ESF Scientific Report

Programme: ESF Micro-dice Exchange Grant

Title of the project: Deformation heterogeneities in ice and 2-phase rocks evaluated by a full-field FFT model.

Author (Summer Intern): Prabhat Kumar(Department of Geology & Geophysics, Indian Institute of Technology, Kharagpur-721302, INDIA)

Host and Supervisor in France : Dr. Maurine Montagnat, Laboratoire de Glaciologie et de Géophysique de l'Environnement / LGGE, UMR 5183, 54 rue Molière, BP 96, 38402 St Martin d'Hères cedex, FRANCE

M.Sc Supervisor in India: Professor Manish A. Mamtani (Department of Geology & Geophysics, Indian Institute of Technology, Kharagpur-721302, INDIA

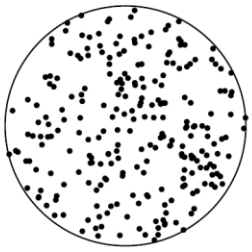
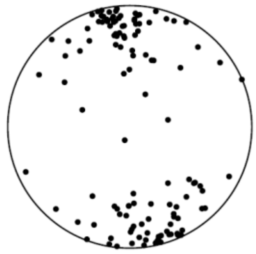
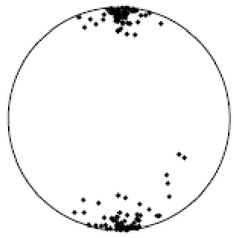
Purpose of the visit

The primary purpose of the visit was to make use of this opportunity to put my theoretical knowledge into practice while gaining experience in a scientific working environment. Specifically to understand the working and to get experience of the full field FFT approach CraFT modelling software, and to use this knowledge to model the deformation behaviour of polycrystalline ice to estimate the strain and stress heterogeneities at a granular scale. The modelling was to be carried out on artificial texture microstructures created with the help of same modelling software using different Tessellation techniques and different degrees of Texture Anisotropy, and then model them using the same conditions that were used while performing the test on real microstructures, to get model results. The purpose was to quantify the differences in the response of different tessellation microstructures with different degrees of texture anisotropy on deformation by characterizing their strain and stress field with various ways which will be specified later.

Description of the work carried out during the visit

The visit started with me learning how to use the full field FFT approach CraFT model, using various model examples given in the software, and a thorough practise using the User Guide provided with the software. I also visited the Laboratory of Mechanics and Acoustics, situated in Marseille, France for four days in the 5th week of my internship to better understand the working of the CraFT model from Herve Moulinec who himself is the developer of this software.
The work carried out mainly concerns itself with the response of two 2-D artificial microstructures with each having 500 grains, developed using two different Tessellation techniques namely: Johnson-Mehl-Avrami-Kolmogorov or JMAK Tessellation and Voronoi Tessellation. Two sets of phases were applied to both of artificial microstructures. One set being Isotropic with Random c-axis orientation, and the other set was Anisotropic with the c-axis orientation being inclined towards the direction of imposed macro stress.
Thus we had finally four microstructures:
1. Anisotropic100 JMAK microstructure (AJ)
2. Isotropic JMAK microstructure (IJ)
3. Anisotropic100 Voronoi Microstructure (AV)
4. Isotropic Voronoi Microstructure (IV)
Later when the analyses of these microstructures were completed, based on their results we added one more microstructure with more degree of anisotropy which was analysed with only JMAK tessellated Microstructure, because the difference between voronoi tessellation and JMAK tessellation was small. The graphs of Probability density were drawn to check the correspondence of the results in the five experiments that we did, and they overlapped the previous results almost perfectly. So therefore the fifth microstructure to be tested was:

5. Anisotropic150 JMAK Microstructure (AJ2)
The pole plots have been shown Fig 1 of the three Microstructure with different degree of anisotropy used

Random Isotropic Microstructure	Anisotropic Microstructure(AJ)	Anisotropic Microstructure (AJ2)
		

<u>Fig 1. Stereograph of the c-axis orientation of the grains</u>. (.) Denotes the position of poles on the stereograph

The JMAK tessellation was done using a growth rate of 0.7 and the time interval of appearance of the seeds for the growth of grains was set to be 0.05 seconds. The voronoi tessellation was done with the same time interval of appearance of seeds of 0.05. These parameters were chosen such that the microstructure obtained resembles the real microstructure of ice.

