# Heat Treatment and Surface Hardening - II


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## Lecture – 33
## Linear regression (least squares) method to find the value of n and k in Avrami equation

Continuing with the last lecture, where we had shown how to obtain the best fit parameters a naught and a 1 of the linearized equation of the Avrami relationship.

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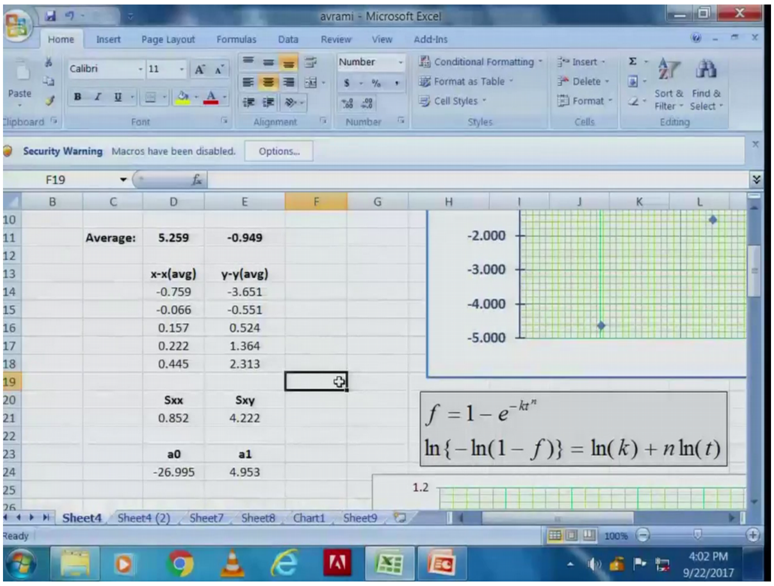


And we had obtained a naught which is log natural log of k, as minus 26.99 and the parameter a 1 which is nothing but the slope n in the avrami equation of 4.95. Now let us see let us see the result by plotting this line on to the On to our graph along with points we have.

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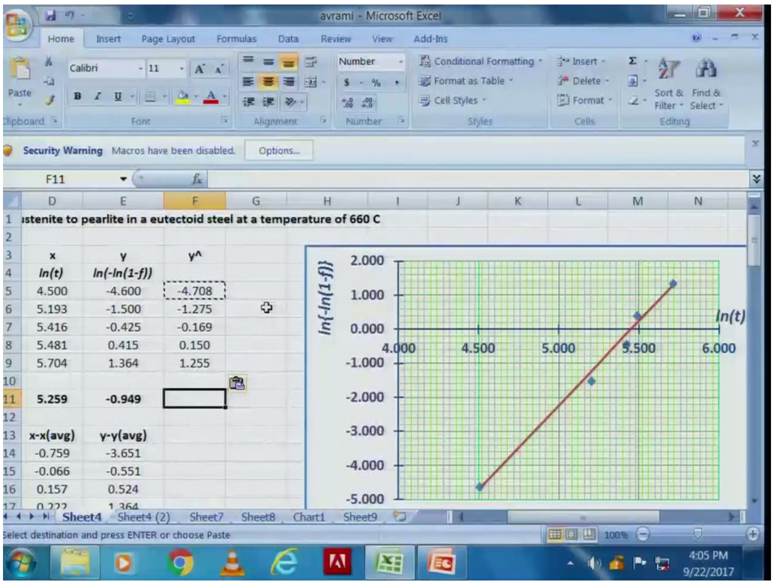


So, let me call the estimate for y for the individual x values as y cap, and below which I will make a plot of a 0 plus a 1 x for the individual x values.

So, the first value that I will get I will choose the cell d 24, and anchor it plus a 1 which is an e 24 anchor this as well multiplied by the corresponding x value which is there in cell d 5. So, this gives me an estimate of minus 4.7 against what we got from our measurement of minus 4.6. I will copy this formula to the other cells to get the estimate for the other x values as well and this is what one gets.

