KNOWLEDGE INCUBATION FOR TEQIP, IIT KANPUR

TEQIP Workshop on High Resolution X-Ray & Electron Diffraction

February 1-5, 2016

TEQIP workshop on High Resolution X-Ray and Electron Diffraction was held from 1st – 5th February, 2016 at IIT Kanpur. The aim of this workshop was to provide in-depth theoretical knowledge about the principles of the advanced diffraction techniques and provided information about the state of the art equipment available at the Department of Materials Science and Engineering and Advanced Centre for Materials Science of IIT Kanpur. The workshop included classroom sessions from eminent experts as well as tutorial sessions and hands-on training on data analysis along with visit to the facilities at the Department of Materials Science and Engineering.

In addition to providing information about the structure of materials, lab-scale X-ray diffraction can also provide information about preferred orientation of crystallites or texture, types of phases present, as well as determination of the lattice parameter, micro-strain, residual stresses and dislocation density in the bulk samples. In addition, different X-ray techniques can provide a wealth of information for thin films e.g. crystallinity, epitaxiality, layer thickness, orientation relationship between substrate and thin film as well as size, shape and distribution of zero dimensional quantum dots and other nano structures

TOPICS DISCUSSED

- Structure of Materials
- Introduction to X-Ray Diffraction
- Introduction to Rietveld Analysis
- Reciprocal Space Mapping and Rocking Curve
- X- Ray Diffraction Line Profile Analysis -1
- X- Ray Diffraction Line Profile Analysis -2
- X- Ray Diffraction Line Profile Analysis -3
- X- Ray Diffraction Line Profile Analysis -4
- Introduction to SEM
- Introduction to TEM
- Introduction to HRTEM
- Introduction to Crystallographic Texure
- Introduction to Electron Back Scatter Diffraction
- Microstructural investigation of SPD processed materials - A case study
- Hands on with Rietveld refinement
- 2D XRD and Hands on with XRDLPA-1
- Hands on with XRDLPA

LIST OF SPEAKERS

- Prof. Rajesh Prasad, IIT Delhi
- Prof. AshishGarg, IIT Kanpur
- Prof. Gouthama, IIT Kanpur
- Prof. K. S. Suresh, IIT Roorkie
- Prof. ShashankShekhar, IIT Kanpur
- Prof. TamasUngar, Hungry
- Prof. K. Biswas,IIT Kanpur
- Prof. A. Subramanian, IIT Kanpur
- Prof. NileshGurao, IIT Kanpur

PARTICIPATING INSTITUTES

Institute	Number of Participants
ISM Dhanbad	1
NIT Kurukshetra	1
MNNIT Allahabad	6
V.S.S.U.T, Burla	2

HBTI, Kanpur	2
KNIT Sultanpur	1
DeenbandhuChhotu Ram University of Science and Technology, Muthal	1
NIT Raipur	2
FET, MJP Rohilkhand University Bareilly U.P.	2
NIT Rourkela	2
V.N.I.T. Nagpur	6
IIT Roorkee	4
IIT Bombay	2
Z.H. College of Engg. & Technology, AMU – Aligarh	1
PEC university	4
NIT Tiruchirappalli	3
OsmaniaUniversity	1
IIT Madras	2
DMSRDE, Kanpur	2
Total	**45**

WORKSHOP SCHEDULE

February 1, 2016

Time	Event
8:30 – 9:00 AM	**Registration**
9:00 – 9:30 AM	**Inauguration**
9:30 – 11:00 AM	**Structure of Materials** ***Prof. Rajesh Prasad, IIT Delhi***
11:00 – 11:30 AM	***Coffee Break***
11:30 – 1:00 PM	**Introduction to X-ray Diffraction** ***Prof. Rajesh Prasad, IIT Delhi***
1:00 – 2:00 PM	***Lunch Break***
2:00 – 3:30 PM	**Introduction to Rietveld Analysis** ***Prof.AshishGarg, IIT Kanpur***
3:30 – 4:00 PM	***Coffee Break***
4:00 – 5:30 PM	**Reciprocal Space Mapping and Rocking Curve** ***Prof. AshishGarg, IIT Kanpur***
7:30 PM Onwards	**Workshop Dinner**

