# Electrochemical Energy Storage
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## Module - 03
## Lithium batteries
## Lecture - 14
## Properties of Electrode Materials (Case Study: alloy as anode)

Welcome to my course Electrochemical Energy Storage and this is module number 3, where I am teaching the Lithium Batteries and today is lecture number 14, where Properties of Electrode Material, I will be describing as a Case Study of alloy as anode.

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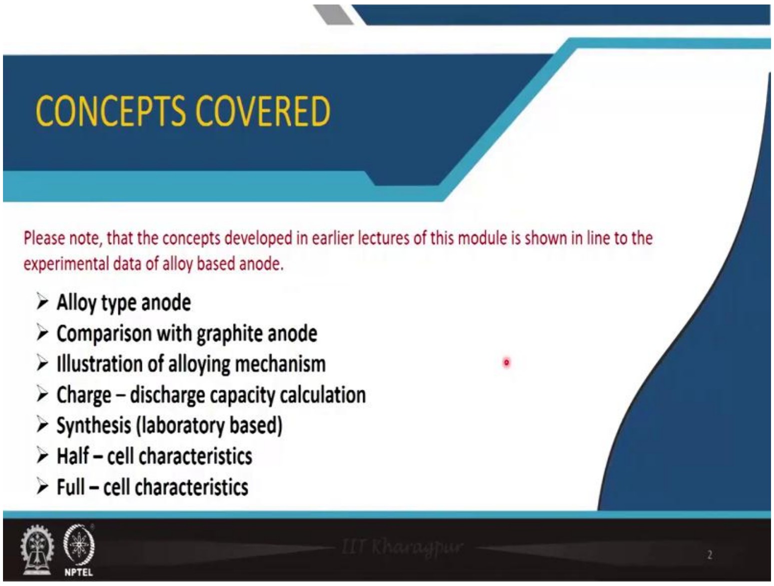

CONCEPTS COVERED

Please note, that the concepts developed in earlier lectures of this module is shown in line to the experimental data of alloy based anode.

- Alloy type anode
- Comparison with graphite anode
- Illustration of alloying mechanism
- Charge – discharge capacity calculation
- Synthesis (laboratory based)
- Half – cell characteristics
- Full – cell characteristics

So, alloy already I have introduced in my earlier classes. Now, you will have to note that the concept that we developed in part of our earlier lectures particularly in this module that is shown in line to the experimental data of alloy based anode. I have already introduced alloy based anode and you can remember silicon is one of them, tin, antimony, germanium, they form alloy with lithium.

So, we will introduce that; and how the electrochemical properties of this alloy, they compare with graphite anode that will be discussed. And then again, I will revisit the alloying mechanism which I have taught as a part of my earlier classes. Then, from the charge discharge capacity, how you can estimate the capacity; theoretical capacity from charge discharge profile that will be taught.

And how this alloy material you can synthesize in a laboratory, because still they have not commercialized. So, whatever data we could accumulate is the data that we have procured from our laboratory experiment. Then, how is the half-cell performance of this particular anodes, and finally full-cell characteristics. So, these are the concepts that I will cover in this course, in this lecture I mean.

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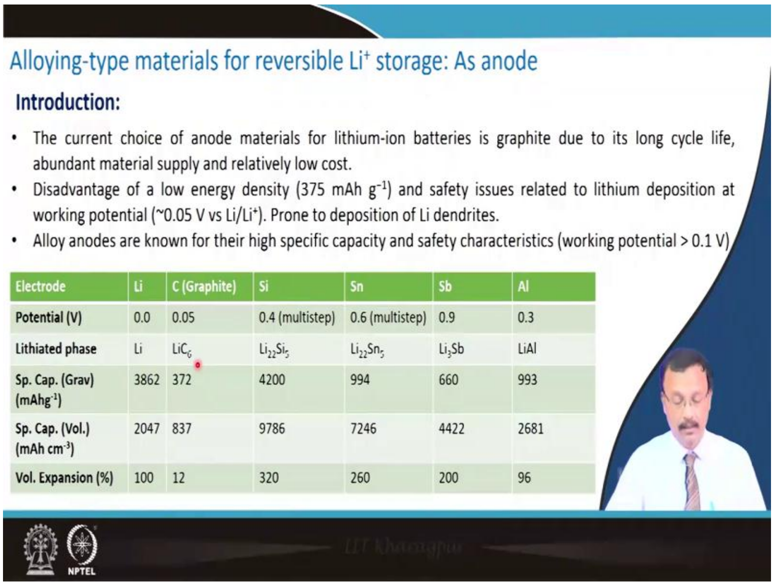

Alloying-type materials for reversible $Li^+$ storage: As anode

**Introduction:**

- The current choice of anode materials for lithium-ion batteries is graphite due to its long cycle life, abundant material supply and relatively low cost.
- Disadvantage of a low energy density (375 mAh $g^{-1}$) and safety issues related to lithium deposition at working potential (~0.05 V vs $Li/Li^+$). Prone to deposition of Li dendrites.
- Alloy anodes are known for their high specific capacity and safety characteristics (working potential > 0.1 V)

| Electrode | Li | C (Graphite) | Si | Sn | Sb | Al |
|---|---|---|---|---|---|---|
| Potential (V) | 0.0 | 0.05 | 0.4 (multistep) | 0.6 (multistep) | 0.9 | 0.3 |
| Lithiated phase | Li | $LiC_6$ | $Li_{22}Si_5$ | $Li_{22}Sn_5$ | $Li_3Sb$ | LiAl |
| Sp. Cap. (Grav) ($mAhg^{-1}$) | 3862 | 372 | 4200 | 994 | 660 | 993 |
| Sp. Cap. (Vol.) (mAh $cm^{-3}$) | 2047 | 837 | 9786 | 7246 | 4422 | 2681 |
| Vol. Expansion (%) | 100 | 12 | 320 | 260 | 200 | 96 |

So, as you know these alloy type materials, they are useful for reversible lithium storage and this we will use as anode because of their potential criteria. Now, the current choice of anode material for all commercial battery as you know they are graphite or MCMB. And this is mainly due to their reasonably well long cycle life and of course, the materials are cheap and they are having low cost. So, it is economic for us to use them.

Now, the disadvantage that is their low energy density; in particular the capacities only 375 maximum milli Ampere hour per gram. And there are certain safety related issues and that is due to the deposition of lithium, particularly at the working potential which is very close to 0 Volt versus lithium redox. And then, it is proned to the deposition of lithium dendrite at that low voltage instead of forming the so called anode alloy.

