Advanced Material Characterization by Atom Probe Tomography and ElectronMicroscopy

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Week-06
Lecture-16

So, welcome to this class. In the last class, we briefly went through the introduction of the reconstruction of the needle specimen. It briefly described the point projection model and how this model can be used in a reverse point projection model. which is used to reconstruct the actual needle specimen after the field evaporation. Okay.

So, as mentioned in the last class, the reconstruction has two important aspects. One is the lateral positions. Another one is the depth coordinate. Okay. So, fundamentally, the first approximation

is that only the atoms that are protruding most from the surface are field evaporated. Okay, so which is subjected to a strong electric field at the local atomic scale. So, the atoms which are protruding most as compared to the neighboring atoms, those get field evaporated. Okay? This particular assumption, okay, underpins the shell model.

The shell model, which was proposed by Moore in 1967. Okay? So, here the atoms are actually likely to evaporate. They are likely to evaporate if they belong to a thin shell at the surface. Okay.

So, if this is a shell, then there should be a thickness of the shell, a thickness of the shell. This thickness is directly related to the penetration of the electric field into the surface of the specimen. Okay? So, The atoms protruding at the surface get field-evaporated, and it was assumed that they belong to a thin shell.

Okay? And that thickness of the shell is directly related to the penetration of the electric field into the surface of the specimen. Okay? And this penetration depth, this penetration depth, okay, is of the order of sub- It is much, much less than the D-spacing of that particular crystal structure.

Okay? This thickness corresponds to the skin depth. Skin depth. Now, this electrostatic electric field F Okay, so, we know that the electrostatic electric field is proportional to the surface charge density, which is sigma e divided by epsilon not.

Okay, this is the electrostatic field. And E0 is the dielectric permittivity. Dielectric permittivity. Okay. And surface charge density is nothing but the number of charges in a thin shell with a thickness of dp.

Okay. So, the dp corresponds to the Penetration of the electric field, the distance of penetration of the electric field into the surface of the specimen. Okay? So, here then the dp is given by ne divided by Fe0, where ne corresponds to the electron density of the volume. Okay.

And the penetration depth can be calculated to be in the range of a few picometers, which is less than the interplanar spacing of the crystal structure of the specimen. Okay. So, this shows that theoretically the atoms get field evaporated. By layer by layer or atom by atom, layer by layer from the outermost shell towards the inside, okay? So, the sequence—so here the important aspect is the sequence. The sequence in which the ions are detected relates to the depth of atoms removed from the sample surface.

So, this sequence is very important to understand the depth at which these atoms are removed from the original sample. So, most of the protocols... Most of the protocols rely on the exploitation of this particular order or the sequence of the detected ions. That is how the Z-depth is created. So, we will just go through some of the equations to understand how this Z is calculated.

So, before going to the Z, we know that the detector coordinates will be given by XT and YD. So, this enables the XY position of that particular ion, and with the study of the sequence—the protocols for the sequence of the removal of atoms—that gives you the Z position. This is how we get the XY and Z position in three dimensions. And the mass-to-charge ratio gives the time of flight, okay? So here, each ion which is detected will have an atomic identity, and

And also, the most important point is the atomic volume. Okay, so this particular atomic volume is used to determine the Z or the depth of the Z sequence of the removal of atoms from the tip surface. Okay, so basically, the reconstruction—the process of reconstruction requires the first important point: the knowledge of the radius of curvature for each ion detected. The evolution of the radius of curvature of each ion detected is necessary to compute the original location at the specimen surface. Okay.

So, due to the—you know that the shank angle is not zero. Okay. The shank angle—the specimen gets, so as these ions get, the atoms get ionized and field-evaporated, the specimen gets blunted. Okay. Blunted means the radius of curvature or the radius increases, or the curvature decreases.

So, to maintain—due to which there is a reduction in the radius of curvature, it means that the electric field also drops. Okay? And this induces a drop in the detection rate. Okay, so to counterbalance this detection rate—if you want to keep a constant detection rate—then the voltage is increased, high voltage is applied during the experiment to maintain a constant detection rate because there is an evolution of radius or an increase in the radius as the field evaporation progresses.

Okay, if we assume that the electric field is homogeneous, across the specimen surface, and this electric field is very close to the evaporation field of that particular material. Then, actually, the radius of curvature you can get by the equation V divided by KF Fe. Okay. Assuming that the electric field is homogeneous and it is near the evaporation field of that particular material,

you can get the instantaneous radius, which is given by the voltage applied divided by the field factor Kf and Fe, which can be estimated. Okay. So, As we described, Kf is the field factor, okay, and Fe is the evaporation field, which we are assuming is a constant for a given material. Okay, and here the voltage

Here the voltage... So here the voltage can be given as the DC voltage, which is applied, plus the pulsed voltage in HV pulsing. Now we will talk about the depth coordinate. Z, okay, and this Z is actually deduced from the ion evaporation sequence which we just

now described about the importance of the sequence of atoms, correct? So this is deduced from the ion evaporation sequence as the ions are removed.

atom by atom, or we can say layer by layer, the specimen surface becomes farther from the detector, okay? The specimen surface becomes farther from the detector. For each ion added to the reconstruction, during the process, the emitting surface shifts by dz, okay? Okay, and the Z tip, which I plus 1, we can write as equal to Z tip for the ith atom plus dz. So, this is the equation we use for defining Z, and that evolves during the field of operation where the surface shifts automatically.

opposite to the detector, and opposite to the detector as the evaporation takes place. Okay. So, the calculation of depth increment is the one term which is used to calculate the depth, and it is the volume analyzed. Okay. So, this analyzed volume, analyzed volume—

is the sum of volumes for each evaporated ion, which can be given by omega i. Okay, so volume evaporation can be given as the number of ions evaporated, their summation of volume, which can be equal to what we can write as NeVf divided by this one. Okay, so here omega corresponds to the average atomic volume. and NeVAP corresponds to the total number of evaporated ions. Okay. So, we know that not all the evaporated ions will be detected.