The modelling exercise was carried out under a macro stress of -0.5 MPa applied in the 'yy' direction till the overall strain in the y direction (Eyy) reached 1%. The model cannot account for the dynamic recrystallization processes that becomes active in the Ice upon deformation to a degree of greater than 1% in the applied stress direction, thus the deformations in ice only up to 1 % can be successfully modelled with the help of full field FFT approach.

Various Graphs and plots were plotted for all the microstructures at four different levels of deformation achieved (overall strain E22 – 0.1%, 0.5%, 0.75%, 1%) to characterize the Strain and Stress Field. They are:

1. Schmid Factor vs. Equivalent Strain/Equivalent Stress

2. Distance to Grain Boundary vs. Equivalent Strain/Equivalent Stress

3. Probability Density Graphs of Equivalent Strain/Equivalent Stress

4. Probability Density Graphs for the different components of Strain and Stress Tensors (mainly Exx, Eyy, Exy and Sxx, Syy, Sxy)

5. Full field map of any strain and stress component along with equivalent strain and stress.

Also various useful results were calculated from these plots to quantify the character of the graphs or plots. All the plotting and calculation of the results were achieved through MATLAB Programming.

After obtaining these secondary Graphs/Plots and calculated results, these were finally used to create the final graphs/plots and results which would be suitable and easily comparable, which I shall present in the 'Description of the main results' section.

<u>Description of the Main Results obtained:</u>

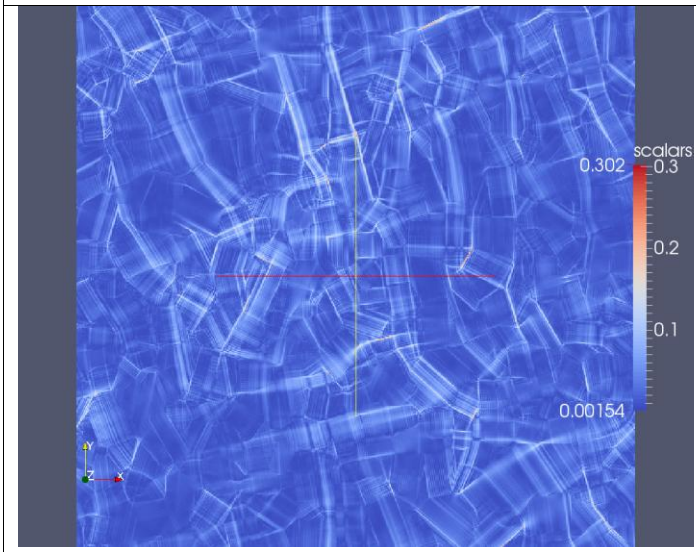
Though there were several graphs and results obtained, there are few main results which I would present in my Final ESF report.

I would now only present the final results obtained for the Equivalent Strain and Equivalent Stress, though similar exercise was carried with all the components of the Stress and Strain Tensors.