So, for example, at an x value or log t value of 5.19 our measured response y was minus 1.5 well and the predicted response now is minus 1.27. Similarly at a x value of 5.7 the response was 1.36 and the predicted response is 1.255. And on the right hand side you can see the graph has been plotted with the straight line passing through these set of points. This line now is considered as the best fit line obtained from this least squared technique or the linear regression technique.

Now, we also want to get some kind of a measure of how good this fit is. So, there are various measures for that and we will just take a look at one of the measures of the goodness of fit. And let us see how the good does goodness of fit can be evolved on the board first.

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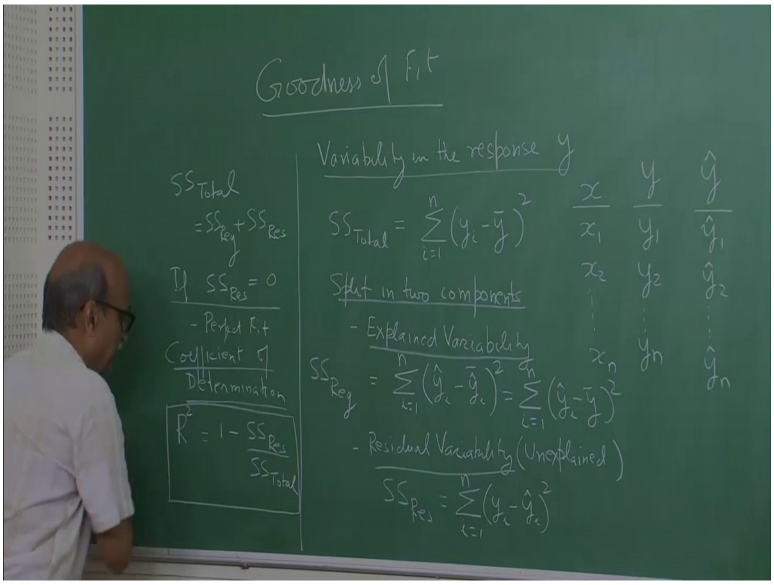


So, looking at the goodness of fit measure for our regression line. Let us consider the variability in the response y.

The variability in the response y, the total variability in the response y can be understood in the following way. Let us say this is the measured response and this is the predicted response. So, I will have y 1 y 2 and so on till y n number of data points that I have corresponding to each of them, I will have the response y 1 cap y 2 cap to y n cap. And of course, this is corresponding to the independent variable x which in this case is log t is x 1 x 2 to x n. So, the total variability in the response y i will write it as sum of the squares total or some of the deviations of the square total can be written as summation i equals 1 to n y i minus y bar square. This is the total deviation of the measured quantity against from the average value of the response.

Now, this total response can be split in 2 components. What are these 2 components? Well the first one is what we can call as explained variability. And what is this explained variability? Well as our independent variable x changes our response y also changes. That is as per the model as per the linear relationship this is called as the explained variability and this could be written as summation i equal to 1 to n y i kept the predicted value of y or the predicted value of the response at the I th response, minus the predicted average value squared. This I will call it as SS regression. That is this is a variability that is explained by the regression model.

Now it so, happens? That this is one of the properties of the least squares that, the average value of the predicted response is the same as the average value of the measured response y bar. And hence I can simply write this as i is equal to 1 to n y i cap minus y bar squared. So, this is the first component of the total variability the response y. The second component is what is called as the residual variability. That is an alternatively one can also call it as the unexplained variability. And this is simply abbreviated as sum of the squares of the residuals which we have already seen, and which is equal to sum over one to n y i the measured response minus the predicted response and the square of this.

Now, it can be shown, it can be shown that SS total is equal to SS regression plus SS residual. This is fairly easy to show by adding the explained variability and the residual variability together and proving it that this is equal to the total variability. Now what does all of this mean? When if my residual variability SS residual is equal to 0, if this is the case, then I have a perfect fit which means the straight line passes through the point all the points exactly.