February 2, 2016

Time	Event
9:30 – 11:00 AM	**X-Ray Diffraction Line Profile Analysis-1** ***Prof. TamasUngar, University of Budapest, Hungary***
11:00 – 11:30 AM	***Coffee Break***
11:30 – 1:00 PM	**X-Ray Diffraction Line Profile Analysis-2**

	Prof. TamasUngar, University of Budapest, Hungary
1:00 – 2:00 PM	***Lunch Break***
2:00 – 3:30 PM	**Introduction to SEM** ***Prof. K. Biswas, IIT Kanpur***
3:30 – 4:00 PM	***Coffee Break***
4:00 – 5:30 PM	**Hands on with Rietveld refinement**

February 3, 2016

Time	Event
9:30 – 11:00 AM	**X-Ray Diffraction Line Profile Analysis-3** ***Prof. TamasUngar, University of Budapest, Hungary***
11:00 – 11:30 AM	***Coffee Break***
11:30 – 1:00 PM	**Introduction to TEM** ***Prof. A. Subramanian, IIT Kanpur***
1:00 – 2:00 PM	***Lunch Break***
2:00 – 3:30 PM	**Introduction to HRTEM** ***Prof. Gouthama, IIT Kanpur***
3:30 – 4:00 PM	***Coffee Break***
4:00 – 5:30 PM	**2D XRD and Hands on with XRDLPA-1**

February 4, 2016

Time	Event
9:30 – 11:00 AM	**X-Ray Diffraction Line Profile Analysis-4** ***Prof. TamasUngar, University of Budapest, Hungary***
11:00 – 11:30 AM	***Coffee Break***
11:30 – 1:00 PM	**Introduction to Crystallographic Texture** ***Prof. NileshGurao, IIT Kanpur***
1:00 – 2:00 PM	***Lunch Break***
2:00 – 3:30 PM	**Hands on with XRDLPA**
3:30 – 4:00 PM	***Coffee Break***
4:00 – 5:30 PM	**Visit to FIST XRD and SEM facility**

February 5, 2016

Time	Event
9:30 – 10:30 AM	**Introduction to Electron Back Scatter Diffraction** ***Prof. ShashankShekhar, IIT Kanpur***
10:30 – 11:30 AM	**Microstructural investigation of SPD processed materials - A case study** ***Prof. K. S. Suresh, IIT Roorkie***
11:30 – 12:00 PM	***Coffee Break***
12:00 – 1:00 PM	***Valedictory function***

SUMMARY OF FACULTY FEEDBACK

Workshop

Questions	***Excellent***	***Good***	***Ordinary***
Clarity of communication about workshop	04	06	00
Organization of the sessions	03	07	00
Quality of lectures	07	03	00
Effectiveness of discussions	03	07	00
Effectiveness of learning experience	02	07	01
	Appropriate	***Short***	***long***
Duration of workshop	08	02	00
	Definitely	***May***	***No***
Would you like to have more such sessions?	08	02	00
Would you like e-lectures by experts on special topics?	06	01	00
Suggest specific topic that you would like additional expert lectures on	➢ Experimental procedure for SEM and TEM ➢ Metal recovery from waste ➢ Power plant materials. ➢ Use of spectroscopic techniques to analyze combustion generated pollutant. ➢ Heat transfer. ➢ Advanced functional materials ferroelectric. ➢ Thermodynamics of interfaces in metals and alloys ➢ Nano alloys ➢ Small angle scattering (SAXS) ➢ Polarized light microscopy ➢ Dielectric spectroscopy ➢ Dynamic mechanical analysis (DMA) ➢ More lectures on SEM, TEM and structural charges with temp		

Additional Suggestions	➢ Lab demonstration for XRD and SEM, TEM ➢ Lab session must be more ➢ Discussion part must be more. ➢ It will be better if you could organize such workshops during summer and winter vacation. ➢ There should be a fully dedicated workshop on XRD line profile analysis (may be from Prof. Unger's group)

