



## **Simulation of the CNFs multilayer coating particle distributed in three dimension**

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### **Abstract**

In modern thin-film technology, spray coating plays a crucial role in fabricating flexible electronics and photovoltaics. Surface-sensitive scattering methods deduce the complex interface and multilayer structure. Spray coating was applied to create functional layers, from novel latex colloids to complex biomaterials templates. There is a strong need to go beyond a one-dimensional analysis and investigate the use of simulation-based research. The real-space structure is modelled (size and distribution of the nanostructures in three dimensions), the scattering pattern is calculated and compared to the experimental data. Hence, this project aims to simulate the scattering pattern based on established algorithms and image analysis, CNFs tubes orientation, silver nitrate particle distribution using Born-again simulation software.

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## 1. Introduction

over the last few decades, sustainable materials have gained increasing attention for future flexible, biodegradable, yet disposable electronics. Cellulose nanofibers (CNF) have favourable properties such as lightweight, thermal stable, and good mechanical strength. These properties make CNF a very promising precursor for creating high-performance bioinspired materials and nanocomposites due to their earth-abundant bio-based origin and biocompatibility. Here we are working on the control distribution of silver nitrate particles on CNFs. Silver nanoparticles (AgNPs) and AgNP-based composite materials have attracted growing interest due to their structure-dependent optical, electrical, catalytic, and stimuli-responsive properties.

## 2. Theory & Measurement

1<sup>st</sup> we install bornagain software. This software provides a generic framework for modelling multilayer samples with smooth or rough interfaces and various embedded nanoparticles. In my part of the work, I have to arrange random cylinders over Si-based substrate. The lying cylinder structure should be like randomly placed spaghetti.

1<sup>st</sup> I selected the sample option of this software. I have then started the arrangement of cylindrical CNFs randomly that it should be formed a spaghetti-like structure. I have taken the following coordination point to get a single spaghetti structure.

**Dia-5\*nm, L-50\*nm, Film Thk.-200nm**

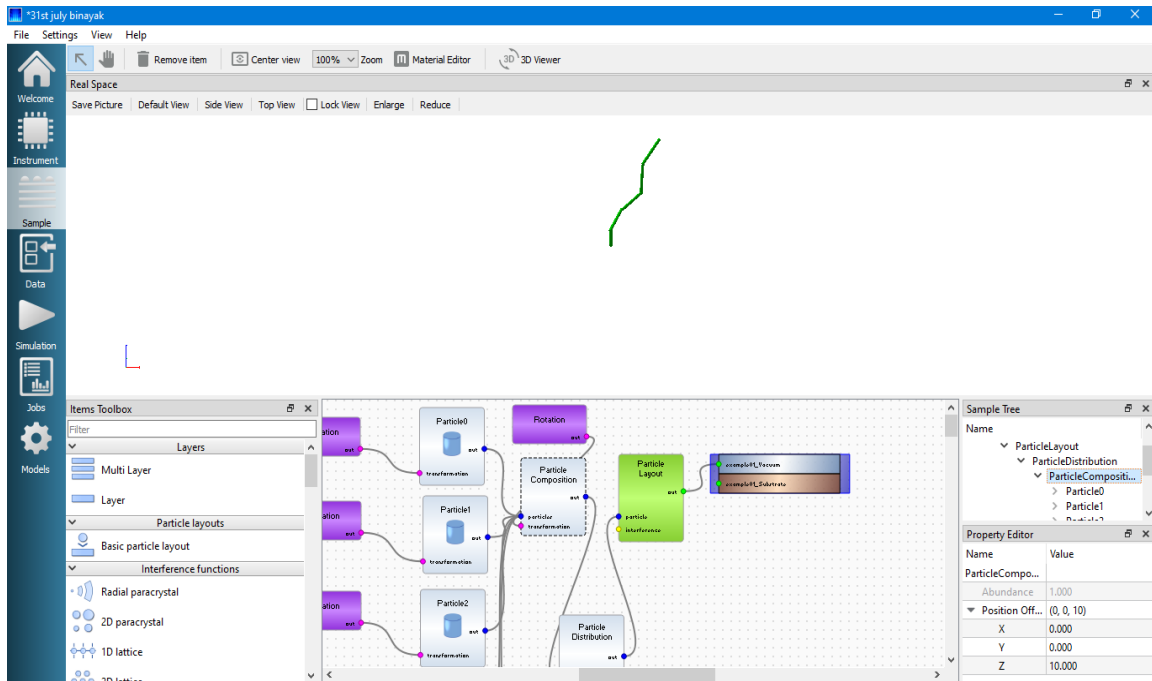
particle\_1\_rotation=Y(90\*deg), Coordination- x,y,z-(0\*nm, 0\*nm, 7\*nm)

particle\_2\_rotation Euler(60\*deg, 60\*deg, 0\*deg), Coordination- x,y,z-(48\*nm, 2\*nm, 7\*nm)

particle\_3\_rotation=Euler(30\*deg, 60\*deg, 0\*deg), Coordination- x,y,z-(85\*nm, -20\*nm, 30\*nm)