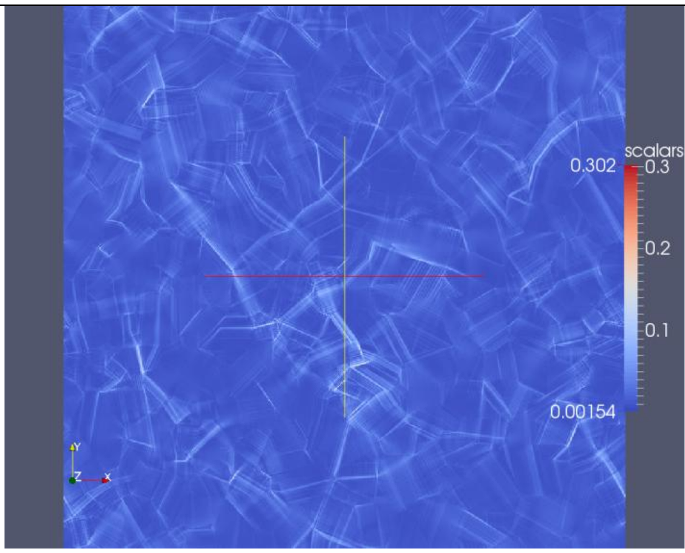
Full-Field Image of the Equivalent Strain at 1% Eyy for all the microstructures are shown in the next page.

<u>Fig 2. Full Field Image of Equivalent Strain</u>. (Scalars represent the colour scale along with the magnitude of Equivalent Strain)