Teaching

Which subjects do you teach?	➢ Material Science ➢ Principals of extraction metallurgy, iron and steel making, mineral processing ➢ Heat and mass transfer, power plant engg,Gas Turbine & Jet propulsion. ➢ Combustion generated nano organic carbon. ➢ Electromagnetic Theory condensed matter physics ➢ Thermodynamics of materials, advanced composite materials, advanced experimental techniques engineering metallurgy ➢ Polymer Sc. & Tech., Polymer Composites. ➢ Structure Prop. Relationship of polymer. ➢ Engineering Physics ➢ Composite materials, Measurement and Control,	
What is average student to teacher ratio in your institute?	➢ 40:01 ➢ 20:01 ➢ 17:01 ➢ 15:01 ➢ 18-20:01	
Questions	***YES***	***NO***
Do you have additional support for teaching (tutors, graders, teaching Assistants, etc)?	04	06
Do you give class projects for UG classes?	08	02
Do you give class projects for PG classes?	07	03
Do you have sufficient resources for laboratory courses?	03	07

	Sufficient	***Inadequate***	
Is the library/journal/e-connection support adequate?	02	08	
	Definitely	***May* be**	***No***
Would you like to have common (TEQIP) repository of course material?	10	00	00
Would you like to visit IITK to participate in and develop course material (existing or new)	08	02	00
Would you like to participate in creation of the repository material (course files/lab. Manuals/question bank/etc)	08	02	00
	e-courses	***Workshops***	***Content***	***none***
How can IITK effectively help you prepare	07	07	03	
How can TEQIP help improve yourteaching?	➢ By teaching-learning methodology ➢ Helping us to provide materials & scope related to our subject area. ➢ By teaching-learning process ➢ TEQIP should start initiative to make a webpage where the experimental/research facilities/resources purchased with TEQIP grant should be listed(institute wise) and should facilitate the testing of sample from TEQIP institution free of cost. ➢ To attend workshops, visiting faculty position at IIT, IISc, financial support. ➢ Even organizing such workshops (support financially) ➢ By organizing the workshops on Teaching methodologies and on basic subjects of importance.			

Research

Questions	***Definitely***	***Maybe***	***No***
Would you like to visit an IIT for a visiting-faculty/ post-doctoral fellow, if offered (via-TEQIP)?	10	00	00
Would you like to share/use research infra-structure at IITK, if made available?	10	00	00
Would you like to conduct collaborative research with IITK?	10	00	00

Would you like lectures by experts (Indian and international) on niche research areas/topics?	08	02	00
Do you want special-topic conferences?	07	03	00
How can TEQIP help improve your research?	➢ By collaborative research work visiting research programme ➢ Provide research facilities during the project work. ➢ To support financially to interact and collaborate with researchers through workshops. ➢ TEQIP should take care of consumables TA/DA sample testing for student/ faculty. ➢ By allowing us to use the advanced facilities at IIT Kanpur. ➢ Allow us to use research facility at all IIT's and provide funds for doing research. ➢ By providing facility available in different TEQIP institutions.		

SUMMARY OF STUDENTS FEEDBACK

Workshop

Questions	***Excellent***	***Good***	***Ordinary***
Clarity of communication about workshop	18	7	00
Organization of the sessions	21	04	00
Quality of lectures	21	04	00
Quality of posters	12	11	00
Effectiveness of discussions	11	14	00
Effectiveness of learning experience	12	12	00
	Appropriate	***Short***	***long***
Duration of workshop	20	01	02
	Definitely	***Maybe***	***No***
Would you like to have more such sessions?	22	01	01
Would you like e-lectures by experts on special topics?	20	03	00

