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A Data-Driven Approach for Modelling the Relationship between Fabrication Parameters and Critical Currents of REBCO Coated Conductors in a Real-Scale Pulsed Laser Deposition System

Takanobu Kiss

*Director,
Research Institute of Superconductor Science and Systems,
Kyushu University, Fukuoka 819-0395, JAPAN
kiss@sc.kyushu-u.ac.jp*

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KYUSHU UNIVERSITY



Coauthors

Kyushu University

M. Yang, Z. Wu, S. Sera, Y. Tanaka, K. Higashikawa

Faraday Factory Japan

R. Valikov, M. Nakamura, V. Petrykin, S. Lee

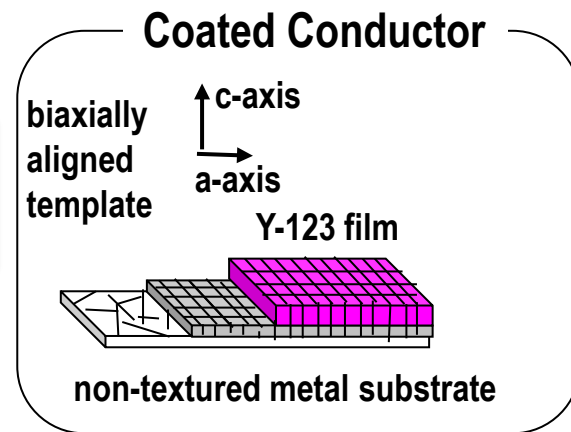
CC manufacturing is now in the transition to meet mass production



Opening new factory on April 19, 2023

Requirements for stable and reproducible operation of multiple production lines.

Quality Assurance (QA) and Quality Control (QC) in mass-production become urgent issues.

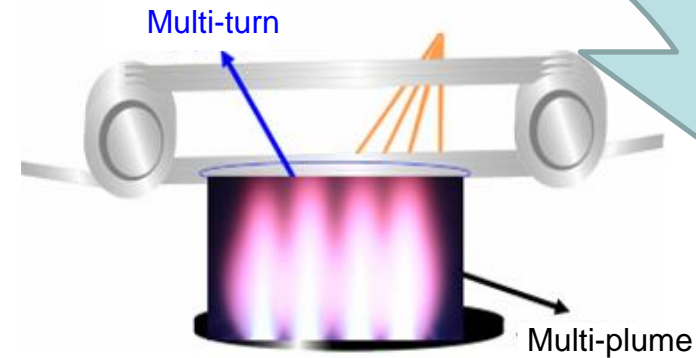
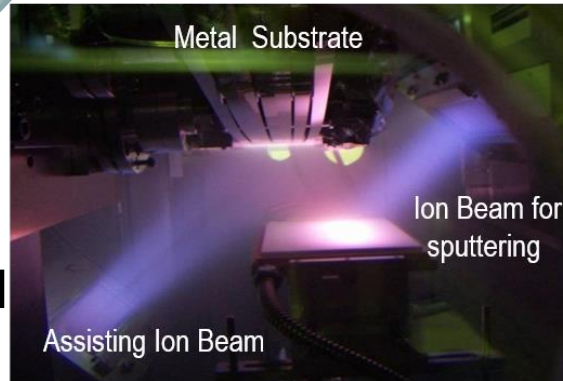


Issues of wire production process (ex: IBAD-PLD)

Input

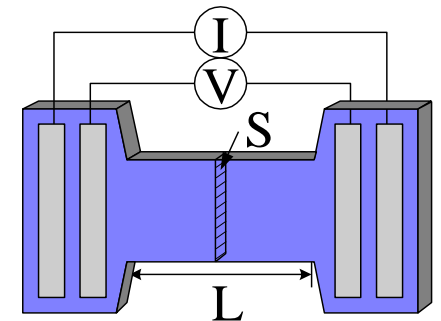
Control Parameters

- Subst. Temp.
- Laser Power
- Pressure
- Wire Traveling Speed
- And more ...



Output

Critical Current
(Practical Performance)



Unknown governing equations due to non-equilibrium and complex processes

Issue of I_c characterization:

Time consuming **slow measurement**.

Some time difficult at low T due to very large I_c

Our method in this study: A new methodology to realize digital model for CC production process by data driven approach coupling high throughput measurement and ML

Combinatorial sample

Condition 4 Condition 3 Condition 2 Condition 1
Param 1, 2 Param 1, 2 Param 1, 2 Param 1, 2
..

Long REBCO CC

$I_{c4}(B, T)$

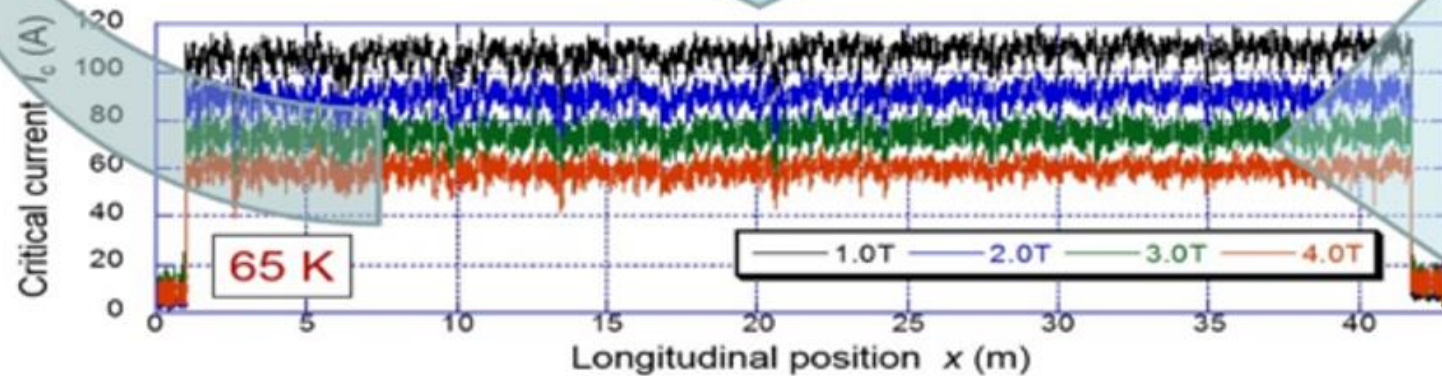
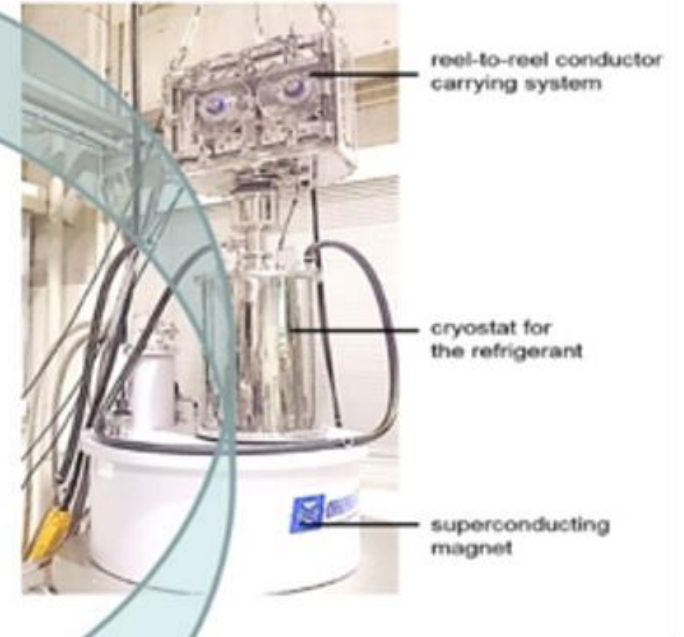
$I_{c3}(B, T)$