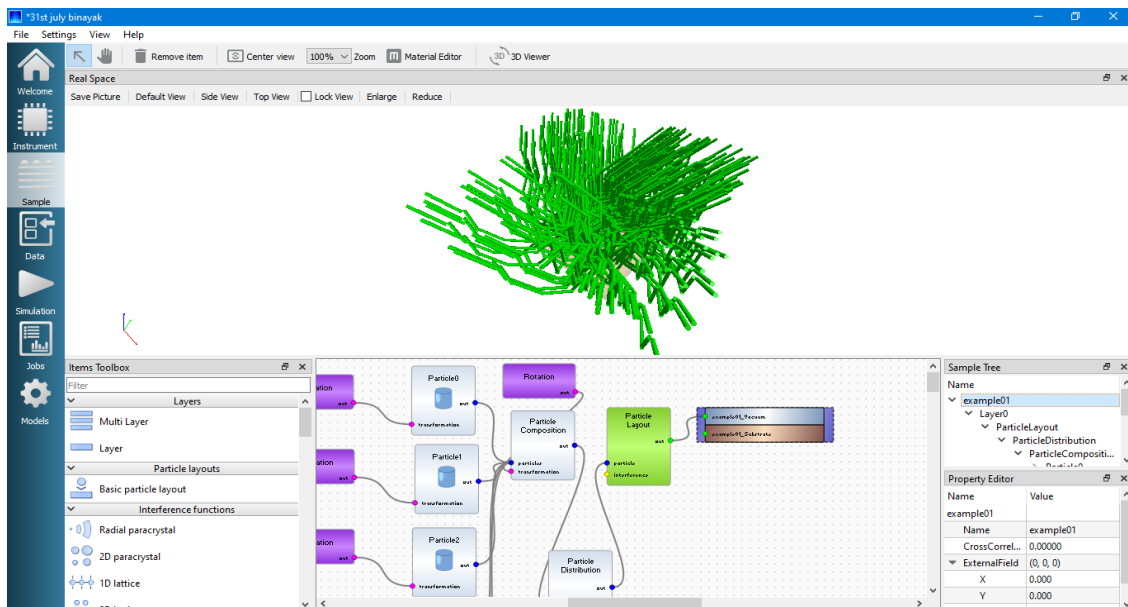
particle\_4=X (0\*deg), Coordination- x,y,z-(106\*nm, -55\*nm, 50\*nm)

particle\_5\_rotation = Euler(35\*deg, 45\*deg, 0\*deg), Coordination- x,y,z- (110\*nm, -55\*nm, 100\*nm)