Suggest specific topic that you would like additional expert lectures on	➢ Transmission Electron Microscopy ➢ Analysis of TEM microscopy ➢ Ferroelectric, Dielectric and Magnetic properties of materials. ➢ Texture for welding sample and corrosion part ➢ Analysis of characterized data. ➢ Stud y of nanomaterials characterization. ➢ Energy based materials function on its structure like thermo electric methods. ➢ AFM, APM and X-Ray Tomography. ➢ X-Ray diffraction advanced topics like X-Radia, X-ray Tomography ➢ Do more experimental include it propagation. ➢ Fatigue and fracture analysis of alloy processed by SPD. ➢ HRTEM ➢ Solidification. ➢ More lectures on micro & Macro texture. ➢ In detail lectures on texture EBSD reciprocal space. ➢ Molecular dynamics simulations (LAMMPS)
Additional Suggestions	➢ Need some more lectures on EBSD in future ➢ 5 days is slightly too long. ➢ The course work during workshop should be lab oriented ➢ Time spent for complex topics like reciprocal space mopping & LPA can be more. ➢ Do more experiments. ➢ Also explore the new soft skill other than exp. work. ➢ Including of SAED for cubic materials ➢ May be included hands on practices ➢ A dedicated workshop on molecular dynamics simulations involving experts from inida and abroad will be good for exposing students like us to simulations like us to simulations domain. ➢ Operating procedure of HRXRD & HRTEM ➢ Regarding microscope TEM no clarity in discussion.

Learning

Questions	***Yes***	***No***
Do you get enough class projects?	19	03
Is the learning adequate?	16	02
Do you have sufficient resources for laboratory	10	06
What is your area of specialization	➢ Texture ➢ Texture of stainless steels ➢ Physical metallurgy; coating ➢ Welding behaviour & phase transformation. ➢ Polycrystalline Transparent Ceramics. ➢ CNT/Polymer composites. ➢ Materials Characterization. ➢ Half time to lecture of the programme and other half time of laboratory visit. ➢ Fatigue & fracture. ➢ Physical & Mechanical Metallurgy. ➢ Nanocrystalline Materials ➢ Metallic glasses. ➢ Characterization of materials ➢ Microwaves ➢ Wear (thermal spray coating) ➢ Ultra high temperature ceramic composites ➢ Nanomaterials	
	Sufficient	***inadequate***
Is the library/journal support/e-connection	14	06

	Definitely	***Maybe***	***No***
Would you like to have common (TEQIP) repository of course	21	01	00
Would you like to visit IITK to attend specialized courses?	23	00	00
Would you like MOOCS/e-resources based courses?	22	01	00

How can TEQIP help improve your learning?	➢ By lecture experts from this improves my knowledge ➢ By listening the valuable lectures given by the experts on various topics. ➢ Expand to depth to which analysis can be done. ➢ Yes, it provide us platform to interact with expertise ➢ So many minds on simple platform makes me more inquisitive about topic. ➢ Yes, it provide us platform to interact with expertise & share their experience with us. ➢ Organize workshops on latest trends in research co-related to real world applications. ➢ By conducting more specific workshops like the we attend at IITK ➢ Help to explore new stuffs ➢ Ideas generated for different process ➢ Run the learning course quality in region wise IIT ➢ Please give proper hands on. ➢ Conduct frequent workshops like this on varied topics. ➢ Demonstrating equipments for practicality. ➢ Provide or organize some core experimental course like SEM, optical Microscopic. ➢ Conducting workshop like this. ➢ Student like us should be given more exposure to these kind of expert talks which help to enhance interaction. ➢ Organize additional training program ➢ Preferences (books, journals) by lecture.

Research

Questions	***Definitely***	***Maybe***	***No***
Would you like to visit an IIT for a short visit /internship/post- doctoral stint ,if offered (via TEQIP)?	25	00	00
Would you like to share/use research infra-structure at IITK, if made available?	25	00	00
Would you like to conduct collaborative research with IITK faculty?	24	01	00
Would you like lectures by experts (Indian and international) on niche research areas/topics?	25	00	00
Do you want special-topic conferences?	25	00	00