You can remember in one of my earlier lectures, involving gold and lithium, the alloying characteristics; we have summarized all possible reactions at different voltage regime. So, at low voltage, the formation of lithium deposition under potential deposition forming of lithium alloy, they are all applicable.

So, it is no exception with that. And alloy anodes are known for their high specific capacity and safety characteristics. So, working potential is always more than at least 0.1 Volt. So, I have, you have the less possibility of forming the alloy or forming electro deposition of lithium and stuff like that.

So, here this table is very important. Here, I have tabulated the electrode material with potential first, then what are the lithiated phase, then you can calculate the gravimetric specific capacity. Also, you can calculate the volumetric specific capacity using the formula I described earlier and volume expansion also can be estimated.

So, the example is carbon that is graphite, that is pretty well-studied and well-known and it has been commercialized by Sony. Then, apart from that, this silicon, tin, antimony and aluminum. You can see their potential whether they are multistep or not that you can easily identify from their respective phase diagram. So, we will see a one to one correlation.

Then, what are the types of alloy that basically forms at different potentials, so that has been given. Then, you can calculate the specific capacity using the Faraday law, if you know the molecular weight and if you know the number of electron that is being exchanged.

Then, with a certain constant, I will describe it; you can estimate this. So, I leave it on you to estimate the specific and volume metric capacity which has been shown in this table, based on those composition. And also, volume expansion you will have to tackle.

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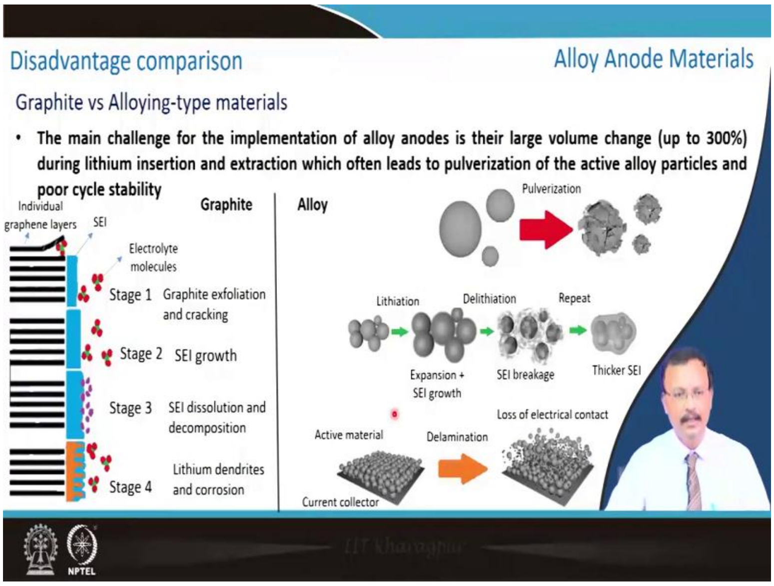

Disadvantage comparison

Alloy Anode Materials

Graphite vs Alloying-type materials

- **The main challenge for the implementation of alloy anodes is their large volume change (up to 300%) during lithium insertion and extraction which often leads to pulverization of the active alloy particles and poor cycle stability**

Now, if you compare this graphite with alloy type of material, this also is a recap. Because already I have spoke about it several times. So, if you see the layered graphite, there are several steps of the formation of this so called solid electrolyte interface. So, you can have the stage 1, where you can see the SEI has formed due to electrolyte decomposition.

And usually, the solvated lithium, the solvated anion, they are actually disintegrated. But if not, then there is a possibility for graphite exfoliation and that leads to the crack of this layered structured material. So, SEI growth which is good because it will not expose the unreacted graphite but at the same time it will be pervious for lithium ion inter collation. So, SEI growth is unavoidable particularly at lower voltage. Then, sometimes this SEI dissolution takes place and it also decomposes.

And once it does that, then you know this layer is formed. Sometimes, it exposes the lithium sorry the graphite here and electro deposition of lithium instead of intercalation, that is another problem and that can form the dendritic structure.

And by this time, you know that if dendrite forms, then they are not a layer by layer growth. But they are a some kind of sharp needle like structure which is floppy in nature that also disintegrate; that can puncture the separator and there could be internal short circuit which can lead to the thermal runaway of the battery.

Now, if you want to replace graphite with alloy, then you will have to tackle this problem. First one is the volume expansion upon lithiation and beyond the critical size you will see pulverization takes place. So, it is disintegrated, and that can lead to the formation of the thicker SEI and not always this SEI will be pervious to lithium ion. So, that is another problem.

And due to the combined effect of this pulverization as well as this kind of SEI formation followed by their disintegration, what happens that from the correct collector, this electrode material is delaminated as you can see here. So, you are losing the active material and this will certainly affect the capacity.

So, these are the major problem which already I have described. So, this picto-graphical view certainly will allow you to understand this mechanism more clearly.

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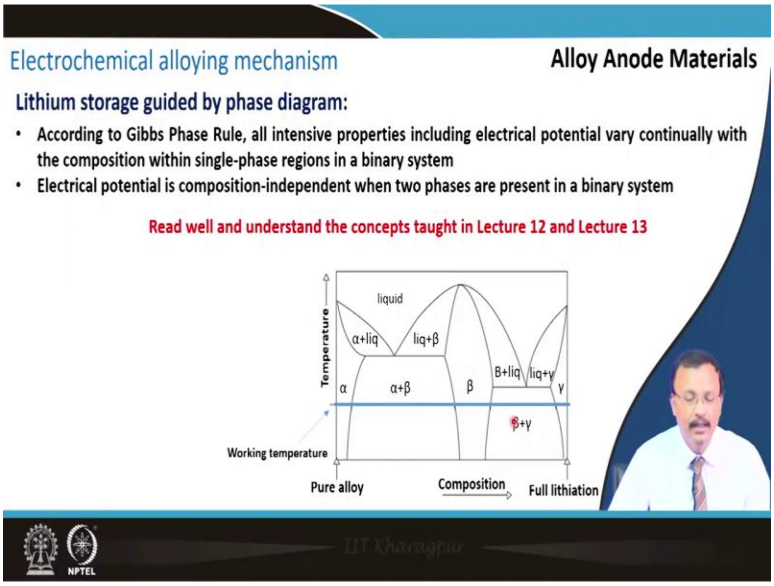
Electrochemical alloying mechanism

Alloy Anode Materials

**Lithium storage guided by phase diagram:**

- According to Gibbs Phase Rule, all intensive properties including electrical potential vary continually with the composition within single-phase regions in a binary system
- Electrical potential is composition-independent when two phases are present in a binary system

Read well and understand the concepts taught in Lecture 12 and Lecture 13

Now, again, I will go back to my general phase diagram and I will ask you to read well and understand the concept that was taught in lecture number 12 and 13; that how to understand the voltage profile once at a particular temperature, you start to change the lithium ion concentration.