$I_{c2}(B, T)$

$I_{c1}(B, T)$

Faster material development

Process Informatics



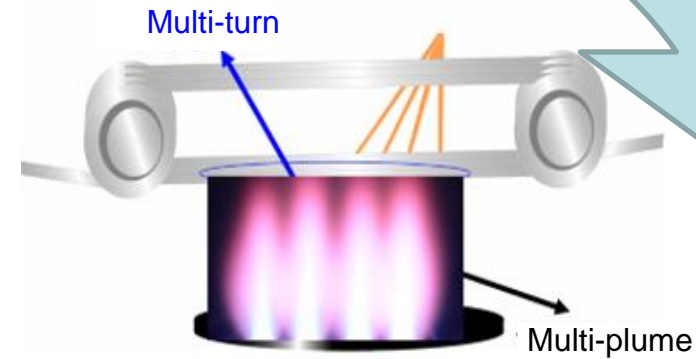
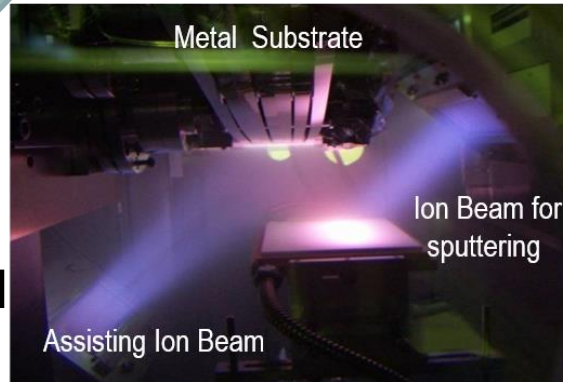
High throughput measurement of I_c (10-20 data/sec) at *operando* condition.

Our method in this study: A new methodology to realize digital model for CC production process by data driven approach coupling high throughput measurement and ML(cont'd)

Input

Control Parameters

- Subst. Temp.
- Laser Power
- Pressure
- Wire Traveling Speed
- And more ...



Output

Critical Current
(Practical Performance)

Unknown governing equations due to non-equilibrium and complex processes

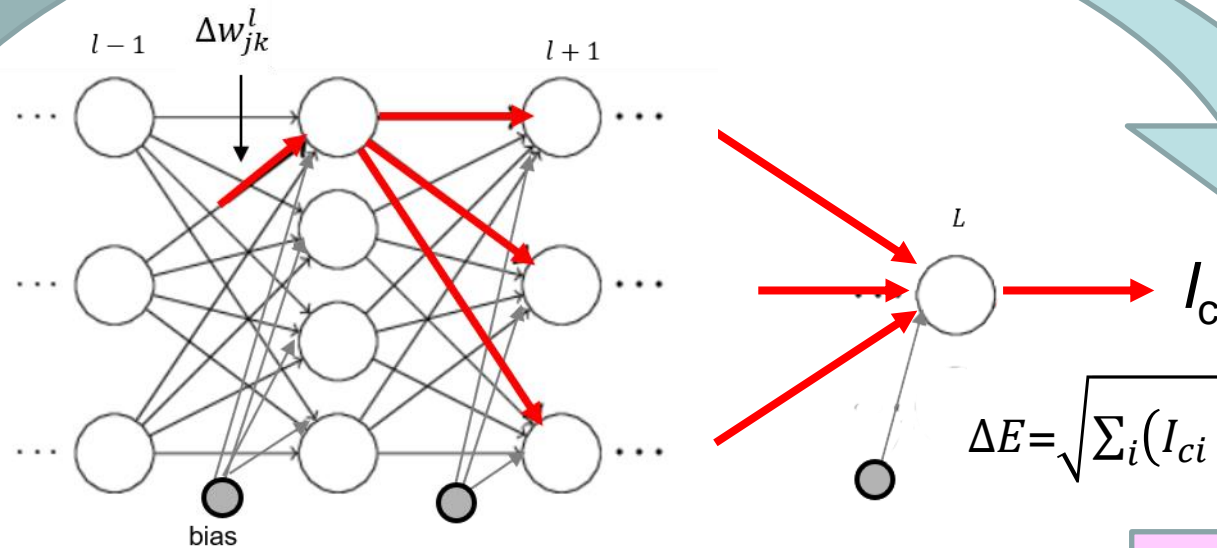
Our method in this study: A new methodology to model CC production process by data driven approach coupling high throughput measurement and ML (cont'd)

Input

Control Parameters

- Subst. Temp.
- Laser Power
- Pressure
- Wire Traveling Speed
- And more ...

$x_{1,i}, x_{2,i}, x_{3,i}, \dots$



Deep Neural Network Model

Output

Critical Current
(Practical Performance)

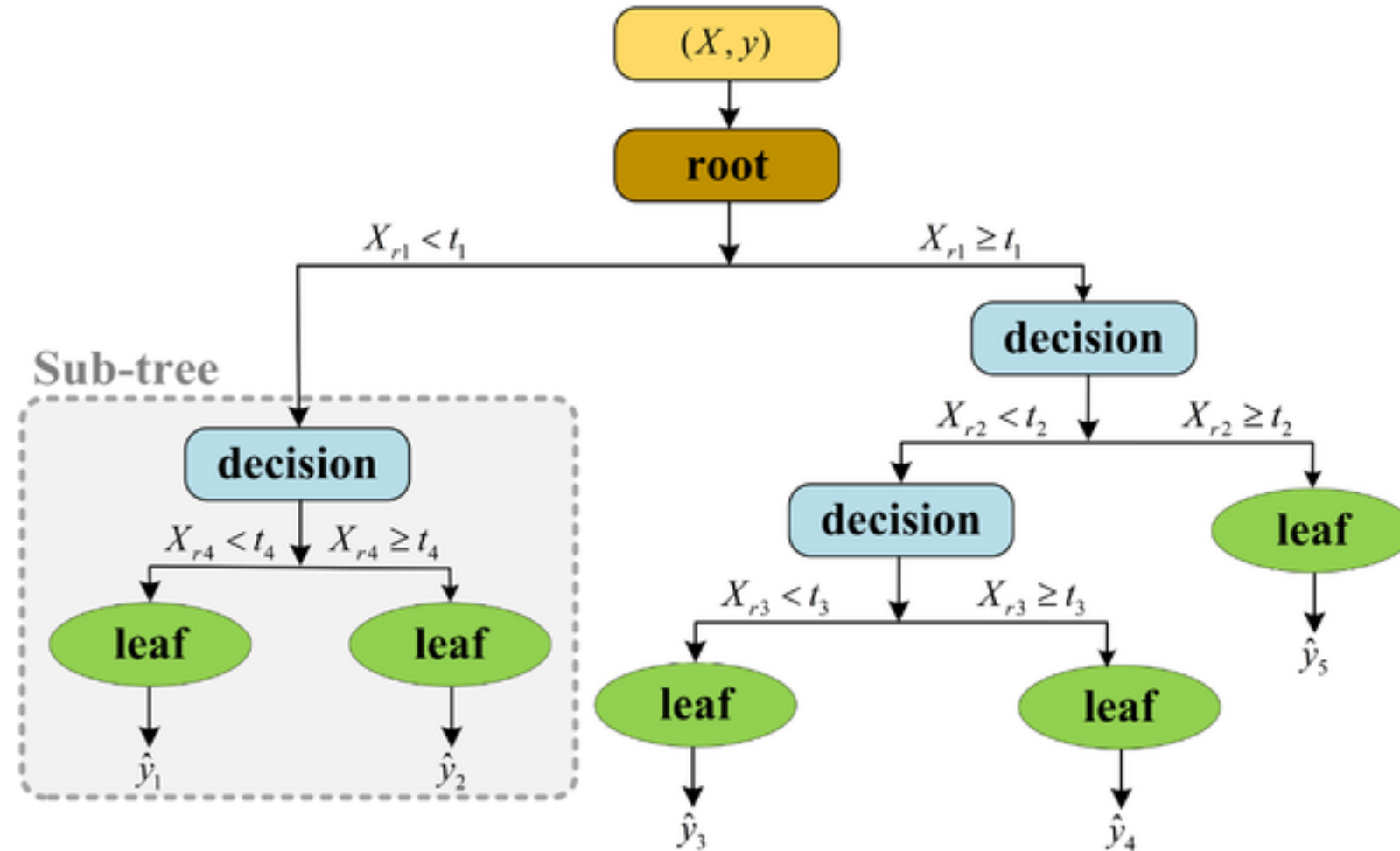
$$\Delta E = \sqrt{\sum_i (I_{ci} - \widetilde{I}_{ci})^2}$$

\widetilde{I}_{ci}

$$I_c = f(x_{1,i}, x_{2,i}, x_{3,i}, \dots)$$

The model is trained, i.e., the weight and bias in each neuron are determined to minimize the error, ΔE (=rms), between model output and training data.

