

Advances in Additive Manufacturing of Materials: Current status and emerging opportunities

Prof. Bikramjit Basu

Materials Research Center, Indian Institute of Science, Bangalore

Lecture 45

welcome back to this NPTEL course on additive manufacturing. In the introductory lecture on this course, I mentioned that in this course, I will be also covering some of the emerging concepts and emerging topics in the field of additive manufacturing. one of such emerging topic is artificial intelligence and machine learning. this is more related to data science. what I am going to do in today's lecture, I will introduce you to the fundamental concept of data science in reference to AI and ML as they are relevant for this course for the additive manufacturing subject. I would like to upfront mention you that for more details you can also refer to these textbooks that is understanding deep learning by Simon Prince.

Then another textbook is StatQuest illustrated guide to machine learning by Joshua Starmer and third one is machine learning yearning that is Andrew Ng. Further there are also NPTEL courses by Professor Sudeshna Sarkar, Introduction to Machine Learning and then also another course on Machine Learning Stanford lectures by Andrew Ng. additive manufacturing what you have learned so far particularly in the context of metal 3D printing. that there are two approaches that what we learnt one is called directed energy deposition.

essentially you focus your laser beam and then laser beam interactions with the materials is also synchronized with this powder delivery at the molten pool. there are different parameters which you remember that you I am sure that you know you have seen this movie this video of the additive manufacturing process. of the DED based additive manufacturing processes for metal 3D printing and this specific facility is also available at Indian Institute of Science. what are the different parameters of importance? One is this argon gas flow rate that is through which this powder is delivered and what is the particle size distribution, powder feed rate, laser power, spot size, laser scanning speed. what you can see these are like different variables .

The optimization of these different variables for any specific materials to be manufactured with a particular design needs to be done each time. what it means that there are large number of intuitive tailoring of these variables and then also what we call trial and error approach. or another term I just used is intuitive tailoring of the different parameters clearly you can understand from this particular slide that large number of experiments to be needed to optimize these parameters essentially for this directed energy deposition process. Now another technique or another manufacturing technique which you have also learnt in earlier lecture is called LPBF that laser powder based fusion processes. And this laser powder based fusion processes, there are processes which are also used is called SLM, SLS, selected laser melting, selected laser sintering, DMLS, these are all synonymous.

As far as the operation of these techniques are concerned they are all synonymous. if you also remember that from this is like SLS system, this is like SLM or SLS system of an Indian company. essentially you can see that this particular machine operates like a powder based fusion processes. You can see that laser beam is scanning this powder bed and layer by layer this powder bed is being manufactured in the Z direction. Here again if you see that what are the parameters or variables that are important is the particle size distribution, laser power, laser

spot size, laser scanning speed and many of the parameters what you see for SLM and SLS are also identical in nature with the DED process except the fact for the DED is the powder feed rate that is also important or argon gas flow rate that is also common to both the things.

It should be very clear like in DED SLM, SLS, DMLS techniques also need large number of experiments before these parameters are optimized to manufacture a designed construct. metal 3D printing that one of the things that you have learnt also that after this SLM and DED, the 3D printed parts need to be heat treated. And this post-processing is equally important because one of the main thing that you have learnt in case of metals is that strength ductility combination. strength ductility combination and this as I think that I have already mentioned that intuitive tailoring of a range of process parameters, it results in large data sets and post-processing heat treatment also at different temperature and time that leads to a range of microstructure, composition phase and morphology. And properties are largely correlated with the microstructure.

microstructure property correlation is very important and in this material science literature it is called PSP linkages, process structure property linkages. And then experiments that are involved in establishing PSP linkages for any material essentially generates large volume of data. And traditional trial and error approach or high throughput approaches are highly inefficient. Just to give an example, for example if you heat treat at the heat treatment conditions P1 or P2 and P3, you are quite likely to generate three different classes of microstructure. And you can see that what is the typical temperature versus time profile, the typical heat treatment, you can heat it up, you can hold it, you can cool it down. here these are like different heat treatment profiles that any 3D printed parts can experience and depending on that as I said before few minutes back that it will have different strength-ductility combinations.