So, according to the Gibbs Phase Rule, all intensive properties including electrical properties vary continually with the composition within the single phase region that is alpha and also, within the binary phase region which is alpha plus beta. And electric potential, particularly the equilibrium potential is composition dependent and particularly, when two phase mixture is present in the binary system.

And based on this kind of reaction, you can easily estimate the type of the voltage profile, because you can reconstruct from the phase diagram, the mixing free energy versus composition diagram.

And from there, remember by drawing a tangent, knowing the lithium ion potential in the cathode as well as in anode material and apply to the formula of open circuit potential equal to mu of cathode minus mu of anode divided by faraday constant, you can actually estimate what will be the potential involved.

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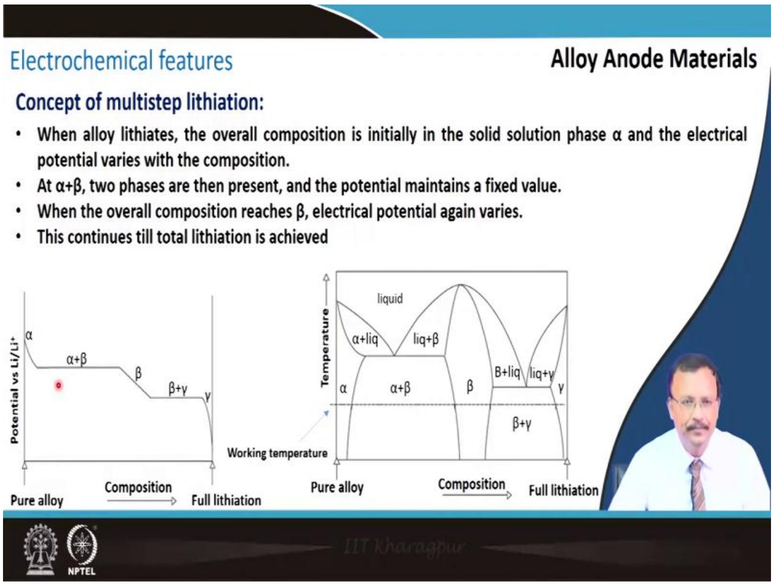

Electrochemical features

**Alloy Anode Materials**

**Concept of multistep lithiation:**

- When alloy lithiates, the overall composition is initially in the solid solution phase α and the electrical potential varies with the composition.
- At α+β, two phases are then present, and the potential maintains a fixed value.
- When the overall composition reaches β, electrical potential again varies.
- This continues till total lithiation is achieved

So, here I have shown the result which is expected when the alloy lithiates; the overall composition is in initially a solid solution phase which is alpha, that is in this region and the electrical potential will vary with composition because you can apply the Gibbs law; the degree of freedom I estimated is equal to 1. So there will be a change a reduction in potential when the lithium concentration is increased in this solid solution.

When two phase mixture is there alpha plus beta, then potential maintain a fixed value, because this has lowest Gibbs free energy. And you remember the line across this composition, where the chemical potential will remain almost constant, so that will lead you to a plateau of the voltage. So, voltage will remain constant and even if you increase the lithium ion content. And beta phase, this is a single phase region; beta plus gamma, two-phase region and again, gamma is a single phase region. So, it will exactly follow the trend which we have seen in case of alpha and in case of alpha plus beta.

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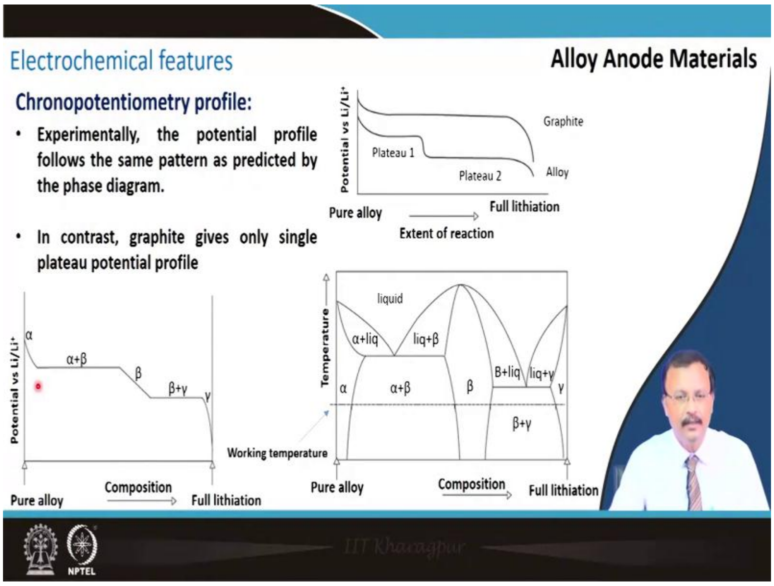

Electrochemical features

**Alloy Anode Materials**

**Chronopotentiometry profile:**

- Experimentally, the potential profile follows the same pattern as predicted by the phase diagram.
- In contrast, graphite gives only single plateau potential profile

So, experimentally, it has been verified in case of graphite as you can see in case of graphite, you have 4 layers, then 3, then 2, then 1 and lithium ion intercalate in it and there is a volume expansion involved here. So, at this particular potential, you can see you can have a plateau and then, when it goes to s 3 or s 2, then you will get another plateau, it is not shown here.

But in case of the two phase mixture, you can have a plateau and then, again another types of mixture, you get plateau number 2 which basically support the theoretical prediction what we have calculated estimated. So, it is in line to that.