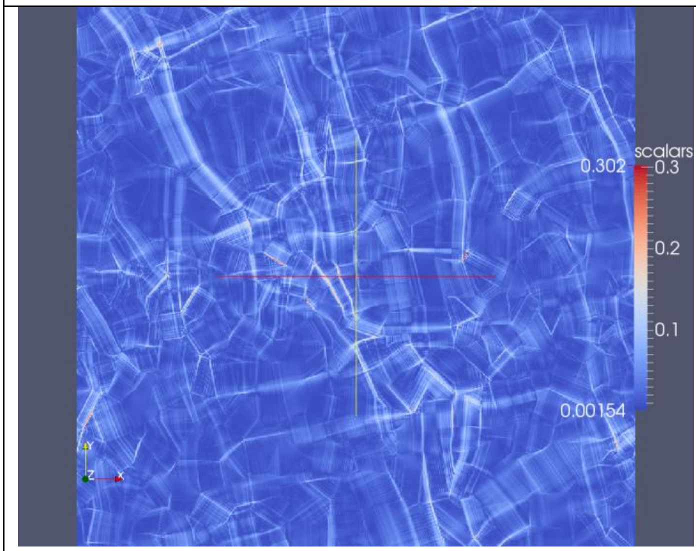
Anisotropic JMAK



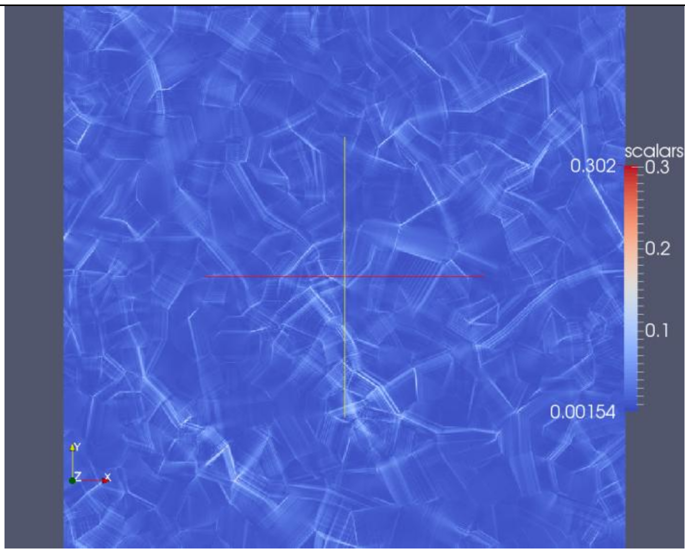
Isotropic JMAK



Anisotropic Voronoi

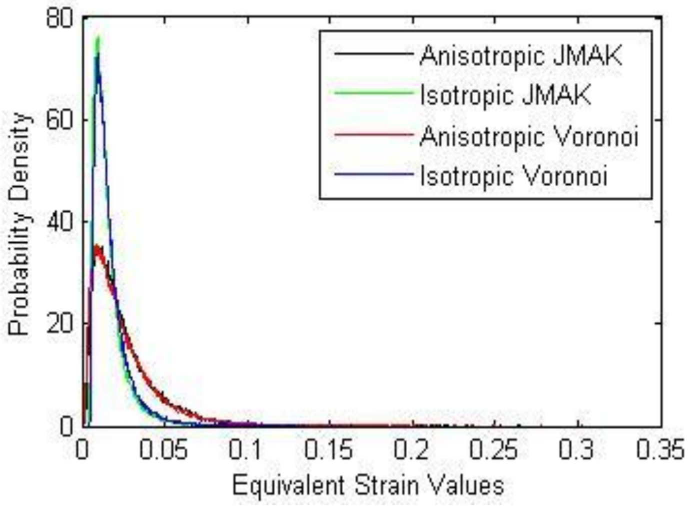
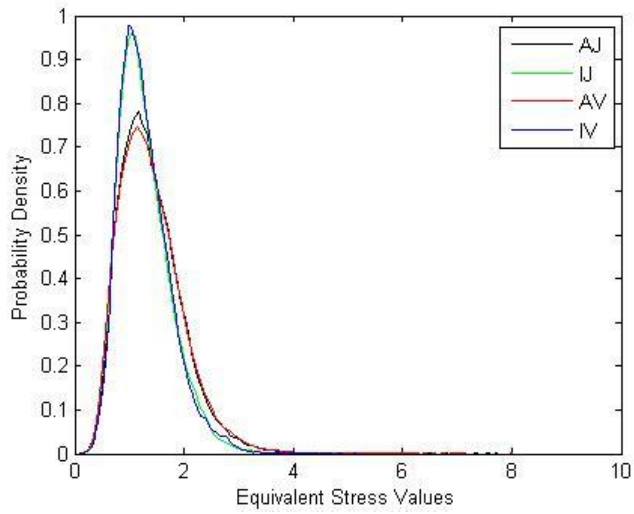


Isotropic Voronoi



The full field map of the Equivalent strain shows the differences in the evolved strain heterogeneities in different microstructures. Similarly the full field maps of the Equivalent Stress, and of the different components of the stress and strain tensors were obtained.

Fig 3: Probability Density vs Equivalent Strain/Stress at 1% Eyy

Equivalent Strain (at 1% Eyy)	Equivalent Stress (at 1% Eyy)
	

A few results explaining the graphs of Fig 3 are given below. Eeq represents Equivalent Strain and Seq represents Equivalent Stress.