Other model we adopted: Decision tree model

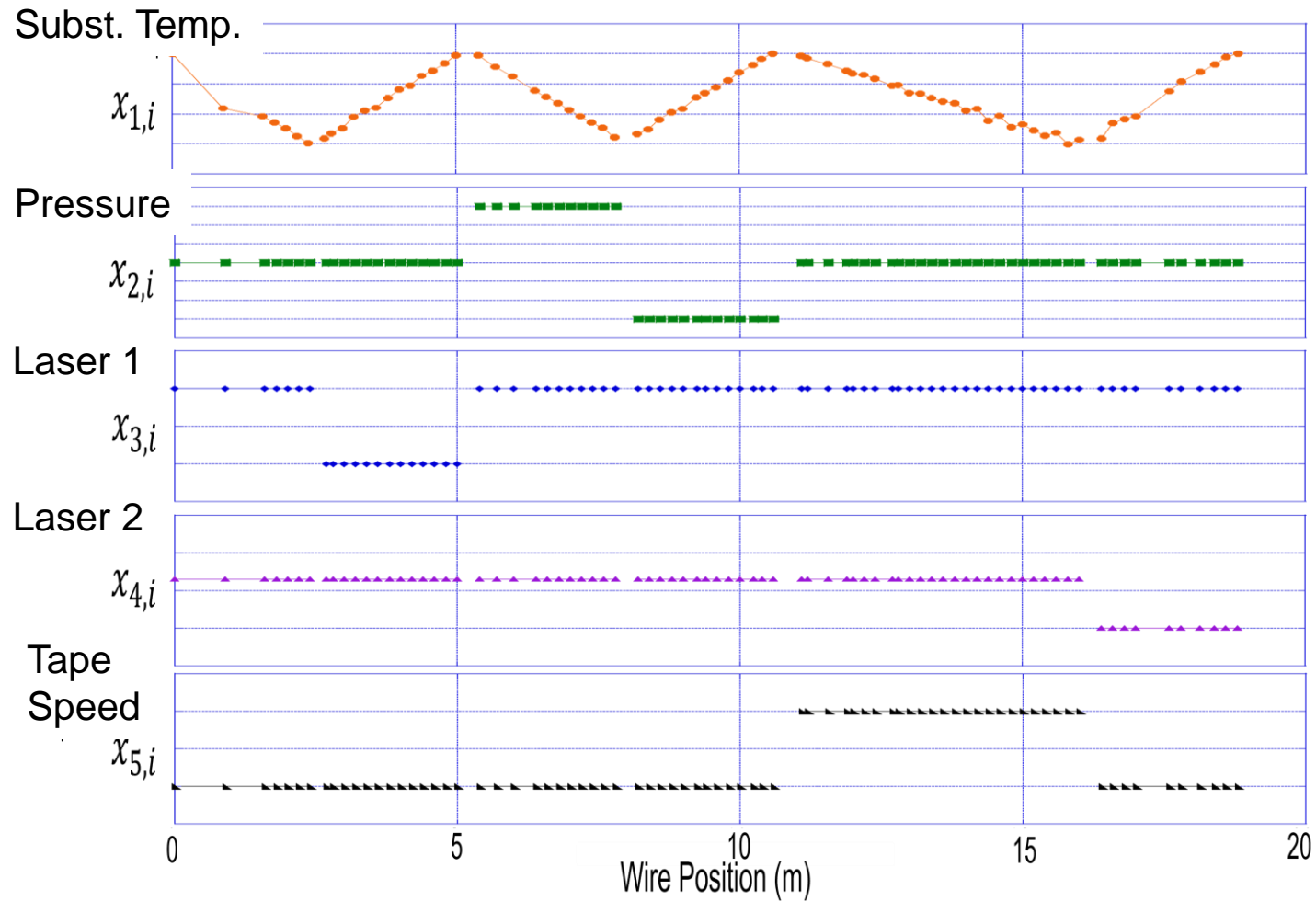


1. Choose a **feature** which **minimize RMSE**
2. Define **split points** to minimize separates **RMSE**
3. Split node
4. The **average value** of all instances in the leaf will be the **prediction**

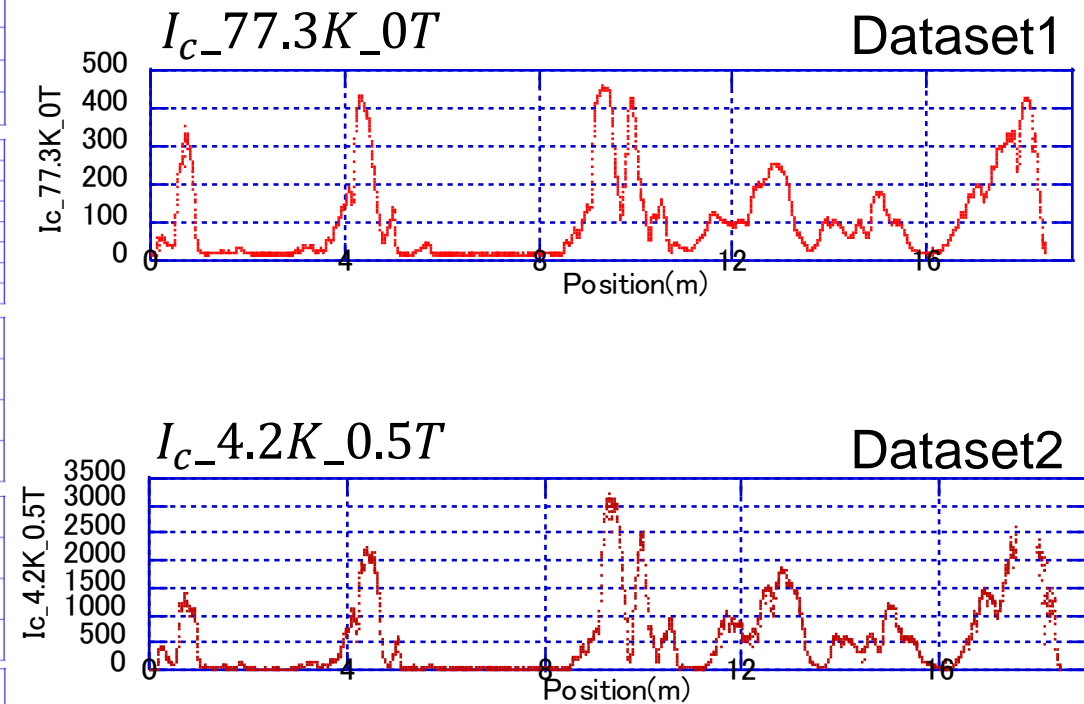
- **Low accuracy, sensitive to outliers**
- **Could be overfitting**

