of problem we have already solved but here we just look into see that when the slip system we define, here we define the slip system means we need to define the slip plane and the slip direction. So slip plane is defined 11 minus 1 that is the plane and direction d is here, is basically here we can define that d is basically 10 minus 1.

And slip plane is 11 minus 1and normal to the slip plane direction n equal to 11 minus 1 and we define the x, y and z axis, x and z axis we need that, now we need to estimate here we can find out the direction cosines lnx, between the two axis n and x, ldx between d and x axis, lnz between n and z axis, ldz between d and z axis, so we can find out all the direction cosines here. Now shear stress tau nd can be represented like that that lnx, ldx, sigma x axis, lnz ldz sigma zz this we simply consider the transformational axis rule in terms of the direction cosine and we have not consider the other components stress, stress component because stress component along y direction it is 0 and all other shear stress component are 0.

So that is why out of 6 component 4 components of the stresses are 0 only we consider the two component of the stress and we can solve this problem. So here we found that shear stress on the slip plane is 9.186 kiloPascal. So this is simply way, once we define the slip

plane and we can found out the stresses acting on the slip plane by considering the system of slip system and defining the different axis or difference, stress state on the specific problem.

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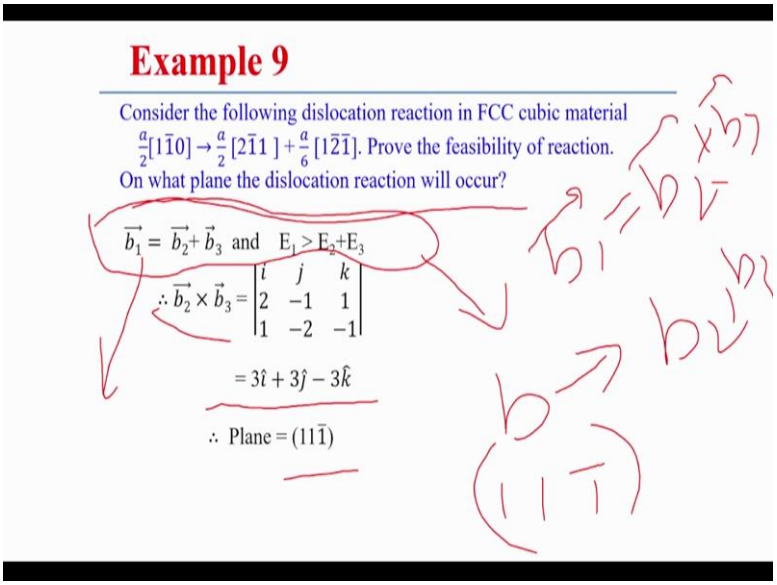

Now finally we consider another problem, let us look into this, consider the following dislocation reaction in FCC cubic material and the reaction is define, dislocation reaction prove the feasibility of the reaction and second question is the on what plane is the dislocation reaction will occur. So first thing is the feasibility of the reaction we have already discussed. To prove the feasibility of the reaction we try to satisfy the first checking, whether it is satisfying the vector sum rule or not, that means left hand side and right hand side, total components of the x, y, z component of the vectors are satisfying or not. Second checking their energy level, what during the reaction whether the energy level decreases or not. If both are satisfied then we can say the reaction is feasible.

Now second part on what plane the dislocation reaction will occur, so in this case here the assuming that b1 is decompose into maybe b2 and b3, now b2 and b3 are Burgers vector or b2 and b3 is define and that work basically partial, so when b2 and b3 is define, if you do the cross product of this vectors between b3 you can found out that this vector 3i plus 3j minus 3k, this indicates actually Millar index of this plane is minus 1, so simply that the reaction will basically occur on this plane 11 minus 1. So this is the way we can check the feasibility of the dissociation of the dislocation and we can define that which plane this reaction, the complete reaction will occur that means b1 is the total full length of the dislocation and b2 and b3 are the partials for this dislocation.

So hopefully we will be able to understand this crystal part of the, first part of the crystal plasticity by looking to the very basic elemental problems associated with the theory and it will be, I think it will be helpful to basic understanding of the concept of the dislocations and how the dislocation is basically influential to explain the different phenomena specifically the strengthening of the part. So this examples are given or explained only to strengthen the knowledge of the application of the very basic elemental theory so far we have learned.

Thank you very much for your kind attention.