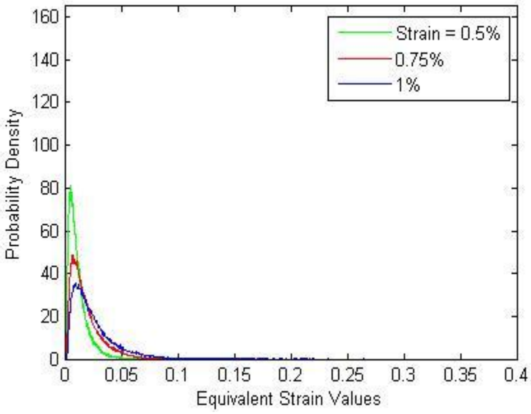
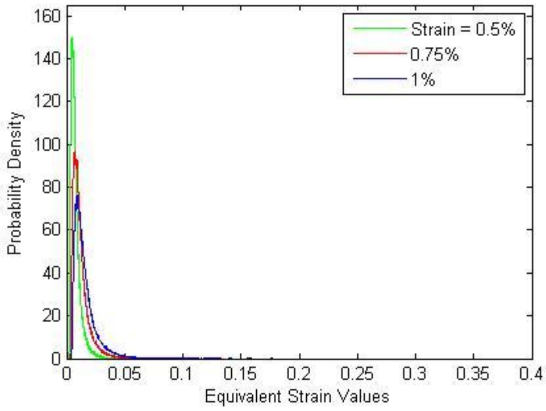
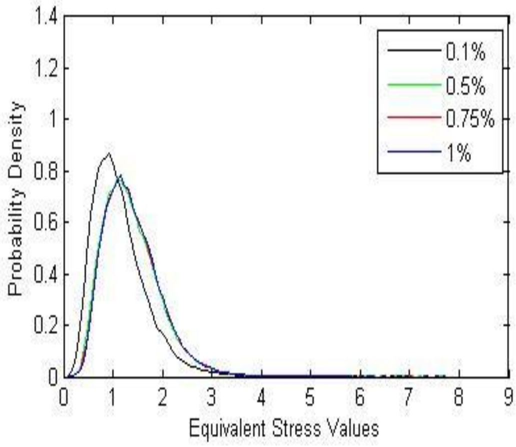
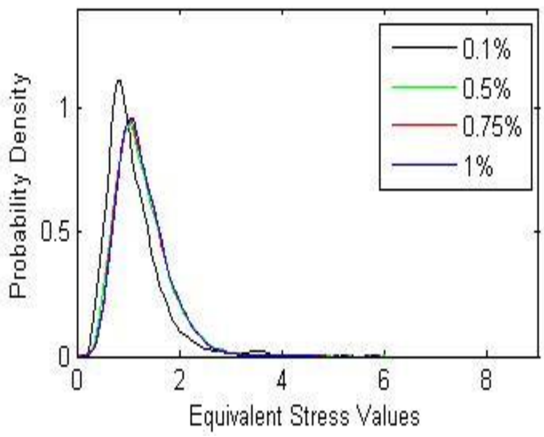
Eeq	Mean	Standard Deviation	FWHM
AJ	0.025377	0.020153	0.023342
IJ	0.015856	0.010422	0.01092
AV	0.02519	0.020982	0.022975
IV	0.017137	0.011214	0.01107

Seq	Mean	Standard Deviation	FWHM
AJ	1.394527	0.570296	1.23125
IJ	1.269502	0.482829	0.957522
AV	1.401162	0.585748	1.289909
IV	1.280962	0.477763	0.953672

We see that the JMAK and Voronoi Microstructures nearly overlap for each Isotropic and Anisotropic case separately; the data related to these figures show some minor differences in overlap. The difference between the Anisotropic and Isotropic case is distinctly evident and interesting. The isotropic microstructure experiences less strain and stress heterogeneities than the anisotropic microstructures. One can also observe that increasing the degree of anisotropy results in increasing the deformation heterogeneities, though the increase in strain heterogeneities seems to be more than the increase in stress heterogeneities.

Since we see that the JMAK and Voronoi tessellations produce almost the same results, so I would only present the results now for JMAK microstructures.

Fig 4. Probability Density vs. Equivalent Strain/Stress

Microstructure	Anisotropic JMAK	Isotropic JMAK
Eeq		
Seq		

Here I shall present the Probability density graphs of equivalent strain and equivalent stress at three stages of their deformation (Eyy reached 0.5%, 0.75%, 1%).We observe that the Equivalent Strain heterogeneities increase with the percentage of overall strain Eyy. Though it is observed that the Equivalent Stress heterogeneities does not change after 0.5% overall deformation is achieved (Eyy=0.5%) , there is a small change or increase in shown in the initial stages i.e. from 0.1% to 0.5%, but we can say that the Stress heterogeneities are set during very early stages of deformation and does not evolve much with increase in the deformation. Also it is very clearly seen that the local strains and stresses can reach much above the macro strain and stress observed even more than 10 times as large as their macro counterparts.