How can TEQIP help improve your research?	➢ I received very new exposure, which I will try to introduce in my journey of research. ➢ I improved certain level by listening lectures. I planned for Nano Indentation characterization by attending TEQIP programme in 2014 ➢ Free facility to use instrument in any TEQIP institute. ➢ TEQIP should emphasize or enhancing workshop interactions so that we can learn more from global experts. ➢ Also I request TEQIP to fund more for participants ➢ Provide lab facility during workshop at extra time after class session. ➢ By providing/organizing workshops for experimental and analysis techniques. ➢ Collaboration & sharing of facilities as well as collaborative cutting edge research work. ➢ Increase no of experimental classes ➢ Analysis must be different. ➢ Give more demonstration to lab visit. ➢ Hands on experience of equipments ➢ Just like this workshop all institutes under TEQIP should share the facilities al low cost than others ➢ Yes, such type of workshop conducted by TEQIP improve our technical skills as well as our research knowledge. ➢ So many new research work by different professor gives lots of information. ➢ Yes, by providing such type of workshop & conferences to enhance my knowledge. ➢ By organizing this type of lectures by expert in the area of texture in future too.

Additional Questions

1.) Would you want in the 3rd phase of TEQIP paid access to high end experimental facilities in specific institutions?	➢ High quality of research always require a well established structured lab. Here we found a good research infrastructure. It always require upgrading the facility with the age of development. ➢ In the 3rd phase of TEQIP we would like to have high experimental facilities in the specific institutes, so that all the TEQIP institutions can avail those facilities. ➢ To enhance the level of research, TEQIP is very good initiative. I have an idea always which we can implement i.e. about the advanced central research facility in India will be very involved in application field. It may be in the form of the whole research city which is publically open not only limited India but internationally. No boundation or limitations should be their which can limit the research in India. ➢ Yes , TEQIP is very useful programme for increase the knowledge of my research in various fields. In this programme, I learnt that the analysis is more important tool for research. TEQIP should be organized quarterly in IIT's. ➢ For sophisticated instrument like TEM, SHRTM more training should be done. ➢ I request concession for NON-TEQIP institutions to attend such kind of workshops. Already we have been passing for experiments facilities, request less the charges for Ph.D. scholars. ➢ Since, there is already a paid facility for access to experimental facilities in almost all the TEQIP affiliated institutes, so now if these institutions provides to the people accessing their facility from other TEQIP affiliated institute then this will definitely help them in many ways. ➢ I wish to have some type of workshop is provided with some experimental facility to participant so that participant can use all information discussed in lecture can utilize in lab work too. ➢ I definitely welcome TEQIP paid access to high end experimental facilities in specific institution. However i have slight reservation in this regard. Rather than explicitly finding for experimentation I also

	would like to suggest that funding simulations in high end computational facilities also would provide as supplement to enhance research quality. I am of the opinion that enhancing simulations research can cut the expenses incorrect in redundant experimentation. But it will be definitely good to have funding from TEQIP to get access to experimentation. ➢ As there is paid access already at may IIT, NIT & TEQIP affiliated institutes ; it will be more encouraging if students / scholars from other TEQIP affiliated institutes will be allowed to test a finite number of samples for free of cost & then the charges should be applied at bare minimum limit. This will encourage various institutes to interact on student level also. ➢ Yes, we could probably have these workshop across the country, to ease accessibility. I also a little clarity regarding TEQIP, as in what/which institutes come under this fold. ➢ Yes, the paid access to high end experimental facilities in remote specific institution. ➢ We would like to access high end experimental facilities like XRD, HRTEM, FESEM etc on payment basis. ➢ I would like to participate in future workshops and conferences organized by TEQIP on advanced analytical technologies for materials characterization and other instrumentation workshops. The experimental facilities database at various institutions may also be prepared & shared so that it may be utilized by researchers. ➢ Yes we want the further TEQIP session, which is very much good to us and help to increase our knowledge and it should be organized regular interval time period. ➢ Yes, I want paid access of high end experimental facility in your institute because I am working on material sciences so I am not have so much facilities. So we want to join your institute facility to do our research work. ➢ Yes, definitely the facilities are exceptional in the access centre and I think that would help a lot.