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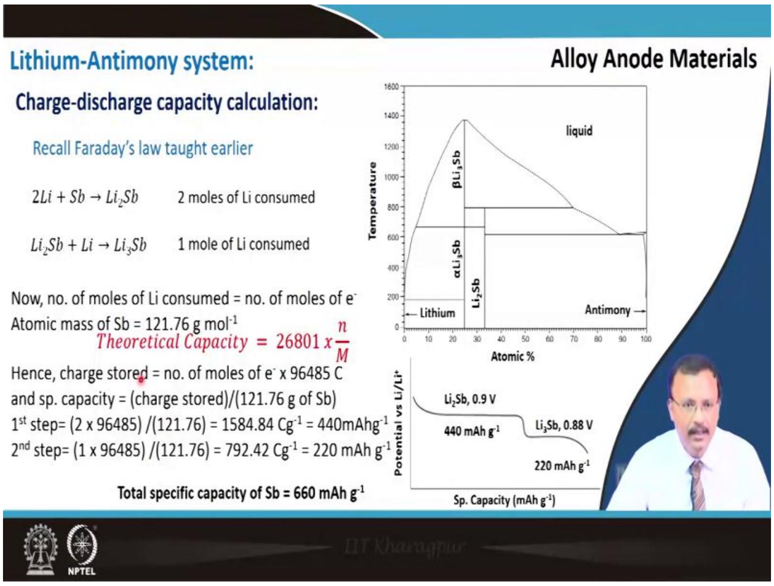

Lithium-Antimony system:

Alloy Anode Materials

Charge-discharge capacity calculation:

Recall Faraday's law taught earlier

$2Li + Sb \rightarrow Li_2Sb$ 2 moles of Li consumed

$Li_2Sb + Li \rightarrow Li_3Sb$ 1 mole of Li consumed

Now, no. of moles of Li consumed = no. of moles of $e^-$

Atomic mass of Sb = 121.76 g $mol^{-1}$

$$Theoretical\ Capacity = 26801\, x \frac{n}{M}$$

Hence, charge stored = no. of moles of $e^-$ x 96485 C

and sp. capacity = (charge stored)/(121.76 g of Sb)

1st step= (2 x 96485) /(121.76) = 1584.84 $Cg^{-1}$ = 440mAh$g^{-1}$

2nd step= (1 x 96485) /(121.76) = 792.42 $Cg^{-1}$ = 220 mAh $g^{-1}$

Total specific capacity of Sb = 660 mAh $g^{-1}$

So, now we will see the example. This phase diagram already I showed you. So, you can see lithium and antimony that basically forms this Li 2 Sb. So, here 2 moles of lithium is consumed. Then, Li 2 Sb again take lithium and form Li 3 Sb, where 1 mole of lithium is consumed. Now, the number of moles of lithium that is consumed that is equivalent to number of electron that is exchanged, you know the atomic mass of antimony which is 121.76 gram per mole.

So, the charge stored is number of mole of electron into Faraday constant. And specific capacity can be calculated as charge stored by your molecular weight, right. So, in first step, what is happening? 2 mole that has been exchanged and this one is your molecular weight. So, you get the capacity in Coulomb per gram and this is also in Coulomb per gram and you can convert from Coulomb per gram; that also I have discussed in one of my earlier lectures in you will get in terms of milli Ampere hour per gram.

$1^{st}$ step = (2 x 96485) / (121.76) = 1584.84 C $g^{-1}$ = 440 mAh $g^{-1}$

$2^{nd}$ step = (1 x 96485) / (121.76) = 792.42 C $g^{-1}$ = 220 mAh $g^{-1}$

So, you get two steps; and you know that at this particular voltage, you are getting 440; in this particular voltage you are getting 220. So, although the voltage is reducing, so the nominal voltage will be somewhere in between but total capacity will be 660 milli Ampere hour per gram.

Now, there is a shortcut formula based on the Faraday law. The theoretical capacity, this constant you can easily estimate from the Faraday law. This also I have illustrated once into number of moles of electron that is exchanged and the molecular weight of the relevant material. So, if you do that, then you can see that you can also get back these numbers without any problem.

So, the calculation of theoretical capacity and the voltage profile, identification of that it is not that problematic if you do the practice quite well.

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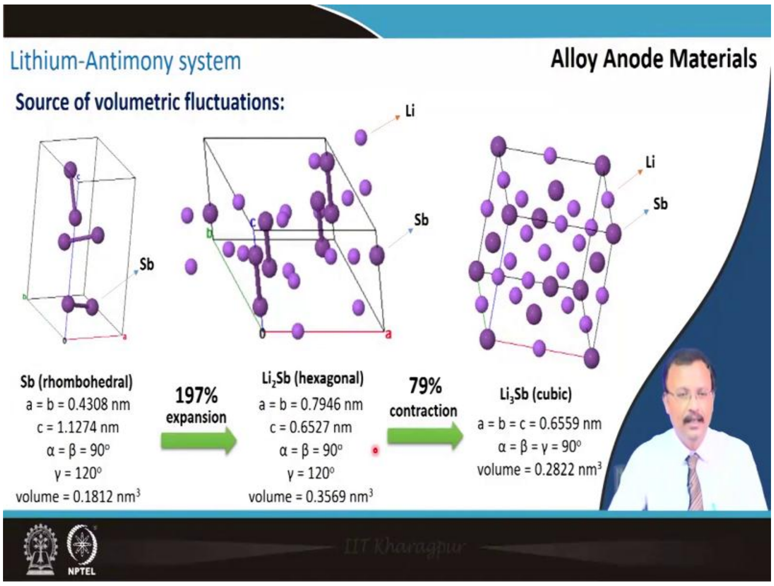

Lithium-Antimony system

**Alloy Anode Materials**

**Source of volumetric fluctuations:**

**Sb (rhombohedral)**
a = b = 0.4308 nm
c = 1.1274 nm
α = β = 90°
γ = 120°
volume = 0.1812 $nm^3$

**197% expansion**

**$Li_2Sb$ (hexagonal)**
a = b = 0.7946 nm
c = 0.6527 nm
α = β = 90°
γ = 120°
volume = 0.3569 $nm^3$

**79% contraction**

**$Li_3Sb$ (cubic)**
a = b = c = 0.6559 nm
α = β = γ = 90°
volume = 0.2822 $nm^3$

Now, the source of this volumetric fluctuation that also can be estimated from the unit cell and here you can see the volume you can calculate for S b and then Li 2 Sb forms. So, from Rietveld refinement of the X-ray diffraction, you can precisely estimate the a, b, c parameter and also, the angle between a and b, which is gamma; b and c, which is alpha and a and c, which is beta, and you can calculate the volume.