Next we would compare the **Equivalent Strain vs Distance to grain boundary**, of every pixel in a microstructure for all the microstructures at 1% Eyy strain. Seeing the results we can clearly say that the concentrations of strain heterogeneities are only slightly more near the Grain Boundaries. We shall observe the results only for the JMAK microstructures.

<u>Fig 5. Equivalent Strain vs Distance to grain Boundary</u>

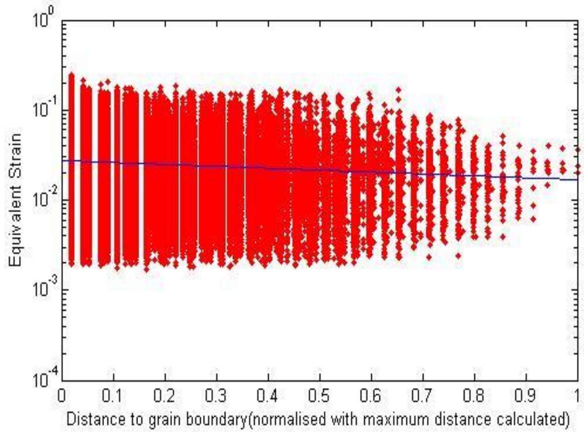
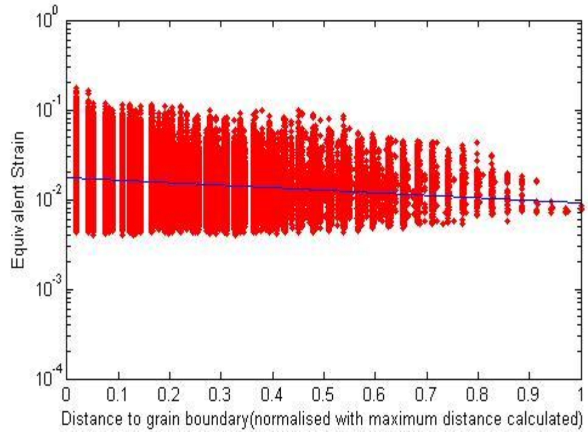
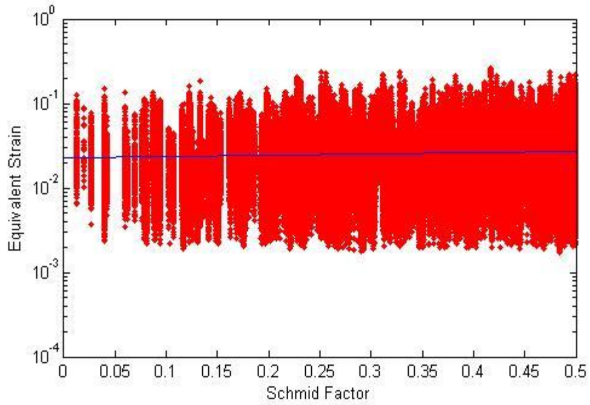
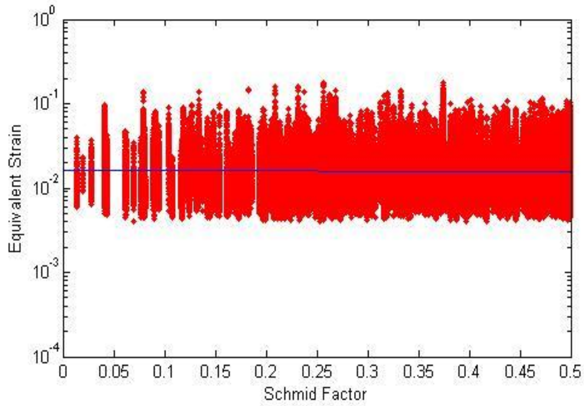
	Anisotropic JMAK	Isotropic JMAK
Eeq		

Fig 6. **<u>Eeq vs Schmid Factor</u>** of the pixels for different microstructures.