So, there will be a detector efficiency. So, we can write it as Nd is equal to Nd is the total number of detected ions, and η is the detection efficiency. Okay? Fine?

So, this is Nd equal to η multiplied by NeVAP. So, the analyzed volume can be related to the geometry of the specimen. Okay? So, here Okay, so the analyzed volume can be related to the geometry of the specimen.

So, here we can give as a, so V_EVAP equals the integral from 0 to Z_max of W_V(Z) dZ. Here, this particular W(Z) is a function describing the increase in the analyzed volume. Increase in the analyzed volume of the specimen as the specimen is field-evaporated. Okay. So, the dZ can be given as the atomic volume divided by nW_bZ.

Okay. So, Most of the new protocols depend upon the evaluation of this WVZ. Okay. Which is the function describing the increase in the analyzed volume of the specimen as the specimen is field-evaporated.

Okay. So, This is the basic thing which is related to how to evaluate the Z. And combining this point projection model with this, which is proposed by Bas et al., a simplified point projection model. Okay, so, we can, as magnification of projection is equal to D by d, which is equal to, which can be written as L by image compression factor divided by R. Okay.

So, here the D is the distance from the ion impact point to the center of the detector. Okay. And the d is the distance between the specimen axis of the projection of the ion into the plane. So, in this figure, it is written, it can be understood. Okay.

So, here the And the projection is equal to D by d, which is equal to L by R. Okay, so D is the distance from the ion impact point. This is the ion impact point to the center of the detector. And d is the distance between the specimen axis and the projection of the ion into the plane. This particular.

Into the plane which is perpendicular to the specimen axis. Projection of that particular ion into the space which is perpendicular to the projection axis. Okay, so assuming that ions are projected along straight trajectories, as we described for the reverse projection model. So, the relationship between x and y position towards xD and yD can be written as x equals xD divided by M projection and y equals yD divided by M projection in two dimensions, correct?

And the field evaporation takes place about a volume, correct? In this figure, you can see that this is your needle, okay? And the field evaporation takes place for a volume, correct? And this field evaporation V_evap can be written as Sa into Da, okay?

So, here the SA is the analyzed area, two-dimensional area, analyzed two-dimensional area, which is, okay? This is SA. And the DA is is the analyzed depth is the analyzed depth which in the schematically it is written as da okay so the size of the region of specimen surface lying within the field of view is called the SA.

Within the field of view, the size of the specimen in two dimensions is represented as SA. And we can tell that volume of evaporation can be assumed to be SA into DA. By small angle approximation, that This SA can be assumed to be the reverse projection of this particular SD, which is projected on the fluorescent screen, on the screen. Correct?

So, the reverse projection of the detector in the plane tangent to the specimen axis can be written as Sa, can be written as SD divided by the magnification of projection squared, as this is an area. Correct? So, This is written. So, SD is the surface of the detector.

SD is the surface of the detector, and M projection is the magnification of the projection. Okay. So, assuming with these equations that the atomic volume is distributed homogeneously across the area—okay, atomic volume—then we can write WVZ as equal to Sa. And from the earlier formula, R is equal to V divided by KF Fe, the evaporation field.

dZ is written as the atomic volume divided by efficiency and this particular function, which is responsible for the projection, and M projection can be estimated by L divided by the image compression vector R, and Sa is equal to SD divided by M projection squared. By using these four equations—these five equations—you can write it as Sa is equal to SD divided by L divided by xi R whole square, which can be written as dz equal to atomic volume L squared divided by SD xi R squared, and dz can again be written by using this equation. We can write it as atomic volume L squared kf squared field evaporation field squared divided by efficiency SD xi squared

voltage applied. Okay, so this projection generates the atomic positions within the plane tangent to the specific tangent to the specimen axis. So, in this figure, as I told you, if you see this particular figure, Okay. So, you are assuming that the atom which is present on the tip surface is projected onto a plane which is perpendicular to the specimen axis. Okay. So, we need to correct this factor because it is a projection. Correct? So, we have now calculated dz

Now, another correction has to be added, which takes care of this plane tangent to the specimen axis. Okay? So, this can be deduced from positions, okay? For the ith ion, for

the ith ion, the dz dash, okay, can be computed as Ri multiplied by 1 minus the square root of 1 minus (xi plus yi) squared divided by Ri squared.

Okay, so for each ion, we can calculate this dz dash, which is a correction that has to be included in the depth calculated by this particular formula. Okay, so the z position of the ith ion can be written as zi equals the summation of dz plus dz i dash. Okay, so this is how the Z coordinate is calculated, based on the assumption that field evaporation is taking place atom by atom or layer by layer. Okay, so in summary, what we have learned is that to build a reconstruction, to build a reconstruction, we need four basic parameters. which have to be calculated.

The first one is the image compression factor. The second one is the field factor. The third is the evaporation field, and the fourth one is the detection efficiency. Okay, and for Z, as I told you, we are assuming that the atoms are evaporated layer by layer, and for this calculation, we are using the atomic volume. We are calculating the atomic volume, and from the atomic volume, we are actually calculating the depth, the Z of the particular ion.

Okay, so, I hope in this class we have explained about the parameters which are needed to estimate the ion position on the detector, especially the x and y position, okay, and the z position which is calculated by the atomic volume. Okay, so, in the next class, we will go through each of the four reconstruction four basic parameters and how to calculate them from the data obtained from the atom probe or the field ion microscope. Okay? So, with this, I will end this class today, and we will meet in the next class.

Thank you.