	➢ Yes, we want the 3rd phase of TEQIP paid access to high end experimentation facility in specific institution as it would help a lot. ➢ Yes it should be here and in all institute to attracting all institute. ➢ Definitely, we would be very much interested for TEQIP paid access to high end experimental facilities in specific institution. ➢ Yes, 3rd phase of TEQIP should be paid access to high end experimental facilities should be created in a every region of India. ➢ Yes we would like access to the above experimental facilities
2.) would they be interested in having high end state art of activity TEM, SHRTM etc at specific institution (in the TEQIP fold so that all TEQIP institutions can access) ?	➢ Particularly for HRTEM, FE-SEM charges for Ph.D. scholars provide less charges. TEQIP workshops must be 06 days. For self sponsoredPh.D. scholars please give collaboration with IITK or IIT organization facilities. It is very difficult to me to carry out experiments in IIT's. As a self sponsoredPh.D. scholar I request please provide collaboration with IITK professors ➢ Yes , I would definitely like to have these high end state art of activity TEM, SHRTM etc if TEQIP can help kin providing this provided the charges for using variables facilities should be as minimum as possible. ➢ I will be great idea to have state of the art activity in TEM, SHRTM atom probe topography and many other equipment at any specific institution. ➢ Al least basic characterization tools such as FEB-SEM, SRD, HRTEM etc should be made available at every TEQIP affiliated institutes. Our institution, VNIT has a good centralized facility of SEM, XRD & thermal analysis equipments that we run on our level. If TEQIP can help, then as a scholar, I would like to have FEB-SEM & at least basic TEM at our institute. This will reduce the trouble for many students for travelling & encourage them to explore the potential these techniques for better research. ➢ Yes, please try to acquire Atom Probe or TEAM.

	➢ Be interested in having high end state art of actively , at specific institution. ➢ After getting adequate exposure in these area, we would like to buy these art of state analytics instruments. Our establishment is also planning to create XRD, FESEM & HRTEM facilities very soon. ➢ PEC university of Technology, Chandigarh is also going to apply under TEQIP-III phase. So PEC also wants some basic facilities like XRD FESEM. ➢ Yes, we all are interested in having all these facilities of TEM, SHRTM which is help us in our Project and Research work. ➢ Yes, some facilities like EBSD and TEM are very much required. As I arrive from a NIT it would be very nice for us to use the facilities because that would even help us make the research facilities at NIT's better. ➢ Yes, interested in having high end state of art of activity like EBSD, TEM, SHRTM which help us in understanding the m/c and technology & help in our research. ➢ We are definitely interested to have the high end state art of activity TEM, at VNIT, Nagpur so make available to access by all TEQIP institution. ➢ Yes, but always centralized facility in each region.

OUTCOME

The workshop was envisaged to introduce participants to the various diffraction techniques using both electron and x-ray to characterize material. 45 participants were registered for the workshop. Participants came from all corners of the country, including NIT Trichy, VNIT Nagpur, PEC Chandigarh as well as IIT Bombay and IIT Madras. The initial feedback from the participants was overwhelming. Each of the participants greatly appreciated the presence and contribution of Prof. Ungar in the workshop. Most of the sessions were interactive with several questions being asked by the participants.

- Prof. Tamas Ungar who is considered the authority in the field of 'Line Profile Analysis' was especially invited for this workshop. Prof. Ungar contributed significantly to the workshop by addressing several lectures and tutorial sessions.
- Structure of materials and basics of X-Ray diffraction was introduced by Prof. Rajesh Prasad of IIT Delhi.
- Prof. Ashish Garg disseminated knowledge related to various advance techniques of X-ray diffraction, including, but not limited to, Rietveld Analysis.
- Workshop also greatly benefited from department's expertise in the field of electron diffraction (viz. TEM, HRTEM, EBSD, Texture). Some students also lend their hand in conducting the tutorial session. Lab-session was meticulously conducted by Lab staff of ACMS and MSE, under the supervision of Prof. Nilesh Gurao.