However this would never really happen, because in all our measurements we always have statistical error. And hence they will always be some finite non 0 variability for the SS residual. Now this gives us a handle to define a goodness of fit, which is also called as the coefficient of determination called as R square, and this is defined as follows R square is equal to 1 minus SS residual divided by SS total. This is a goodness of fit parameter. Let us try to understand what this means, when we have a perfect fit when the sum of the squares of the residuals is 0 you can clearly see that R square is going to be 1, when on n in all other cases SS residual is going to be some finite positive value less than the total variability SS total and hence R square is going to be less than 1.

So, R square is going to be one for perfect fit for all other fits R square is going to be less than 1 and R square is going to vary between 0 and 1. What this means is that closer the coefficient of determination R square is 2 one better is your fit. Further away it is if it is a very, very small number like 0.2, 0.3 then we can consider that the fit is not good and perhaps the relationship, we have chosen does not fit the experimental data.

So, this is one way of checking, that if I have collected experimental data to experimentally verify whether the avrami relationship is valid or not for a particular system, I do this fit and then check the value of the coefficient of determination to see how good the fit is. So, what we will do now is go back to the spreadsheet where we already have the data and calculate for this given data what is the value of the coefficient of determination.

So, let us look at this data and try to get the goodness of fit R square. For that I need to calculate now 2 parameters, SS residual and SS total.

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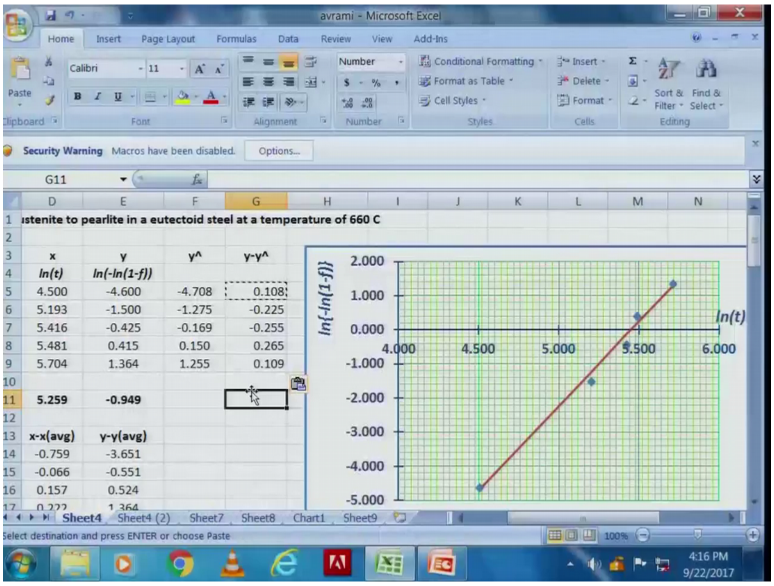


Now in order to first calculate let me calculate SS residual. In order to calculate SS residual I will have to compute y minus y cap. So, let me put in this column here, and this I individually calculate the difference between y and y minus y cap. So, this is e 5 minus f 5 gives me the first difference, and similarly I just have to copy this all of these formulae in the following cells. And I get the individual values of the residuals.