And again, it forms Li 3 Sb having this kind of structure, then you can calculate the volume and you can see that about 197 percent expansion and around 79 percent contraction that takes place. Not only always it is volume expansion, sometimes contraction also takes place.

So, once you prepare the material, do the lithiation, stop according to that voltage, take out the electrode, do X-ray diffraction, identify the alloying phase and then, do Rietveld refinement, calculate the lattice parameter, estimate the voltage, then volume expansion also can be estimated.

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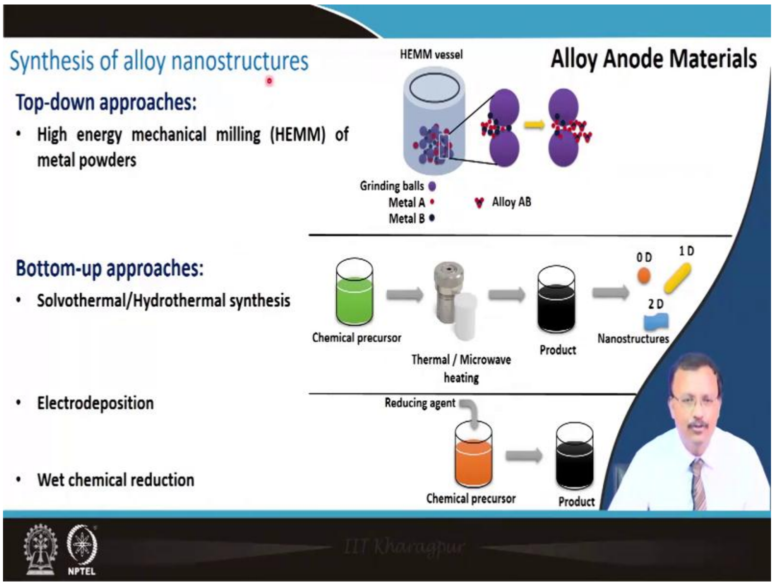

Alloy Anode Materials

Synthesis of alloy nanostructures

Top-down approaches:

- High energy mechanical milling (HEMM) of metal powders

Bottom-up approaches:

- Solvothermal/Hydrothermal synthesis
- Electrodeposition
- Wet chemical reduction

So, synthesis of the alloy nanostructure; this can be done by various route and it can be categorized by two approaches; one is High Energy Ball Mill, you prepare this alloy by solid state reaction and then, do a high energy ball mill to reduce the particle size progressively. So, that is one way. Second is the Bottom-up approach.

So, in bottom up approach, we go for wet chemical synthesis method and solvothermal or hydrothermal synthesis is one of them. And in the laboratory, we have done it by chemical precursor preparation; the batch calculation. We will have to do accordingly; which already I have taught in one of my earlier lectures.

Then, you can do the microwave or thermal heating inside an autoclave just to reduce the processing time. Then you get the product and after suitable calcination, sometimes you add surfactant here also to modulate the growth pattern. And then, finally, you can get various types of structure in 0 d, 1 d and 2 d.

So, this nanostructure, you can prepare by this route. Electro deposition is one of them, you can make by electro deposition. You can make the layers of the alloy materials and wet chemical reduction that is also another way to prepare this kind of alloy.

The challenge is to upscale this material for commercial applications; still it is in the laboratory based research. So, there are lot of scope, scopes to improve their performance and including our group, various other groups in the country as well as in the globe, they are trying to work on this material as a effective alternative for graphitic based material.

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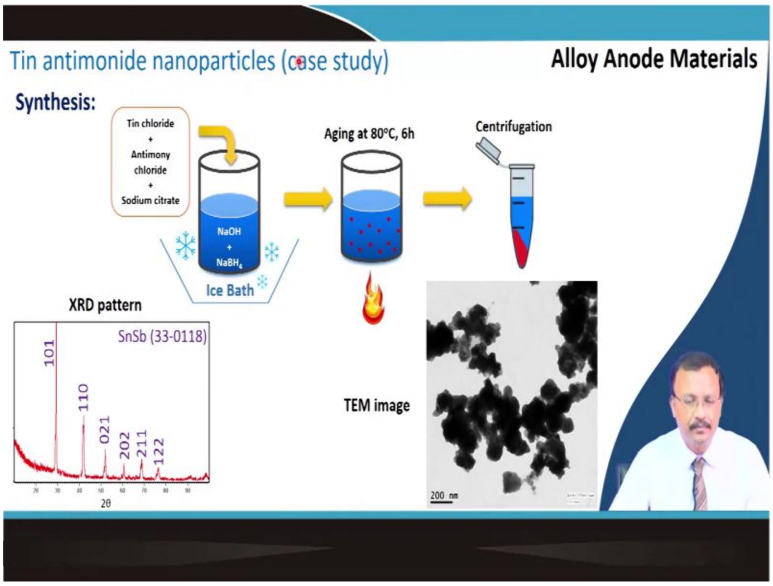

Tin antimonide nanoparticles (case study)

Alloy Anode Materials

Synthesis:

So, as a case study, we did it by a solution based technique; and what we did? We took say tin chloride and antimony chloride mixture in sodium citrate in an ice bath. Then we age here for 80 degree Celsius for 6 hours and then, we have centrifuged it and we got this kind of nanoparticle of tin, antimony, alloy.

And through X-ray diffraction, we can see that they have a phase pure structure and the structure that matches well with the JCPDS finger print. And additionally, we have done Rietveld refinement as well to know their precise lattice parameter, the way I showed for earlier case studies.

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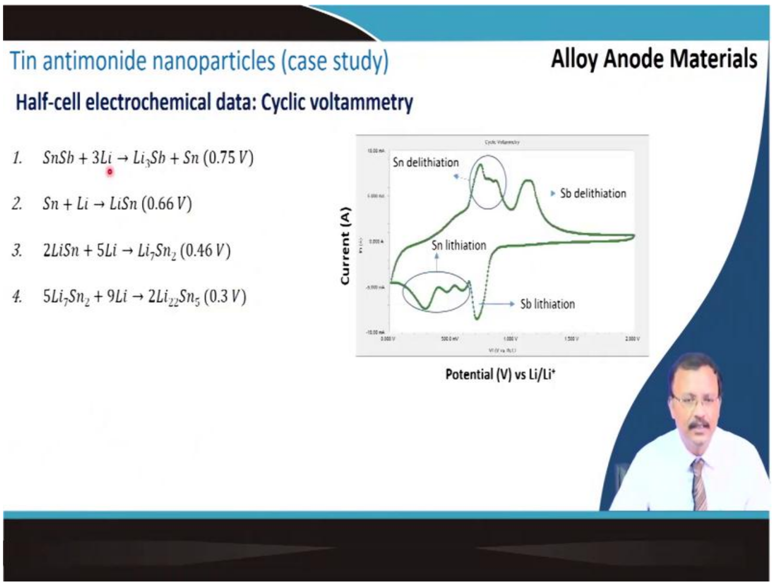

