NOBUGS 2024
23 - 27 September 2024
ILL & ESRF, Grenoble

“Intelligence Terminal” Multimodal Data Analysis System for Synchrotron Radiation Experiments

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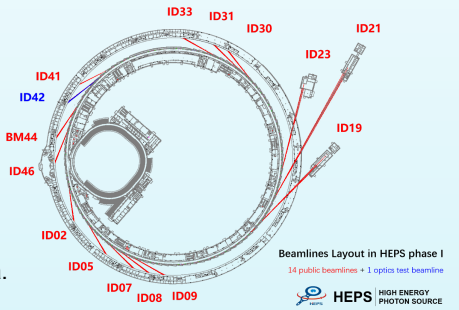

Introduction

Advanced synchrotron radiation (SR) light sources drive cutting-edge scientific research across various fields. The High Energy Photon Source (HEPS) as shown in Figure.1, a fourth-generation SR light source in China, will offer high energy and ultra-low emittance, facilitating sensitive and fast experimental observations at molecular, atomic, electronic, and spin levels. Facing to SR scientific big data challenge, it is urgent to develop artificial intelligence (AI) analysis methods to enhance research efficiency including novel material discovery[1].

To address this challenge, this research focuses on developing “Intelligence Terminal” multimodal data analysis system for SR image and diffraction data. A website of a data processing platform is deployed for SR diffraction, spectroscopy, and imaging based on the Python programming language. Overall, this work aims to analyze advanced SR data quickly and accurately in real-time through advanced AI algorithms, enhancing scientific research.

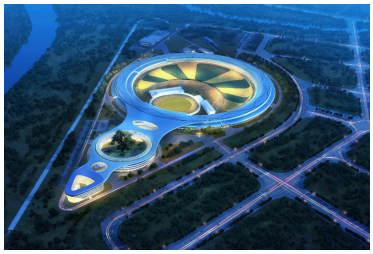

Figure.1 HEPS effect panoramic view.

1. Deep learning analysis of quantitative 3D imaging of single-cell HfO_2 nanoparticles by Nano-CT

Objective: Analyze X-ray nano-computed tomography (Nano-CT).
Method: Implement a novel localization quantitative analysis method based on DL[2].

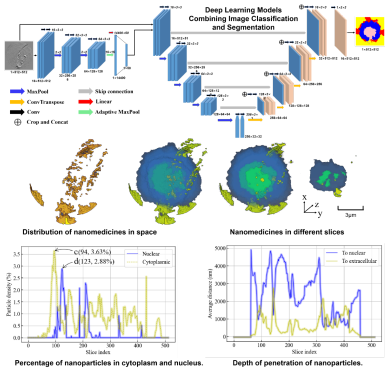

Figure.2 DL combined with Nano-CT imaging aids nanomedicine evaluation and design.

Results:
(1) Achieve localization quantitative 3D imaging analysis.

(2) Demonstrate the notable effect of the nanoparticles in tumor treatment.

(3) Show the potential to explore the localization quantitative 3D distribution information of specific molecules at the nanoscale level.

2. Data-driven machine learning methods for diffraction data

Objective: Extract 3D orientation parameters of nanofibers from the wide angle X-ray diffraction data.
Methods: Develop data-driven ML methods[3].

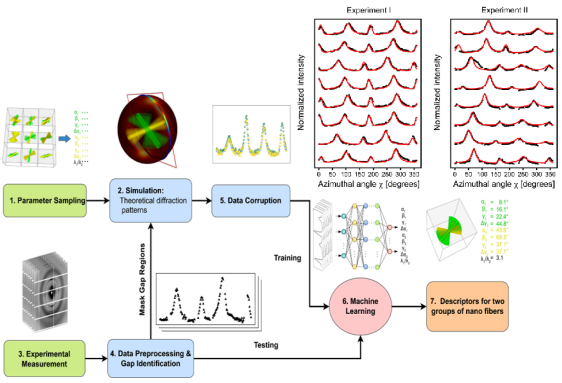

Figure.3 Data-driven ML training methods and results.

Results:
(1) Achieve high accuracy as R^2>0.91.

(2) Fast analysis of experimental data as 10^4 times faster than existing fitting methods.

(3) Be available to be applied in multi light sources and beamlines.

3. Intelligence Photon Source Brain (IPSBrain)

Objective: Build user-friendly interfaces for model functionality.
Method: Embed pre-trained ML models.

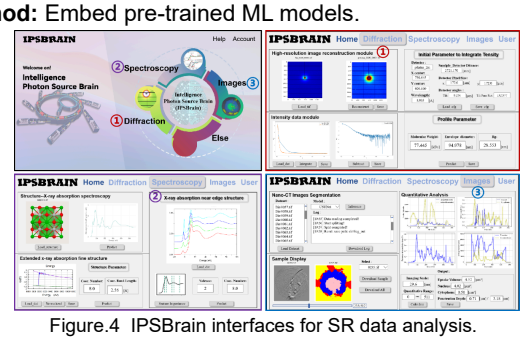

Figure.4 IPSBrain interfaces for SR data analysis.

Advantages:
(1) The convenience and applicability of using trained ML models.
(2) The efficiency of handling big data and further driving real-time online analysis of high-throughput data.

Conclusions

This work focuses on efficient and accurate analysis of SR big data through AI methods.

(1) For image data, we employ DL for localization quantitative analysis in X-ray Nano-CT, achieving 3D imaging of single-cell HfO_2 nanoparticles.

(2) For diffraction data, we develop data-driven ML methods to analyze wide angle X-ray diffraction, enabling accurate and fast analysis.

(3) We build IPSBrain platform to make it convinient for users to deal with SR high-throughput data.

Recruitment:
Title: Overseas Young Talents
Compensation: competitive compensation, benefits and settling-in expenses.
Support: 3~11 million RMB research start-up funds;
Career registration, Beijing household registration;
Provide a uniformly decorated swing space;
Assist in solving children's enrollment and school enrollment.
Subjects: Synchrotron Radiation, Artificial Intelligence, Computer Science, etc.
For more information: https://mp.weixin.qq.com/s/O_RzPP9FdRcdAWFiQqlJIw
For more recultments: https://muchong.com/t-15937556-1
Contact:Mr. Liang (Human Resources Office), E-mail: lianggj@ihep.ac.cn
Prof. Zhao lina (Research Group), Email:linazhao@ihep.ac.cn

Related publications:
[1] Qingmeng Li, Rongchang Xing, Linshan Li, Haodong Yao, Liyuan Wu, **Lina Zhao***. Synchrotron radiation data-driven artificial intelligence approaches in materials discovery. *Artificial Intelligence Chemistry*, 2(1): 2949-7477, (2024).
[2]Zuoxin Xi, Haodong Yao, Tingfeng Zhang, Zongyi Su, Bing Wang, Weiyue Feng, Qiumei Pu, **Lina Zhao***. Quantitative Three-Dimensional Imaging Analysis of HfO2 Nanoparticles in Single Cells via Deep Learning Aided X-ray Nano-Computed Tomography[J]. ACS Nano 18(33): 22378-22389 (2024).
[3] Minghui Sun, Zheng Dong, Liyuan Wu, Haodong Yao, Wenchao Niu, Deting Xu, Ping Chen, Himadri S Gupta, Yi Zhang*, Yuhui Dong, Chunying Chen, **Lina Zhao***. Fast extraction of three-dimensional nanofiber orientation from WAXD patterns using machine learning, IUCrJ, 10(3), 297-308, (2023).

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