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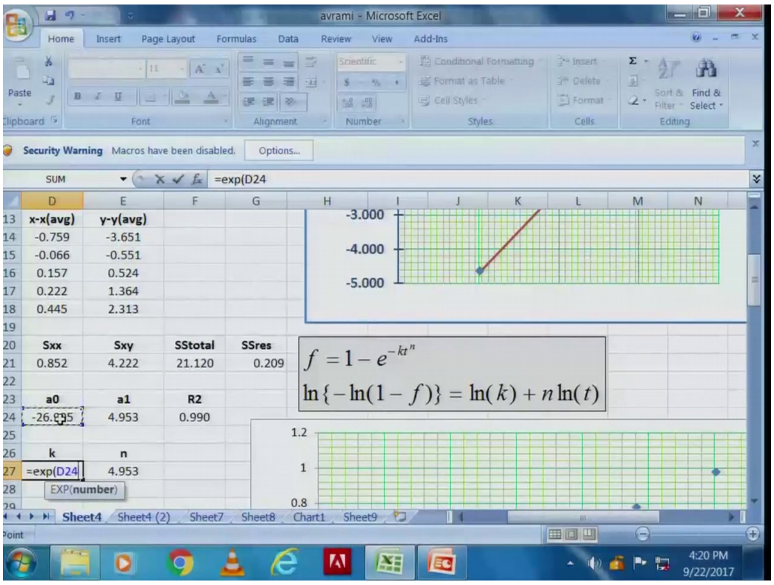


Next let me put down SS total. In this column and let me put down SS residual in this column. So, what is SS total? SS total is the sum of the squares of the deviations y minus y bar, which is nothing but if you look at this column this is y minus y bar y minus average value of y if a the individual. So, I will get it I will use the spreadsheet function sum of the squares of all of these values, and this gives me the total variability of the response y. Now the residual variability that I have to put here, again the same function I can use some of the squares, but of these number y minus y cap. And I get 0.029 as the residual variability.

Next let me get now the value of R squared, the goodness of fit for this particular set of data now this we have already seen R square is equal to 1 minus SS residual divided by SS total to be simply put this relationship 1 minus SS residual divided by SS total. And I get a value of R square is 0.99. This looks like an excellent fit it is very close to 1 and then we can conclude that the data that we had for transformation of austenite to pearlite for at a temperature it was obtained at a temperature of 660 degree centigrade appears to fit the avrami relationships quite. Well now so, far we have determined the parameters a 0 and a 1, but now we want to get the avrami parameters n and k. So, let me get the avrami parameter k here and put the avrami parameter in this column.

So, what is n well if I look at this linearized relationship, n is nothing but the slope pop this line which is nothing but actually a 1. So, we already have the avrami parameter as

4.953 which is quite close to 5. Let us try and see what should be the value of the parameter k in the avrami equation. When the intercept a naught is natural log of k and hence k is equal to exponential of a naught. So, I just have to put this function exponential of a naught which is the value given in cell d 24, and I get a avrami parameter k to be equal to the order of 10 to power minus 12.

Now, we can also see how well this n and k Fit to this data.

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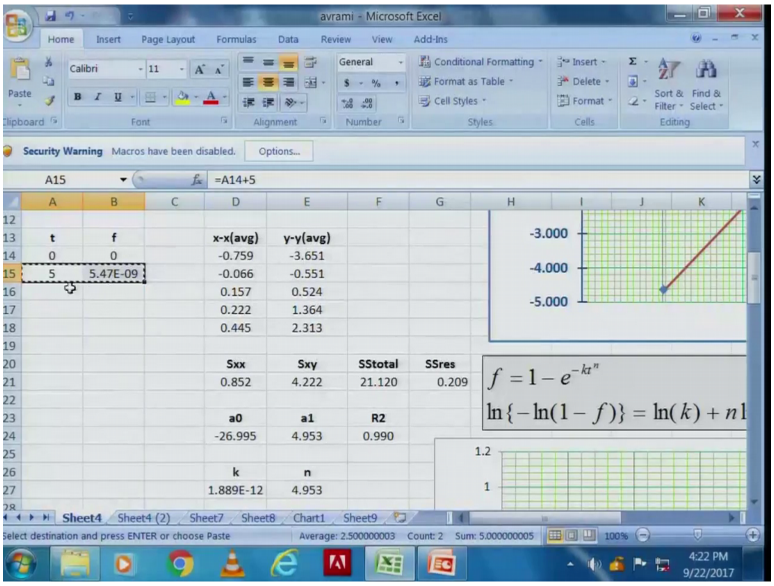