Tin antimonide nanoparticles (case study)

Alloy Anode Materials

Half-cell electrochemical data: Cyclic voltammetry

1. $SnSb + 3Li \rightarrow Li_3Sb + Sn\ (0.75\ V)$
2. $Sn + Li \rightarrow LiSn\ (0.66\ V)$
3. $2LiSn + 5Li \rightarrow Li_7Sn_2\ (0.46\ V)$
4. $5Li_7Sn_2 + 9Li \rightarrow 2Li_{22}Sn_5\ (0.3\ V)$

Now, you can see that this type of reactions can be identified, what is the typical voltage from their cyclic voltammetry curve. So, you can see that there are several reduction reaction that is taking place and there are several alloying reaction that is taking place.

So, the oxidation means lithium is going out from the structure a positive material and if it is coming in, then it is a reduction reaction. So, lithiation part, the alloying part is shown by this and de-lithiation part is shown by this. So, you can clearly identify the voltage and you get this peak.

So, whether it is really Li 3 Sb or Li Sn or Li 2 Sn, if you want to identify that, you will have to stop the measurement right here. So that this phase is affluent and then you will have to do the X-ray diffraction to see whether indeed you are getting this kind of phases.

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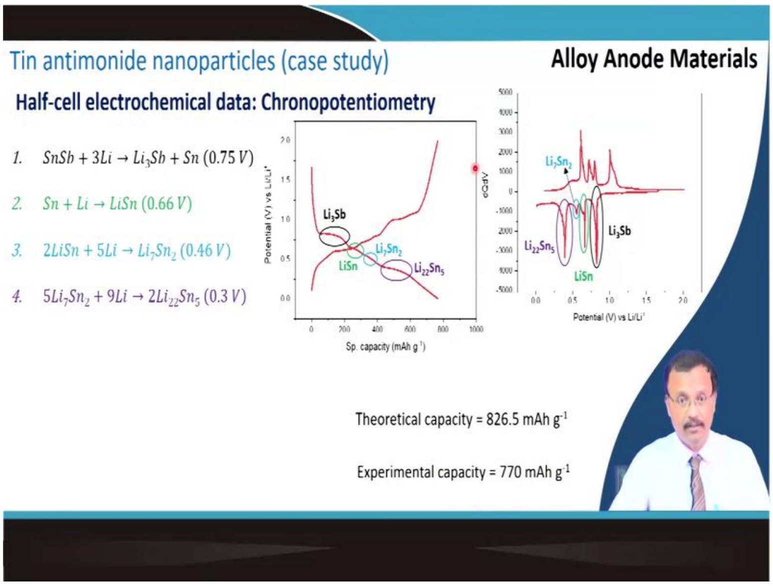

## Tin antimonide nanoparticles (case study)

## Alloy Anode Materials

### Half-cell electrochemical data: Chronopotentiometry

1. $SnSb + 3Li \rightarrow Li_3Sb + Sn\ (0.75\ V)$
2. $Sn + Li \rightarrow LiSn\ (0.66\ V)$
3. $2LiSn + 5Li \rightarrow Li_7Sn_2\ (0.46\ V)$
4. $5Li_7Sn_2 + 9Li \rightarrow 2Li_{22}Sn_5\ (0.3\ V)$

Theoretical capacity = 826.5 mAh $g^{-1}$

Experimental capacity = 770 mAh $g^{-1}$

Similarly, we can do the charge discharge measurement here. The strip kind of structure that easily you can find and which is in line to the theoretical estimation, which I have presented. And I have also introduced the differential capacity plot which will basically differentiate this curve and plot dQdV at each potential.

So, very precisely, you can measure the voltage. The voltage that you have seen here; at what particular voltage this phase is formed that you can experimentally verify by doing this measurement and finally, do the differential capacity plot. Then, you can match this capacity; the theoretical capacity you can estimate, you can estimate the capacity of this one, this one, this one, add it up.

So, the total capacity theoretical should come like this. But experimentally, as you can see that we are getting a bit of from that and there could be various reason, that is a part of our research. But close to the theoretical capacity if you get, then you are conformed that your reversibility is quite good and you have prepared a good quality of sample.

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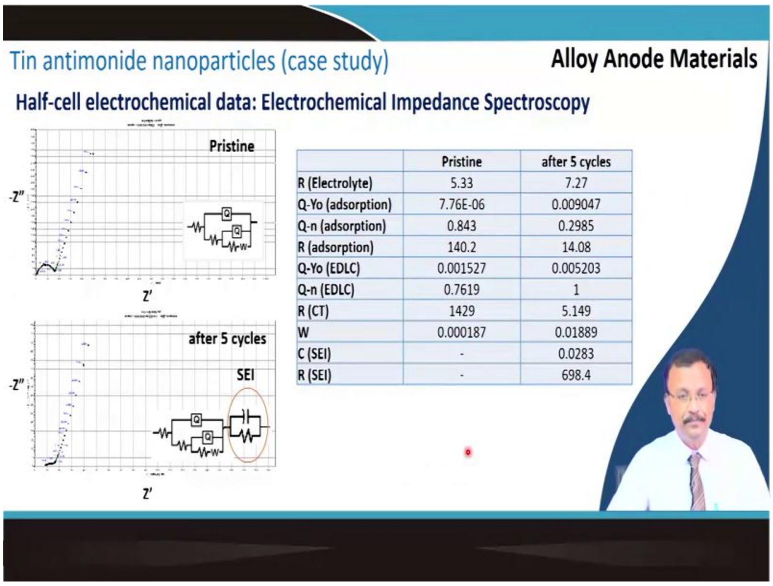

Tin antimonide nanoparticles (case study)

Alloy Anode Materials

Half-cell electrochemical data: Electrochemical Impedance Spectroscopy

| | Pristine | after 5 cycles |
|---|---|---|
| R (Electrolyte) | 5.33 | 7.27 |
| Q-Yo (adsorption) | 7.76E-06 | 0.009047 |
| Q-n (adsorption) | 0.843 | 0.2985 |
| R (adsorption) | 140.2 | 14.08 |
| Q-Yo (EDLC) | 0.001527 | 0.005203 |
| Q-n (EDLC) | 0.7619 | 1 |
| R (CT) | 1429 | 5.149 |
| W | 0.000187 | 0.01889 |
| C (SEI) | - | 0.0283 |
| R (SEI) | - | 698.4 |

Then, we usually dew the half-cell electrochemical data by electrochemical impedance spectroscopy and here as I mentioned, the pristine sample, we can have our own randle circuit equilibrium circuit develop, and there the electrolyte, then charge transfer resistance and additionally, formation of SEI; everything is incorporated and the experimental data is fitted in accordance; and from the fitting cycle for pristine as well as after five cycle, we can see what is the change.