But in actual practice or in actual reality, we need to have a specific strength-ductility combination of a 3D printed part and that targeted strength-ductility combination must be achieved. that was our target. what I am trying to essentially indicate that additive manufacturing process and post-processing processes both together generates large amount of data and this data generation was possible because we essentially invoke more intuitive tailoring of a range of process parameters and this data can be used in the data science approaches and that I am going to show later that how this data can be essentially used in the data science approaches. Then another thing that is important because this one also you have seen some examples in the previous lectures under this course. that total hip joint replacement, THR.

This is a medical device, total hip joint replacement which is used to treat the damaged hip. either the hip is damaged or hip is fractured or hip is broken. essentially by part or fully the total hip joint is to be replaced by femoral stem. This is the natural hip you can see. But then when you put this artificial hip joint then you have a femoral ball head then you have acetabular liner, acetabular socket and so on.

here again the design of acetabulum or design of acetabular cell. is important and why important you can say this is kind of one of the horseshoe shaped cell design. Because these particular things you look at your concentration here, these particular things where acetabular cell is placed that is in direct contact with the host bone. osseointegration or integration of this acetabular cell with the host bone is very important. Now, you cannot do several experiments involving human subjects, so therefore you can only design these different design variants and you can do finite element analysis to generate biomechanically relevant data and then by different design variations it is possible to get a large data sets of Von mises stress, Von Mises strain, displacement at the implant host bone interface and so on.

the idea is that whether this large finite element modeling analysis generated data again can be analyzed using the data science approaches, We are going to see some examples later. what is finite element modeling? That it is an important preclinical tool for testing new designs, important to complement experimental methods, high range of physiological conditions can be simulated and anatomically site-specific results that it can provide. this is essentially the surgical procedure or just to show that how the surgeries that taken place in clinics or in hospitals like you know that first this acetabulum is repaired by placing the cell along with the liner and then femoral head. After that, you put this femoral head into it. This femoral head can be either ceramic or can be metallic.

and then in the virtual implantation and then femoral stem is to be directly inserted if the only the acetabulum is to be repaired then that is that only this is the part and if the femoral stem is also broken so there again the revision surgery case the stem is to be imparted. what in the finite element analysis, this is your region of interest, what is the acetabulum host bone structure and people do lot of this finite element analysis in our group also we have done just to apply the load and degree of freedom and then those things. just to give you some examples of that how much time, how much cost it is involved in Indian context like pre-processing of the CT scan image at least it takes 2 hours, finite element solutions 4 hours, post-processing of the finite element solution data 2 hours and then pre and post-processing data almost like 1000 hours if we consider large amount of data. resources high performance computation platform is 8 lakhs that is for 24 core hours per calculation and considering 4 body weights, 4 bone conditions, 7 designs you need almost like 2000 to 8000 core hours. this is almost like charges also for annual 24000 for 50 core hours that is at presently that is what the charges that are imposed on users at Indian Institute of Science just look at this data and then you see this experimental laser type patient specific implants.

the parameters or variables that I have already mentioned particularly for DED based 3D printing, powder feed rate, scan speed and all. 5 instances, 5 variables for each parameters give you 25 parameters. Powder handling and maintenance is 1 hour, printing 2 hours. total time is certainly up to 100 hours and the cost per print is 8,000. total cost for one 3D printed materials itself is 30,000.

Cumulative cost will be in lakhs INR. what I am trying to say, one is the cost implication. and one is the time, whether it is a computational time or experimental. So, these two simple examples I am trying to emphasize that how much cost and how much time will be involved in this kind of research whether we use the finite element analysis or 3D printing. that places the importance of artificial intelligence and machine learning.

what it does? It predicts the stress and strain based on inputs in seconds, few seconds and can be run on a laptop. parameter optimization in the machine learning if you use then it greatly reduces costs and time and prediction also it allows the structure property prediction. Another example that I can give because I have also spent quite significant amount of time in previous lectures to explain you 3D printing or 3D bioprinting as well as 4D bioprinting. 3D bioprinting essentially I would like to remind you that whenever you see bioprinting that means you are layer by layer printing the 3D biomaterial inks together with cells or biological macromolecules In the 4D bioprinting, you essentially take the 3D bioprinted structure, you give external stimulation and this external stimulation can be either electric field or can be simply photon $h\nu$ or simply can be temperature or can be magnetic field or so on as long as The shape is modified and then functionality of the cell laden scaffolds is also modified. You call it as a 4D bioprinting.