So, let us quickly have a look at this as well. So, let me put it somewhere here. So, let me put time here and the fraction transformed here, this time will start from 0. And the fraction transform is simply the avrami equation 1 minus. And now I am going to use the parameters a n and k that we have obtained. So, here I should put k anchorite multiplied by time which is in cell a 14. No, I should be give you a good idea to put it in brackets. A 14 to power n which is in cell e 27 anchorite and close brackets. So obviously, for time t equal to 0 I must get 0, and let me increments the time by 5 seconds each time. So, for 5 seconds I will copy this formula to cell b 15 and I get a fraction transformed which is a very small value.

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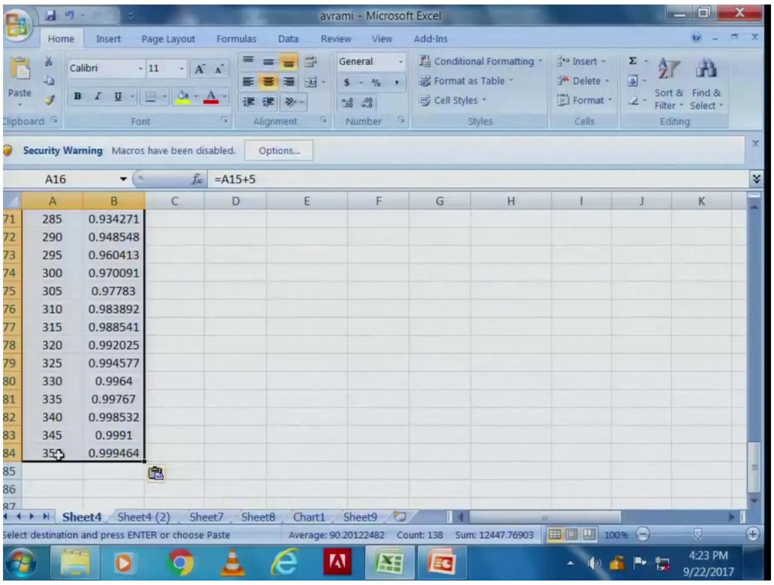


Now, I can copy these values down here paste it here and I get I get a set of values up to 315 seconds. And on the right you will see a graph as I merged of a now the line passing on a graph of fraction transformed versus time in seconds as a curve and it follows quite closely to the experimental data. Now with this we have seen that how we can verify the avrami relationship when we also seen that this technique of regression, can also be used for in many other cases where I have to relate maybe some property to heat treatment or maybe some other microstructural parameter to heat treatment and so on.

Now, with this I will I will close this discussion on the verification of the avrami relationship using experimental data. But one of the things that we needed in order to verify this was that we needed to measure certain microstructural parameters as a function of time. In this particular case we have to measure the volume fraction of perlite formed as a function of time, but they would be other situations where perhaps we have to monitor the grain size versus time grain size versus temperature. And there are many other situations when you give a certain heat treatment to materials we need to quantify the microstructure.

So, what I will do next is that we will look at how we can quantify microstructures. We will look at what is called as quantitative metallography, and this field of quantitative metallography uses tools of an area called stereology. It is a fairly old area more than 50 years old where it was developed by metallurgist and material scientists, an and we will look at various tools by which we can measure how to measure volume fraction, how to measure grain size, how to measure for example, surface area of grain boundaries in a material, how to measure density of dislocations how to measure density of line elements like dislocations as line elements. How to measure number of grains in an area, how to measure particles in an area and so on. It is a very powerful a set of techniques by which we can do these various measurements.

So, what I am going to do would be in the next couple of lectures, I will be discussing the tools used for making quantitative measurements of microstructure. So, I will bring this to a close here this particular lecture, and in the next lecture we will discuss stereology.