As you can see that the electrolyte resistance does not change much and you know you remember this CPE, Constant Phase Element, this part the coefficients are also estimated. Then, you can see the charge transfer resistance that is grossly reduced due to some reason. Why they are reduced, this is again a part of the research; but it happens.

So, these are one of the tools for us to identify at least that after cycling somehow this charge transfer resistance is grossly reduced. From the work book tell we can estimate the diffusion of lithium. It is at the low frequency, so that means, inside the bulk of the anode, how the lithium is getting diffused that we can understand.

And this capacity of the secondary electrode interface which forms after a few cycles not in the pristine, it is not there but how they change. Again, this will give you several insight on your sample that how your sample is behaving in an actual half-cell with the knowledge that we have found it. From using that foundation, you can always have the capability to know more about your sample, what exactly is going on during the experiment by this experimental tool and subsequent analyses.

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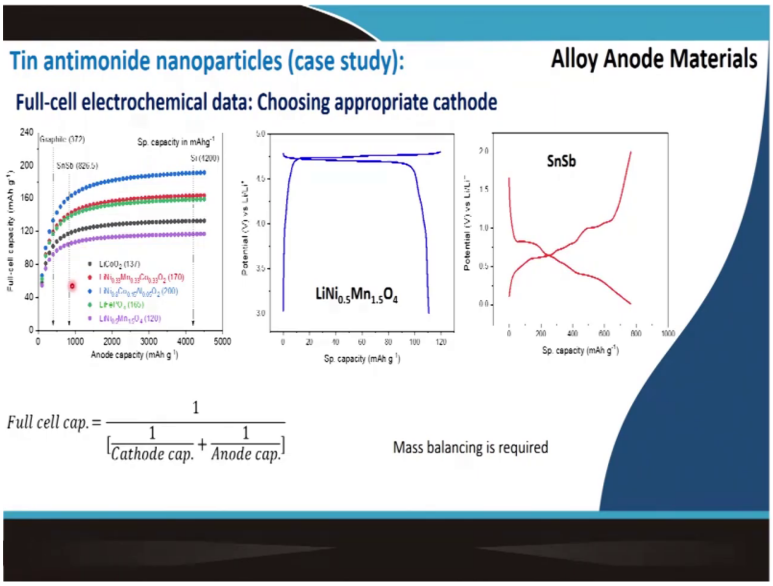

Tin antimonide nanoparticles (case study):

Alloy Anode Materials

Full-cell electrochemical data: Choosing appropriate cathode

$$Full\ cell\ cap. = \frac{1}{\left[\frac{1}{Cathode\ cap.} + \frac{1}{Anode\ cap.}\right]}$$

Mass balancing is required

Now, we will have to check that what will be its performance, when basically you make a full-cell characteristics and this already we have shown for several cathode material, starting from lithium cobalt oxide or 1, 2, 3; lithium, nickel, manganese cobalt and I explained that why lithium manganese cobalt oxide.

Why not only lithium cobalt or why not only lithium nickel. Based on this crystal field stabilization energy, criteria must have remembered. And also, aluminum doped lithium cobalt and several poly anion based material and high voltage cathode.

So, one thing is quite clear that there is no point in excessively increase in the full-cell capacity. So, we were happy with this kind of range less than 1000 that is sufficient for all this cathode as far as their capacity is concerned, they are far lower as compared to your anode material. So therefore, there is no point in excessively increase the capacity value.

And as you can see this high voltage cathode, this is having only about 110 discharge capacity. So, accordingly, you will have to do the mass balancing so that the capacity of this thing, so you take the amount you know the gravimetric capacity, we know that is

110 milli Ampere hour per gram. And the capacity of this particular Sb, Sn alloy is around 800 which we have seen or 700 something.

So, suddenly, you will have to take less mass so that the total charge; charge is nothing but milli Ampere hours. So, the total charge, accordingly you select the amount of mass so that the total charge in anode and cathode they remain same and that will increase the or optimize the full cell capacity. So, this is one example of Sn, Sb, this alloy here you can see we are getting about 700 around and this is pretty low.

So, I will have to make a very thinner anode so that this is mass balance with that. So, this criteria always you will have to follow; not first you will have to measure the half-cell capacity and then, you need to know that how to do the mass balance and then, construct the full-cell.

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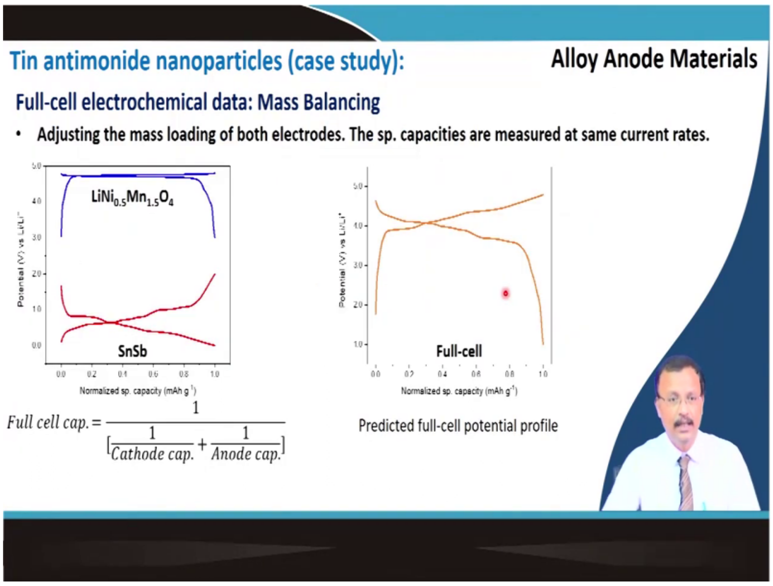

Tin antimonide nanoparticles (case study):

Alloy Anode Materials

Full-cell electrochemical data: Mass Balancing

- Adjusting the mass loading of both electrodes. The sp. capacities are measured at same current rates.

$$Full\ cell\ cap. = \frac{1}{\left[\frac{1}{Cathode\ cap.} + \frac{1}{Anode\ cap.}\right]}$$

Predicted full-cell potential profile

And after mass balancing, you will get something like this; adjusting the mass load of both the electrodes. The specific capacities are measured at the same current rate. So, your capacity is balanced. And one thing is interesting, I hope that you have noticed it that when this one is charged, then simultaneously this is discharged and that is true. Lithium is coming from your cathode site, so it is getting charged and lithium is getting inserted into the anode, so it is getting discharged.