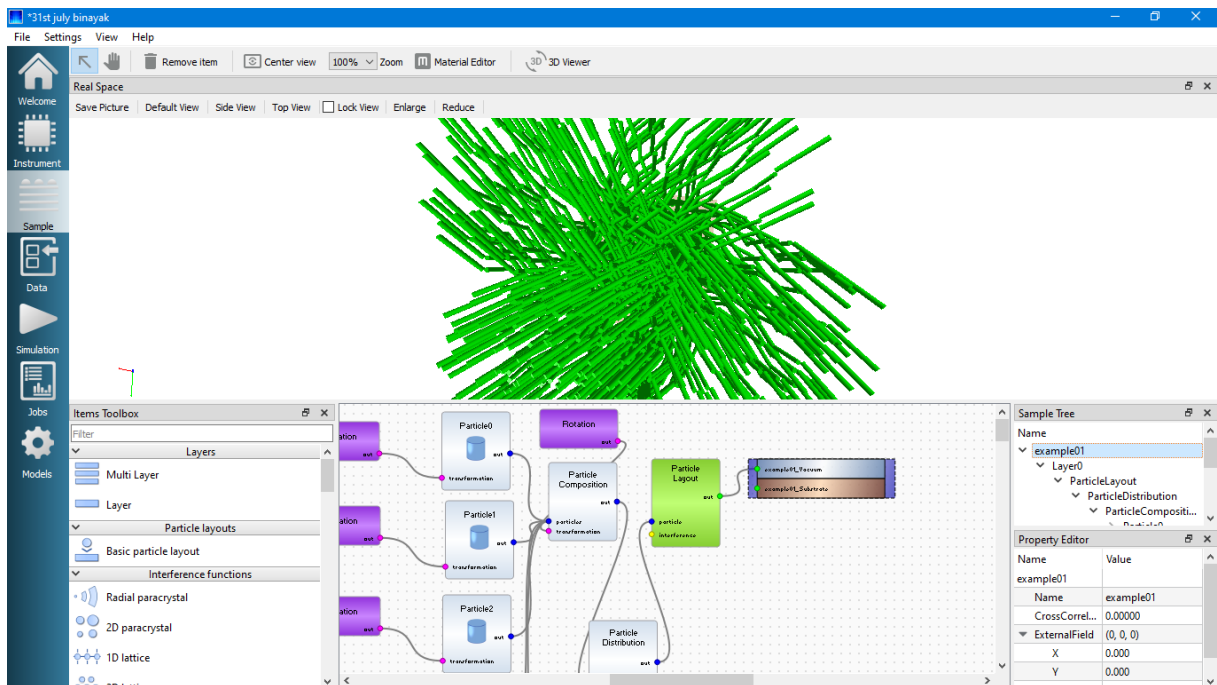


(fig.1- Single spaghetti made up of randomly lying CNF cylinders)

After that, I used the distribution option available in this software to get multiple distributions of the CNFs cylinder structure.

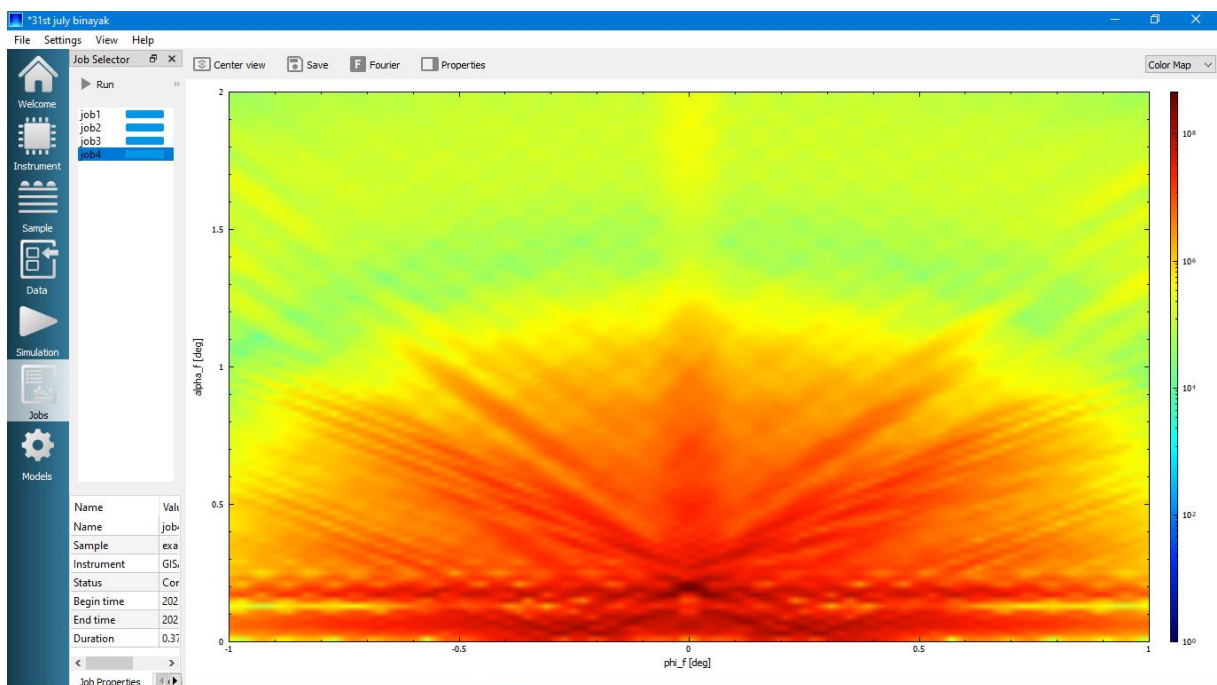


(fig.2- Multiple spaghetti made up of randomly lying CNF cylinders(top view))



(fig.3- Single spaghetti made up of randomly lying CNF cylinders(top view))

After getting a distribution of CNFs over the substrate, I started simulation of scattering patterns.



(fig.4 Scattering Pattern)

### 3. Acknowledgement

I thank DESY for spending two months in their facility between lectures and laboratory experiences virtually. My supervisor gave me this exciting project. And of course, I need to thank all for supporting me during this internship.

## References

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