Training data overview

Parameters



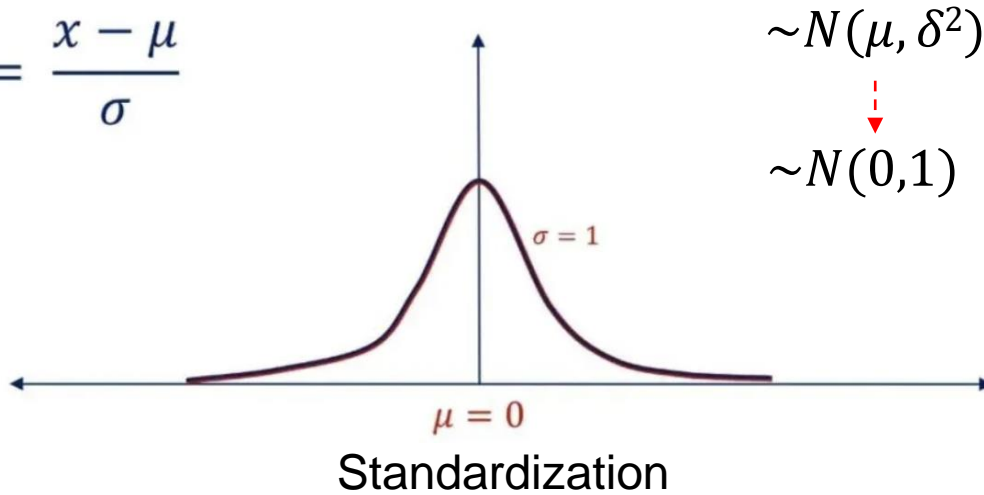
Output



Data preparation

Feature Scaling

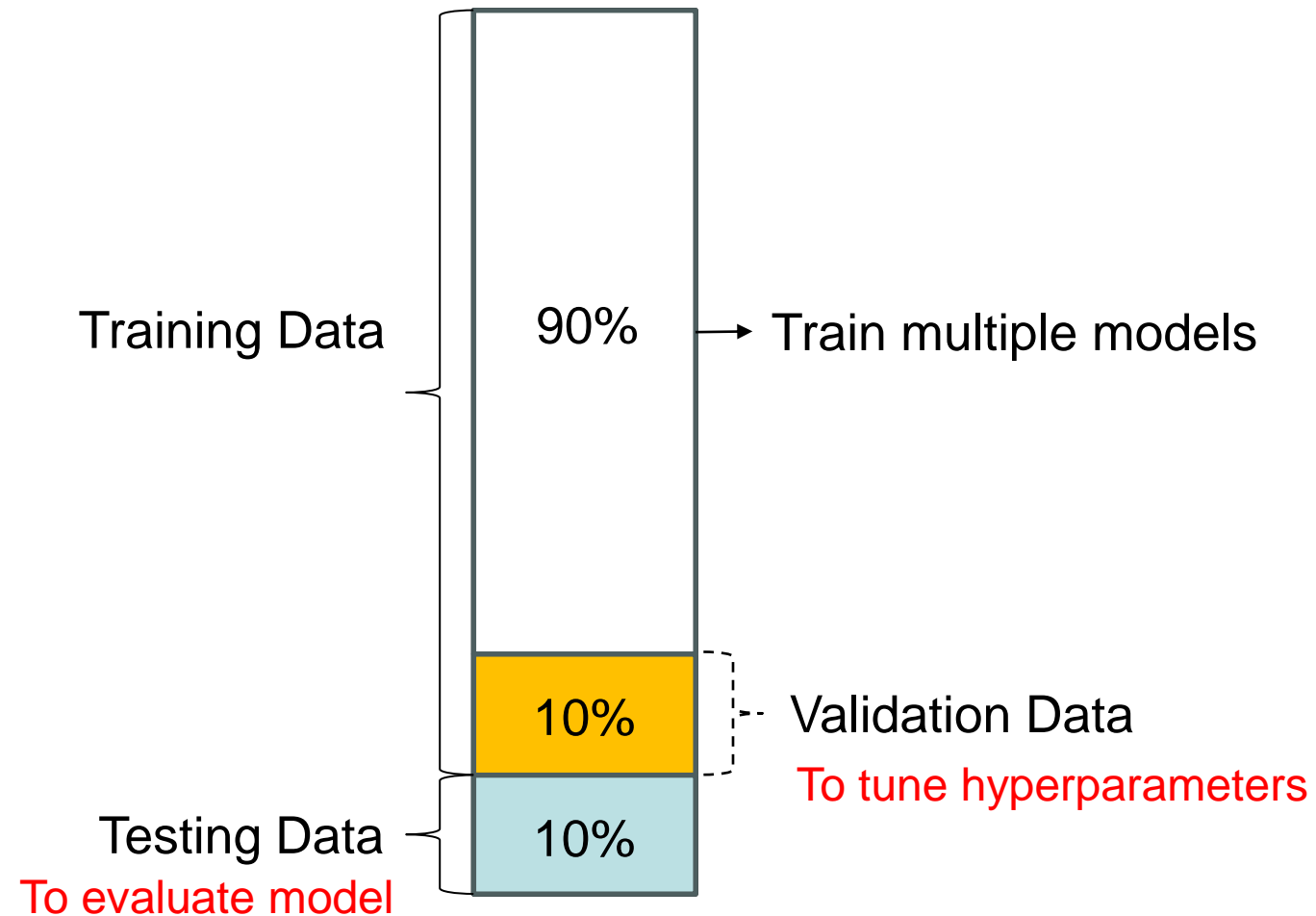
$$z = \frac{x - \mu}{\sigma}$$



$$z = (x - u) / s$$

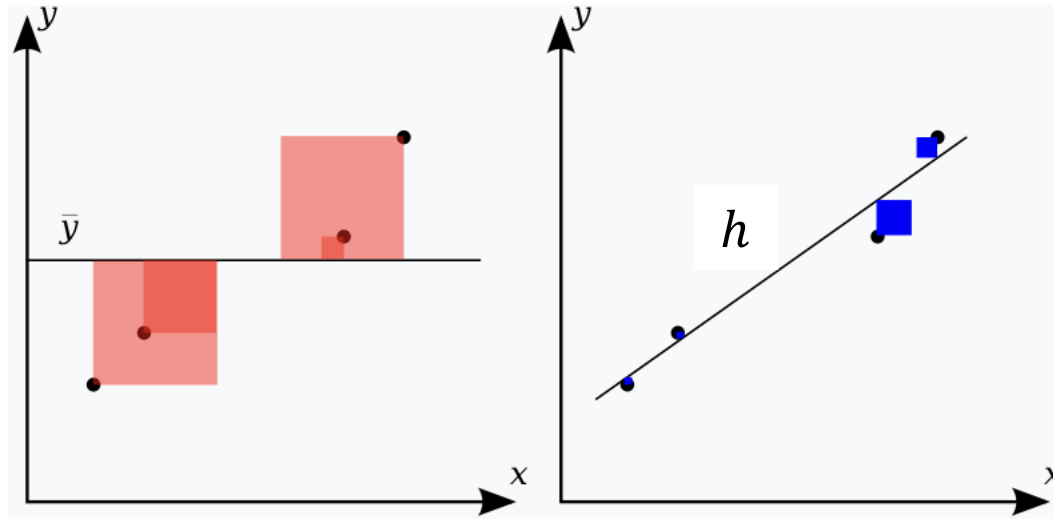
z: standard normal values of x
x: training samples
u: mean
s: standard deviation

Data training needs



Evaluation metrics of regression models

Coefficient of Determination (R^2)



A better model: R^2 that is closer to 1

residual sum of squares:

$$SS_{\text{res}} = \sum_i (y_i - h_i)^2 = \sum_i e_i^2$$

total sum of squares:

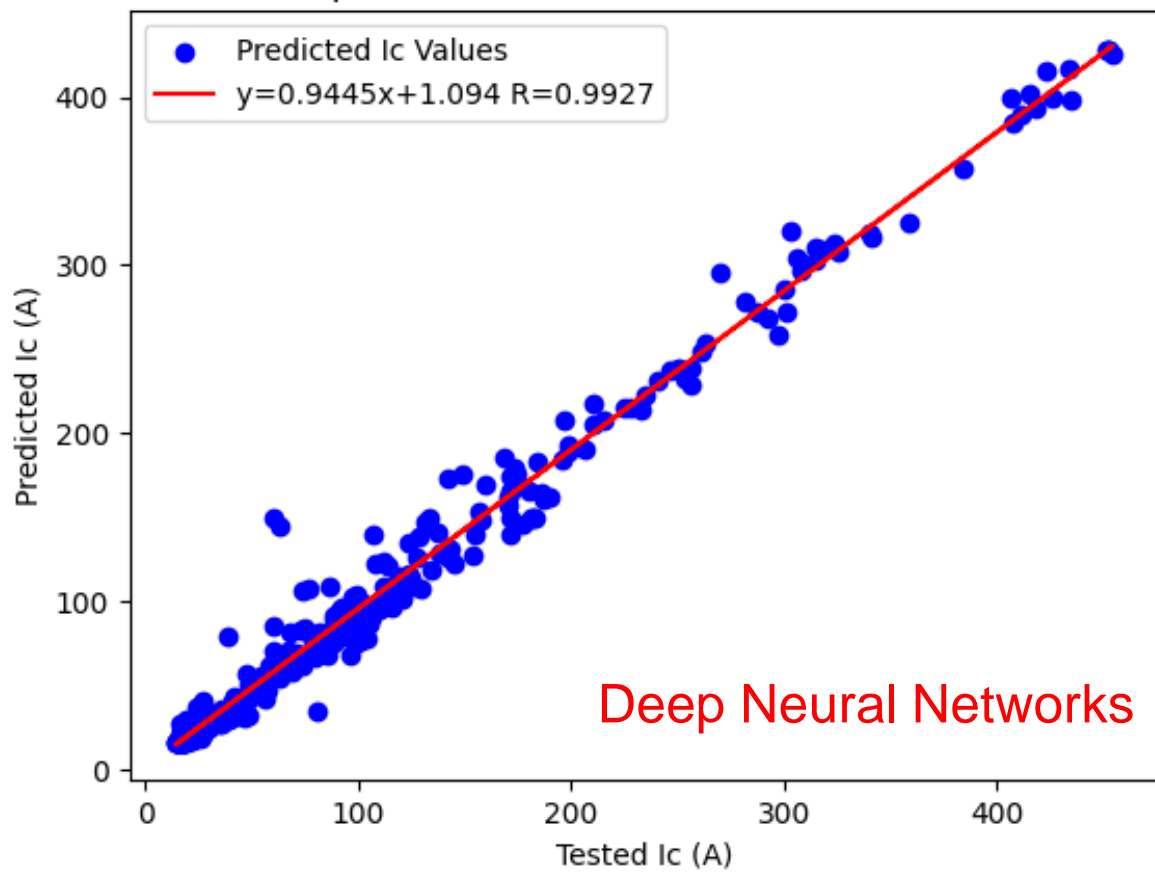
$$SS_{\text{tot}} = \sum_i (y_i - \bar{y})^2$$

$$R^2 = 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}}$$

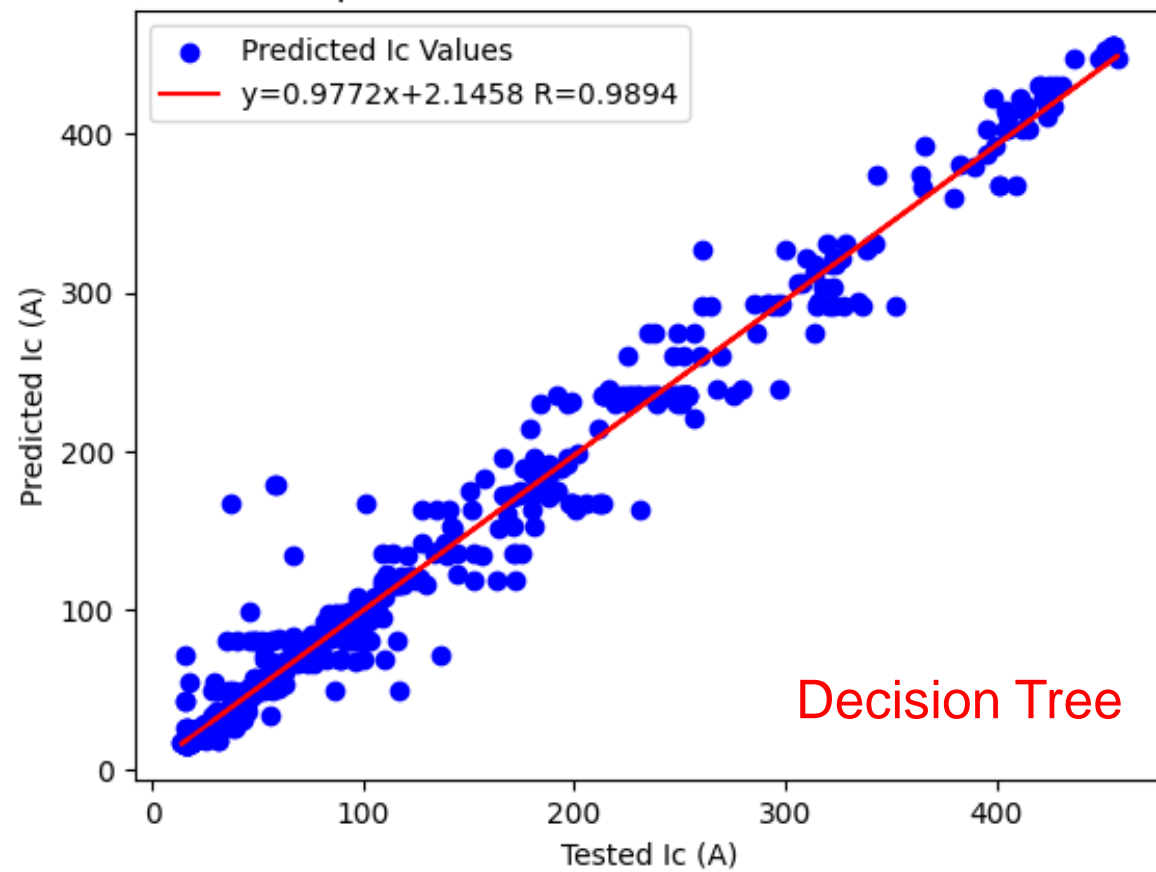
Evaluating predictive performance (I_c at 77.3 K, s.f.)

- ① Linear regression fit of actual I_c and pred I_c
- ② R (Correlation coefficient of actual I_c and pred I_c)