So, charge and discharge then, we will allow you to have the full capacity. And this is the kind of capacity that we are getting and this is a normalized capacity, I have plotted here, not the absolute value; these are all normalized one but at least you can see the shape, you can estimate the voltage.

I am leaving it in on you that at this potential if the voltage is there and the cathode voltage in half-cell is here, so full-cell what is the voltage that you expect? That also, I have theoretically explained in one of my lectures earlier and if not, then again, in some other lecture, I will draw shed light on it. So, this is the full cell that you are getting.

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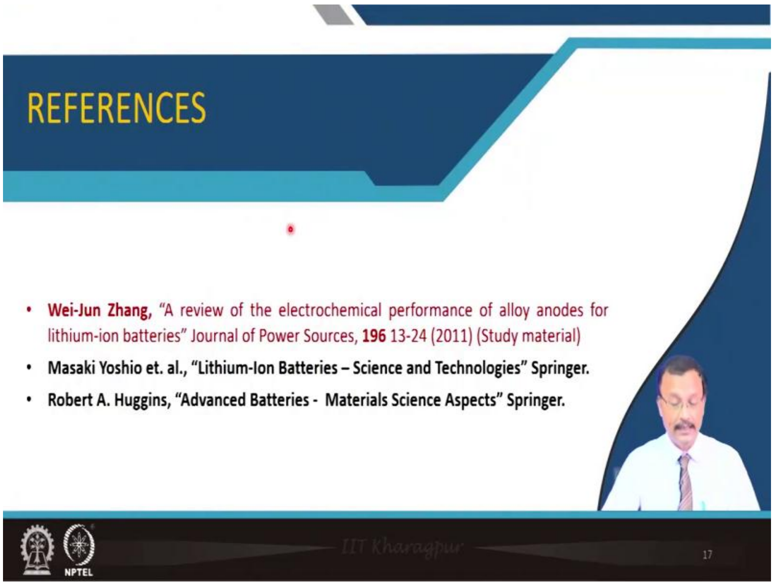

REFERENCES

- **Wei-Jun Zhang,** "A review of the electrochemical performance of alloy anodes for lithium-ion batteries" Journal of Power Sources, **196** 13-24 (2011) (Study material)
- Masaki Yoshio et. al., "Lithium-Ion Batteries – Science and Technologies" Springer.
- Robert A. Huggins, "Advanced Batteries - Materials Science Aspects" Springer.

So, the reference for this particular lecture is "A review article of the electrochemical performance of alloy anodes". So, almost all prominent alloys you will get here. And this is your study material and apart from that, this book is this both the books.

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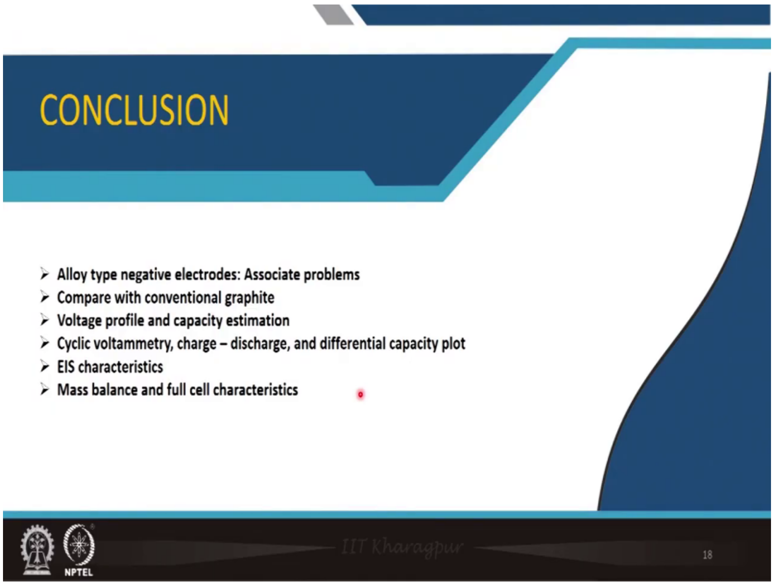

## CONCLUSION

- Alloy type negative electrodes: Associate problems
- Compare with conventional graphite
- Voltage profile and capacity estimation
- Cyclic voltammetry, charge – discharge, and differential capacity plot
- EIS characteristics
- Mass balance and full cell characteristics

Let me conclude this particular lecture. So, first, we have described the alloy type, negative electrodes and what are their associated problem. Then I made an attempt to compare the alloy based anode with conventional graphite. Then again, we have recapped the voltage profile from the phase diagram and that was guided by free energy versus composition diagram. So, this has once been illustrated for your understanding.

And then finally, I showed how to do the capacity estimation. And then, in half-cell configuration, we have described the synthesized alloy material; tin, antimony and how they are synthesized that also has been described. And from the cyclic voltammetry, you can precisely identify the voltage, where the particular alloy reaction takes place because there are multiple alloy reaction is taking place and corresponding to that voltage; you get a plateau voltage plateau because of the two phase mixing. So, that is experimentally verified that indeed it happens like that.

Then, we have shown by ES analysis, EIS analysis, how exactly you can estimate some useful parameter like the resistance for charge transfer, resistance for solid electrolyte interface, estimation of diffusion coefficient of lithium inside the bulk of the material that is also possible; whether the electrolytic resistance is being changed while you cycle your half-cell that can also be estimated. So, that was done.

Then finally, we introduced the mass balance once again, because the anode and cathode, they are very different masses. So, the mass balance is required and finally the full-cell characteristics were defined.

Thank you for your attention.