So this is the most advanced. This represents one of the recent advancement in the field of additive manufacture

in the 4D bioprinting. what are the parameters which are important in 4D bioprinting? You are bioink formulation, printing parameters like 3D extrusion parameters. You remember there are so much examples where I have shown that how gelma based scaffolds can be 3D printed, cross linking treatment, external stimulus. And what are the output here? Output here is the safe fidelity, tissue maturation and biophysical properties.

You remember biophysical properties. I have given you lot of example of the swelling and degradation. One is the enzymatic degradation. I have even shown you that how to do kinetic analysis of the swelling and degradation properties of the GELMA based scaffolds. although this AI ML approaches are I think have started to be used for this kind of 3D, 4D bioprinting.

This is just one such example that predicted mechanical strength and actual mechanical strength. of the Gelma based scaffolds if you do and if you do multilayer perception algorithm it shows some kind of a linearity or 45 degree line but one of the things that you notice root mean square error is fairly high. I will explain to all of you in the subsequent slides that how to essentially analyze the performance of ML algorithm those things I will explain to you in due course of time. there are two things, one is the experimental approach and one is the modeling approach. Now experimental modeling approach essentially both are capable of generating data sets.

perhaps I can comment here that modeling induced data sets are much larger in volume or larger in quantum compared to experimental data sets. And many times in scientific research you need experimental data for calibrating the modeling tools or often if your model predictions need to be validated by experimental results. it goes in a complete circle or reversible manner. And what I have mentioned that is very very carefully you need to remember that AI ML approaches can be used as surrogate to experiments and modeling approach. modeling to predict experimental results, experiment to calibrate the modeling data.

What are the different modeling approaches people use in material science? Related subjects is the DFT, density functional theory, MD, molecular dynamic simulation, FEA, finite element analysis. In experimental library, you can essentially generate large number of materials or their functional property or in the context of biomaterials, you can generate lot of data related to in vitro cytocompatibility for example. Many times we found these data or datasets are essentially available in a very, very scattered manner. And many times people are not reporting metadata. For example, as I said that heat treatment when you do this heat treatment of the additive manufactured parts, you can do heat treatment in argon atmosphere, you can do heat treatment in argon hydrogen atmosphere depending on what type of metals you are handling.

But often this what atmosphere you use for heat treatment that information is missing. Or what is the heating rate that we use for the heat treatment experiment, whether it is a 2 degree Celsius per hour, then heating to some 1000 degree Celsius and holding that for 2 hours versus 5 degree Celsius per minute. people do not even understand the need for this, keeping this metadata. For example, I just gave you two examples. One is the heating rate or what is the heat treatment atmosphere in the heat treatment experiments.

therefore, we need to have a collaborative network to efficiently share, store and analyze the experimental and computational data. The second one is the predictive capability of the biocompatibility based on AI ML approaches. you remember the biocompatibility of the biomaterials that is the compatibility with the desired interactions with the components of the living system like cells, protein, blood, etc. And what we believe that if you go step by step, then you can essentially lead to accelerated delivery of biomaterials and implants. what are the key challenges that has been very carefully mentioned here? One is insufficient and scattered data.

Second one, uncertainty associated with the data. many times suppose you get the strength data or elastic modulus data, you do not get an error bar. you do not know how much there is a scatter in the reported data, what is the scatter in the reported data that you do not get. Third one, you get inferences from the data science approaches that you are going to see in the next few slides as well. In United States, Materials Genome Initiative was essentially announced a few years ago by the White House.