	Anisotropic JMAK	Isotropic JMAK
Eeq		

From the Eeq vs Schmid Factor graphs, we can see that strain heterogeneities do not particularly increase with the increase in the Schmid Factor for the so called favourably oriented grains. This can be explained by the neighbourhood effect and the condition of maintaining compatibility, which hinders the deformations in shape of the grains thus making them accommodate only some determined value of deformation based on the presence and subsequent deformation of the adjacent grains so that no gap is created in the microstructure due to deformation.

These were the main results and concise discussion of the work that I did.

Future collaboration with the host institution

These obtained results with all the primary and secondary results have been carefully arranged and stored for future reference. I am quite interested in the possible applications of this full field FFT CraFT model in the field of Hard Rock Geology, specifically the case with single phase quartzite or double phase quartzite with minor amounts of mica.

I shall be investigating the possible effects of increasing the concentration of mica on the deformation heterogeneities developed in the quartzite as a whole and the possible impacts of increasing mica concentrations on the evolution of crystallography and textures in quartzite. I am also interested in some questions about the possible heterogeneities arising in single material microstructures having a bimodal distribution of grain sizes. Possibly it can answer the questions about quartz vein inside a quartz vein thus having bimodal distribution of grain sizes.

Some more areas where the present knowledge gained through this visit shall be useful , and that I am going to work in near future is investigating the effects of Grain size, grain shape , presence of minor phases such as mica in Quartzite on the evolution of deformation heterogeneities, crystallography and texture development.

My M.Sc. Thesis Supervisor Professor Manish A. Mamtani from Indian Institute of Technology, Kharagpur, India visited the institute LGGE, Grenoble to discuss about future collaborations. The possible areas discussed were in terms of application of this software in the field of Hard Rock geology and related geoscientific areas. In addition the possibility of me being jointly guided for my M.Sc thesis with Dr. Maurine Montagnat (LGGE, Grenoble) as a co-supervisor was also discussed, although a final decision on this aspect has not yet been arrived at.

Projected publication/articles resulting or to result from the Grant

All the results and the data obtained during the visit have been carefully stored in a sound and fully retrievable manner for any future reference. All these data and results may be used when necessary for publishing in any context either by me or Researcher Maurine Montagnat. In October this year, the Structural Geology & Tectonic Studies Group - India (SGTSGI) will be organizing the third Rock Deformation & Structures (RDS-III) conference, which is held once every two years. The target is to present a paper in the conference either by me or my M.Sc supervisor (Prof. Manish A. Mamtani) based on the work done during the visit. An abstract of the above mentioned paper is already submitted to the conference organisers.

Conference Paper (Abstract)

Kumar, P., Montagnat, M., Moulinec, H. and Mamtani, M.A. (2014). Microstructure Modelling using CraFT – Learning from Microdynamics of Ice. Third Rock Deformation & Structures (RDS-III) conference, Dibrugarh University, Assam (India), October 2014 (in-press).

Other comments

Overall this visit was very interesting and quite a learning experience for me. I am quite determined to carry along the things learned here to the future.

References

1. Experimental characterization of the intragranular strain field in columnar ice during transient creep. F. Grennerat, M. Montagnat, O. Castelnau, P. Vacher, H. Moulinec, P. Suquet, P. Duval. 2012 Acta Materialia Inc.

2.Multi-scale modelling of the mechanical behaviour of polycrystalline ice under transient creep. P. Suquet, H. Moulinec, O. Castelnau, M. Montagnat, N. Lahellec, F. Grennerat, P. Duval, R. Brenner. 2012 Elsevier B.V. Selection.

3.Multiscale modelling of ice deformation behaviour. M. Montagnat, O.Castelnau, P. D. Bons, S.H. Faria, O. Gagliardini, F. Gillet-Chaulet, F. Grennerat, A. Griera, R.A. Lebensohn, H. Moulinec, J. Roessigner, P. Suquet. 2013 Elsevier Ltd.