Comparison of Predicted and Tested I_c values



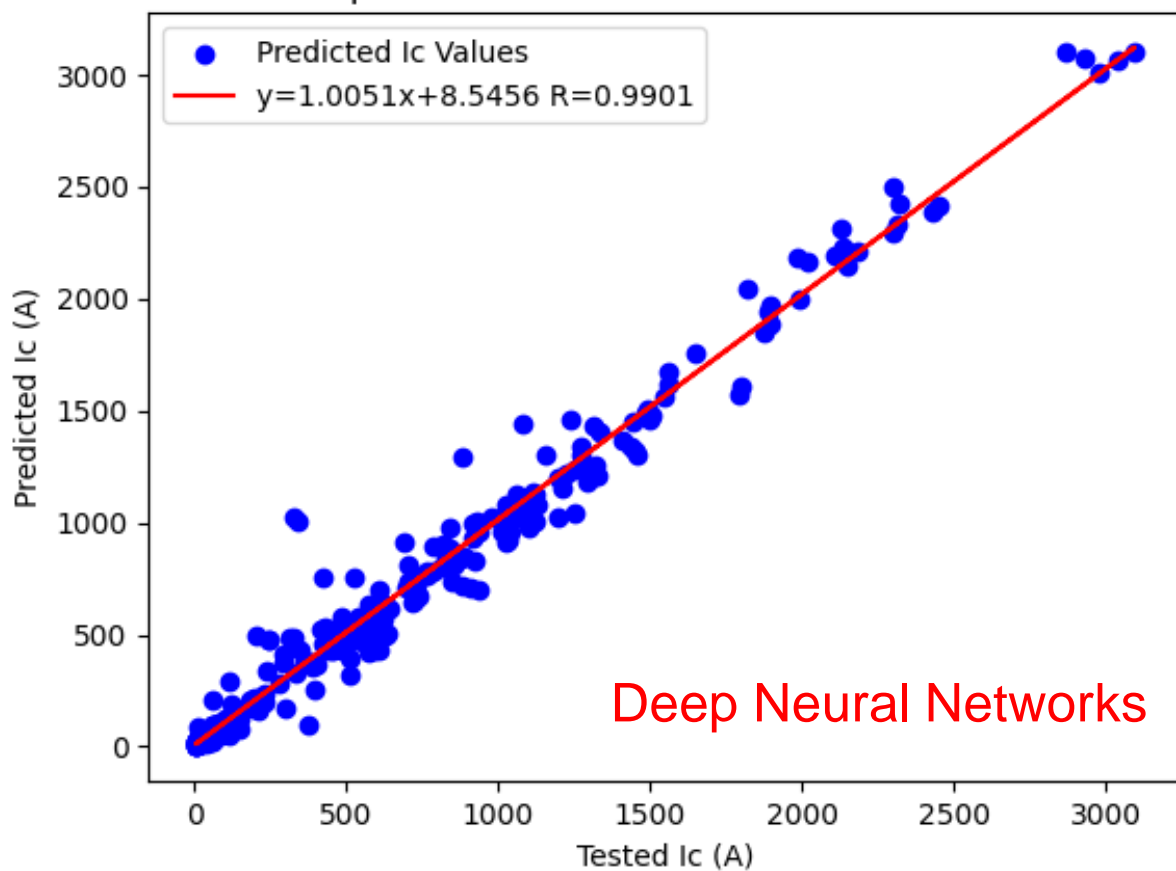
Comparison of Predicted and Tested I_c values



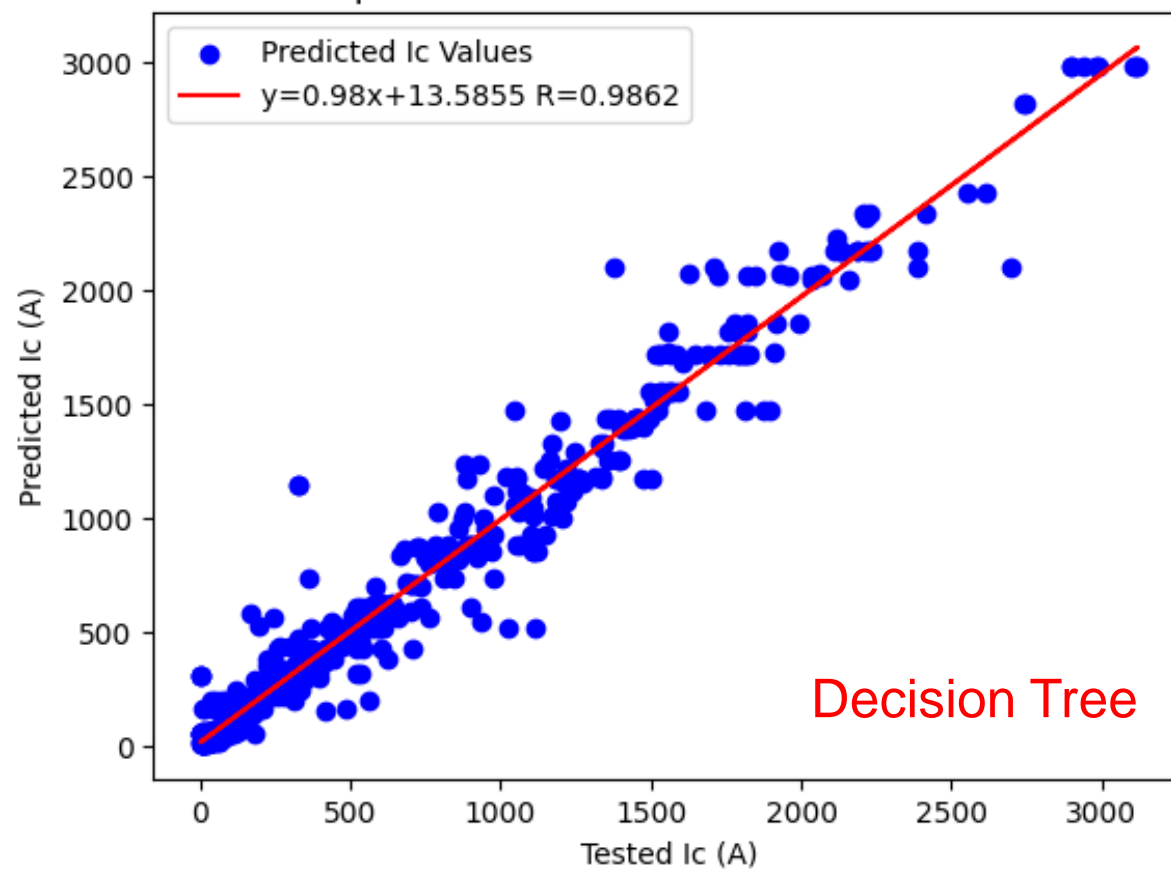
Evaluating predictive performance (I_c at 4.2 K, 0.5 T)

- ① Linear regression fit of actual I_c and pred I_c
- ② R (Correlation coefficient of actual I_c and pred I_c)