And that actually leads to significant research activities by employing machine learning in the material science. Now, one of the things that has been mentioned that US Materials Genome Initiative which has been also triggered by my colleague from University of Pennsylvania, John Mauro, essentially to apply this machine learning to glasses, to glass composition or to predicting glass properties. What they have mentioned in the material genome initiative, the time to market for any component will be accelerated if you use the material genome initiative. The time to market was very before MGI and then after MGI this time to market will be much faster. So what are the three things that has been mentioned? discovery, development and deployment and then this particularly approach material genome initiative, they essentially encompass computational tools, experimental tools, collaborative network and digital data, okay.

one such example from Mauro's group. is for the glass science. those who are aware of that how this glass is essentially multi-component inorganic materials which lack long range order but certainly it can have short range order. And it is multi-component that means it is mostly oxide based materials and this oxides is multi-component oxides. these are mixture of silica, alumina, magnesium oxide and many other oxides which are being added. people use intuitive tailoring of that addition of different oxide component to make the glass stronger that means glass will have better mechanical strength properties or glass will have better modulus properties and so on.

they try to use the different components of these or the different elements from periodic table that is why I think they mentioned that decode in the glass genome and then that will have an impact on the structure. one is the composition, one is the structure and one is the properties. And what are the properties that is mentioned? For example, for any specific glass, if hardness is plotted against the addition of Na_2O , sodium oxide addition, you can see that it goes through a essentially, this is the model and these are the experimental data. And you say that model essentially predicts the experimental data fairly well. it goes up to a linear variation, increasing variation up to somewhere around 20% addition of Na_2O but then after that it drops.

And then why it drops? The answer lies in their variation or in the modification of the structure of this class. this brings me to artificial intelligence. artificial intelligence of science of getting a computer to learn how to perform a task that normally requires human intelligence, That is why you can see that neuron structure here. Machine learning, in general, machine learning are defined as the study of the algorithms with the ability to learn without being explicitly programmed. in the programming language, for example C, C++, you need to run a code, then you have to need to run, you have to debug that program, then it gets output,.

in the machine learning, without even explicitly being programmed, you can generate the predicted values. Then supervised learning, define and learn a mapping from input to output. what is the real level model input, there are some like you know for example the real world input there is some kind of you know house or home, they said 6000 square feet, large area, 4 bedrooms, probably sold for such and such money and now you apply the supervised learning model, then you got what is the predicted price. artificial intelligence is not only for scientific world but also in a day-to-day world unsupervised learning, learn about a data set without levels, unlabeled data

and there you can have a generative adversarial models like GAN models, generative adversarial network models, probabilistic generative models and then you have reinforcement learning with the goal is to take actions to change the state that you receive rewards. I mean these are like different examples, I will come back to this again in the later part of this lecture.

or next lecture. Deep learning that is a subset of machine learning which requires vast amount of data where artificial neural networks in artificial neural networks adapt and learn from the vast amount of data. Often those who are not from data science background they try to use this term artificial machine learning and deep learning in a synonymous manner or in interchangeable manner but that is not true. After look after discussion in this particular lecture you should be able to distinguish artificial intelligence is a large umbrella structure under which smaller domain is machine learning under which another smaller domain is deep learning. Machine learning, deep learning, artificial intelligence, they are not synonymous but they essentially have different meaning which I have already mentioned. Now the question is if you go back to our discussion here, the question is that why are AI-ML and why AI-ML are very important? - if you go back to the earlier examples, these particular things.

Now you would like to know this is your input in the 4D bioprinting and this is your output. You want to establish a relationship between output and input, but scientifically there is no established or any empirical relationship that can correlate safe fidelity with printing parameters, safe fidelity with bio ink formulation or safe fidelity with external stimulus. There is no scientific theory that ever exists which can correlate these two output, one of the output parameters with one of the input parameters or for example, biophysical property. To some extent, you can correlate biophysical property with some of the microstructural property but towards the input parameters, there is no direct relationship. in cases where there is absolutely no relationship between input and output parameters any empirical relationship AI-ML approaches is the only solution and that is the statement I have made in the bold here that AIML most relevant in absence of any established relationship between dependent and independent variables.

With this, I guess you now understand that what is the correlation, what is the relevance of AIML in general. I will come back to you in the next class to continue with this introduction to AI-ML. Thank you.