Comparison of Predicted and Tested I_c values



Comparison of Predicted and Tested I_c values

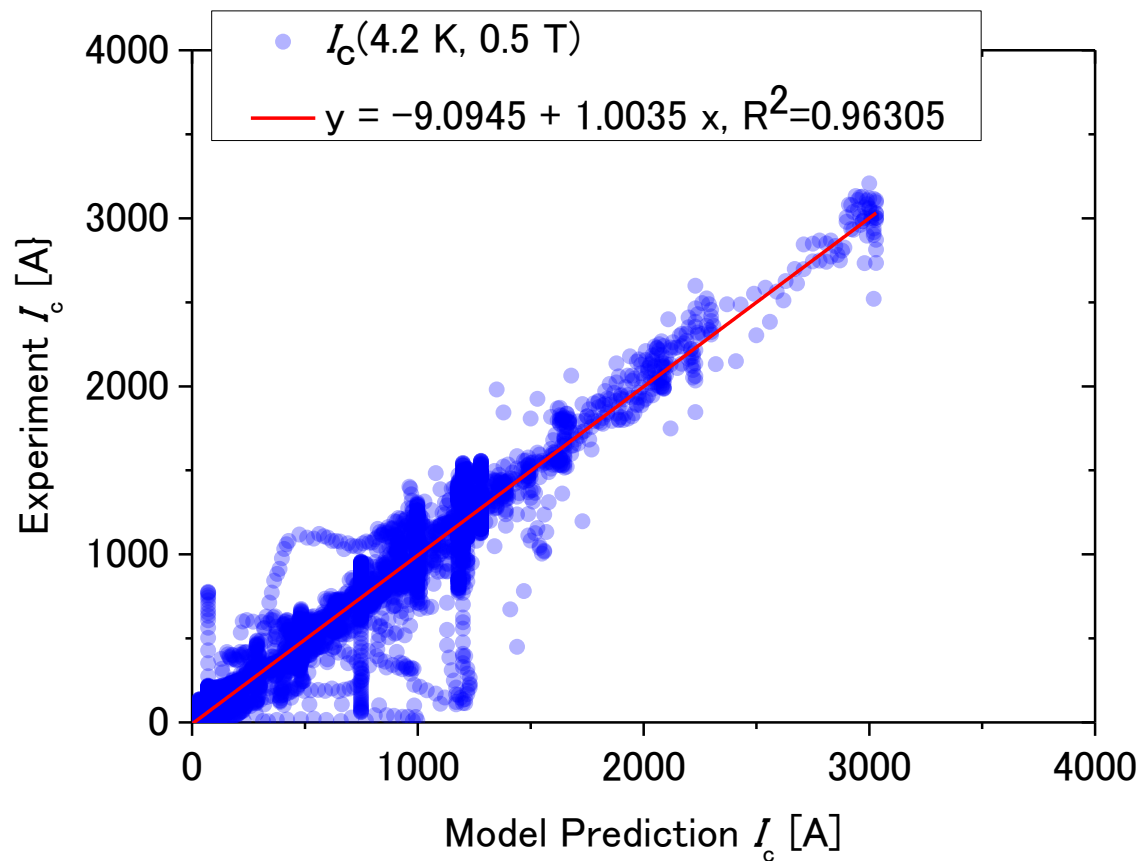


DNN shows better performance

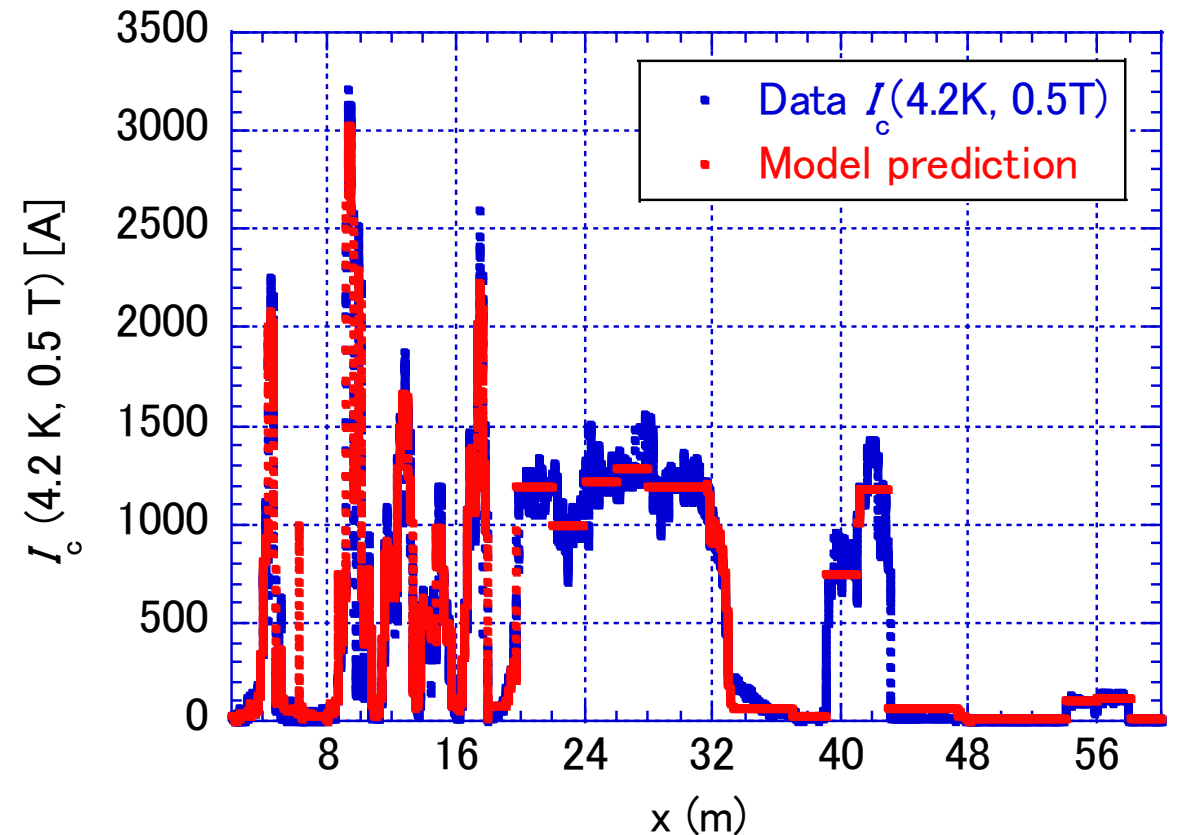
Increase the number of training data for DNN model

24,807 data sets for training
(20 % was used for evaluation.)

High throughput measurement allows us to collect a large number of data for training!

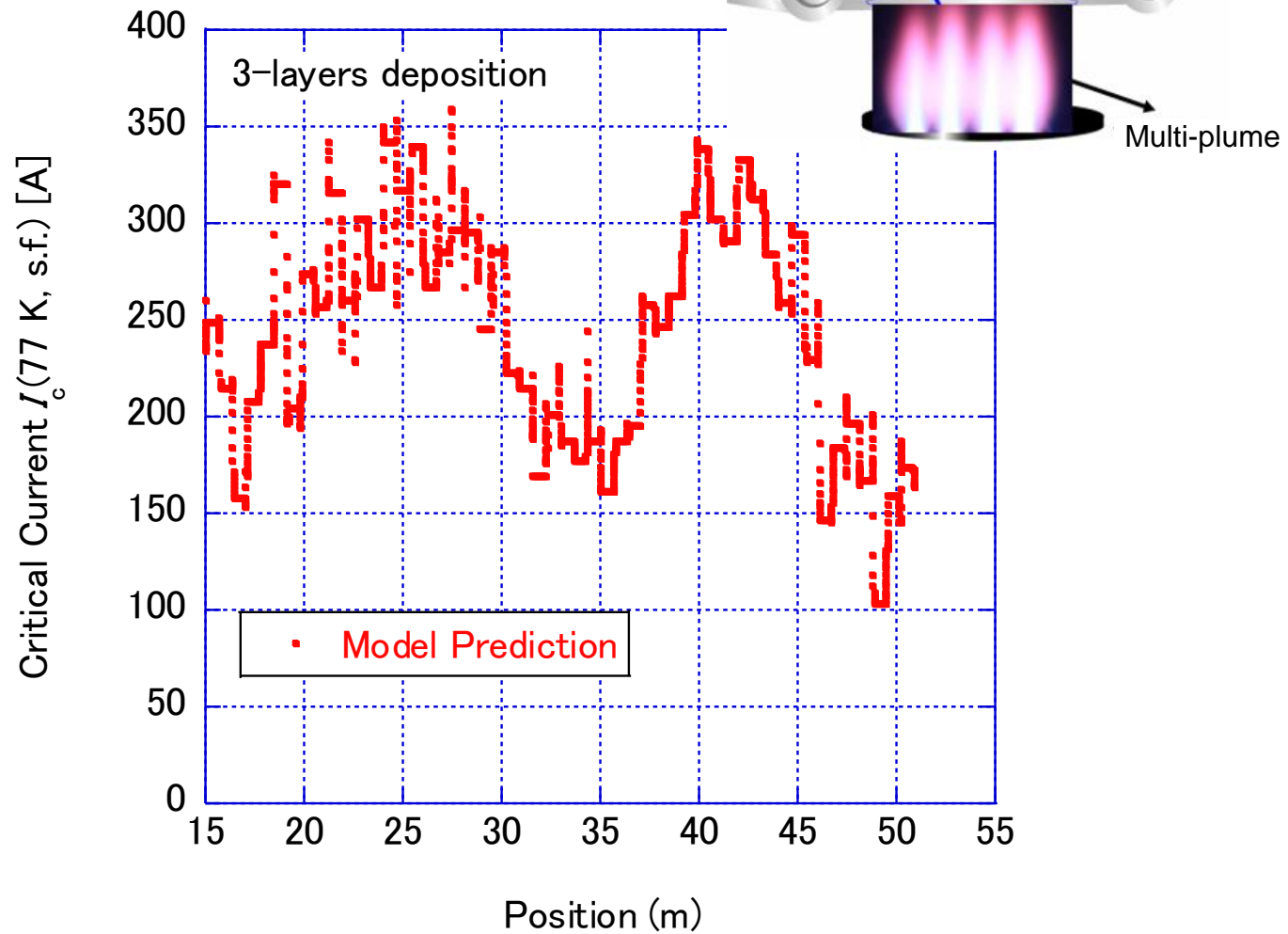


I_c measured continuously at 4.2 K and 0.5 T

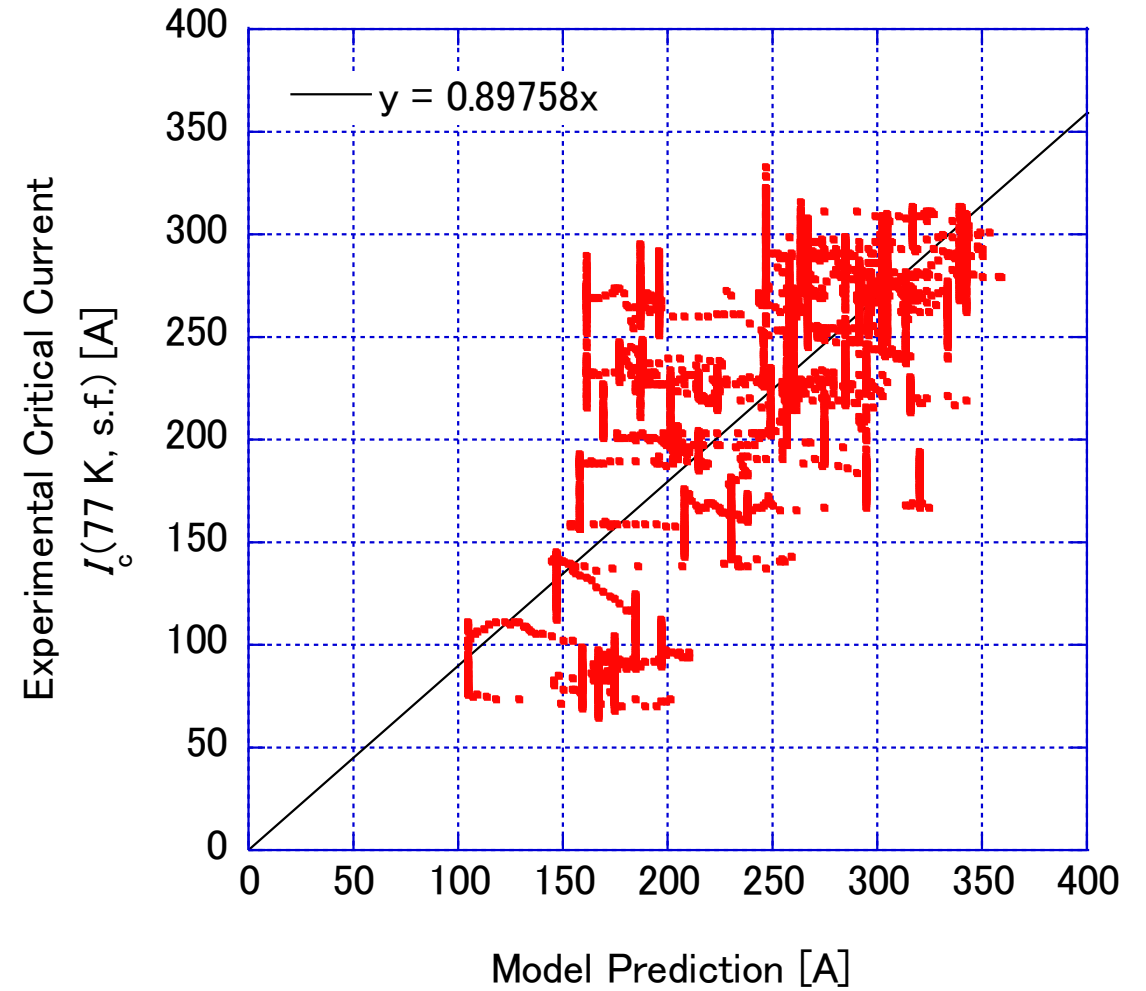
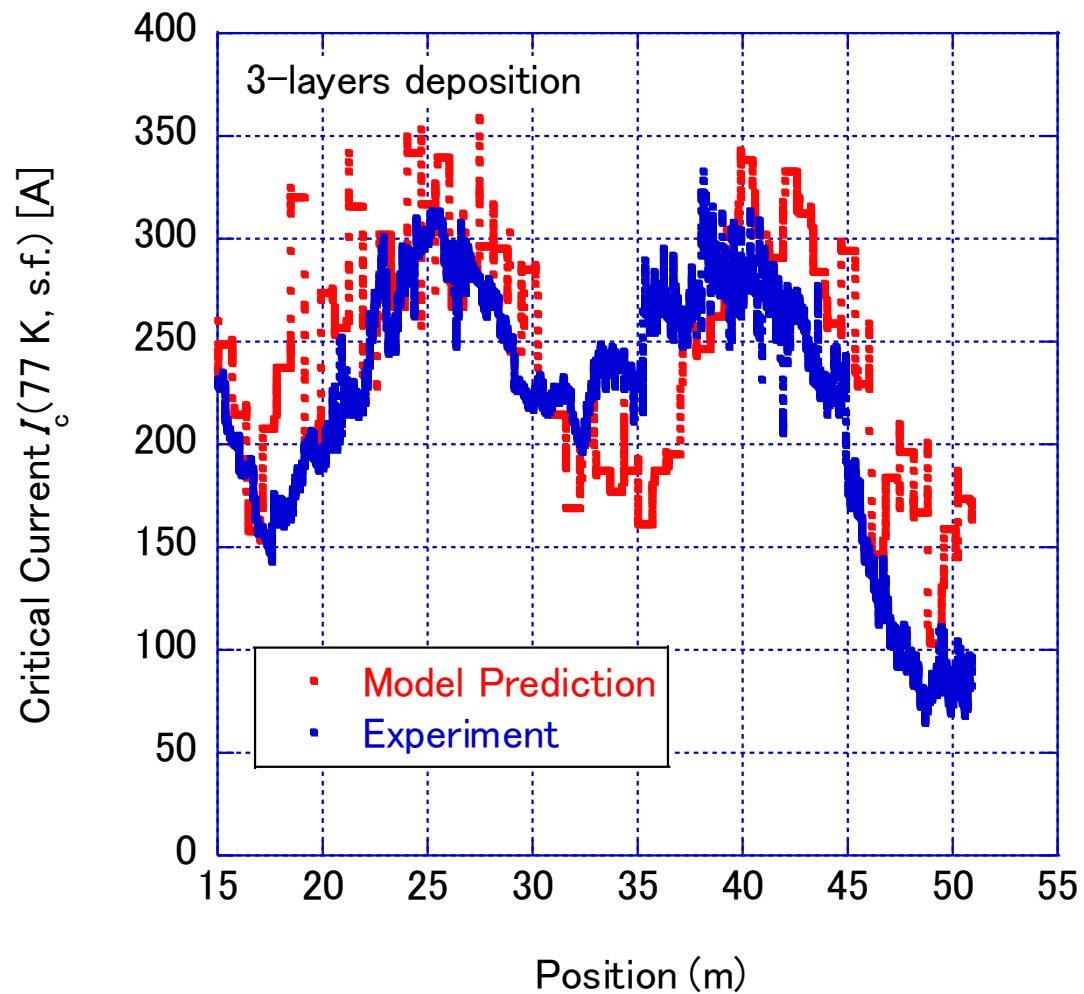


Prediction of multilayer deposition in multi-turn system (separate experiment) by the trained model

3-turn experiment



Prediction of separate multilayer deposition in multi-turn system by the trained model



Summary

1. A novel approach to develop ML models of IBAD-PLD CC production process, which can predict wire performance from input control parameters for deposition, has been demonstrated by data driven approach adopting **combinatorial long samples** and **high throughput continuous measurements of I_c** .
2. Optimum process condition can now be explored *in silico* by using the digital model.
3. This could be a **breakthrough for technological development of mass production of CCs** to cope with such requirements as stable and high speed manufacturing of high performance CCs as well as cost reduction.