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Dynamic Uniformity Modeling in Superconductor Manufacturing via Vector Autoregression Analysis

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Abstract

With high efficiency and low energy loss, high-temperature superconductors (HTS) have demonstrated their profound applications in various fields, such as medical imaging, transportation, accelerators, microwave devices, and power systems. The high-field applications of HTS tapes have raised the demand of producing cost-effective tapes with long lengths in superconductor manufacturing. However, achieving the uniform performance of a long HTS tape is challenging due to the unstable growth conditions in the manufacturing process. In addition, the identification of parameters in the growth conditions that affect the uniformity of HTS tapes remains an unexplored question. To model and analyze the uniformity of HTS tapes, we develop a dynamic uniformity modeling framework that integrates the dynamic statistical uniformity measures and the vector autoregression analysis for identifying important process parameters associated with the tape uniformity. The proposed method is applied to real data from HTS tapes and the key process parameters, such as the tension and substrate temperature, are identified.

Keywords

Critical current, superconductor manufacturing, dynamic uniformity modeling, vector autoregression analysis.

1. Introduction

With high efficiency and low energy loss, high-temperature superconductors (HTS) have demonstrated their profound applications in various fields, such as medical imaging, transportation, accelerators, microwave devices, and power systems [1]-[5]. However, the wide commercialization of these applications has not been achieved yet. For these HTS tapes to be scaled up with high yield and enhanced performance, there must be new and innovative research focusing on quality and process control using data analytics. The high-field applications of superconductor tapes have raised the demand of producing cost-effective tapes with long lengths in superconductor manufacturing. One of the most critical characteristics for such long-length superconductor tapes is the uniformity, which is usually spatial-heterogeneously affected by various process parameters or growth conditions. How to optimally control the growth conditions for producing high-quality and uniform superconductor tapes remains a concern for researchers in superconductor manufacturing.

To produce the HTS tapes with enhanced performance, the metal organic chemical vapor deposition (MOCVD) process has been developed and used as an important approach to manufacturing superconductor tapes [6]-[9]. During the MOCVD process, the substrate tape goes through the chemical vapor deposition in a reaction zone until a layer of superconductor film grows on its surface [1]. In-line quality control tools and multimodal sensors have been set up for real-time monitoring of superconductor tape quality and process parameters in the pilot-scale manufacturing tools [2]. Among different tape quality characteristics such as thickness, width and smoothness, researchers identified one of the most important metrics to evaluate the performance of HTS tapes, the critical current (denoted by I_c), which characterizes the largest electrical current a tape is able to carry [1, 3, 4]. One of the major obstacles in the application of long HTS tapes is to achieve the uniform performance of critical current [3]-[5]. Therefore, for HTS tapes to be produced with large scale, high yield and enhanced performance, it is crucial to develop innovative data analytic approaches focusing on modeling and analyzing the uniformity of critical current. However, analyzing the uniformity of critical current is challenging due to the following reasons.

(1) The uniformity of critical current changes dynamically along different locations of an HTS tape due to the unstable growth conditions, especially in a long tape with a kilometer length. However, existing uniformity measurements were proposed for the whole tape that cannot capture the spatial non-homogeneity in the uniformity

[3, 4, 6]. To precisely quantify the variations along a long tape, this paper proposes a time-series based dynamic uniformity metric that measures the uniformity of critical current within moving windows. The dynamic measure of uniformity is also readily available for modeling the relationship between the I_c uniformity and the process parameters or growth conditions.

(2) The MOCVD is a highly complex manufacturing process that involves multiple time-varying process parameters, such as voltage, temperature, pressure, and residual oxygen concentration. The underlying relationships between these process parameters and the uniformity of I_c remain unclear. There exists a significant challenge in modeling these relationships as the uniformity of critical current and process parameters dynamically evolve over tape with both autocorrelation within measurements and interactions between parameters. To address this challenge, this paper uses a vector-autoregression (VAR)-based approach to capture both autocorrelation within uniformity measures and effects of process parameters. To enhance the interpretability of the uniformity model and inform the process control of MOCVD, a forward feature selection algorithm is integrated that identifies the most important set of process parameters for uniformity modeling.

The rest of the paper is organized as follows. Section 2 formally describes the problem of interest in this study. Section 3 reviews the related literature, and Section 4 introduces the dynamic uniformity modeling framework developed in this study. Section 5 describes the results of our analysis, and the conclusion is drawn in Section 6.

2. Problem Description

Given an HTS tape produced from the MOCVD process with its critical current measurements and process parameters, this paper focuses on modeling the spatial-varying uniformity of critical current and its relationships with the process parameters. To solve this problem, a dynamic uniformity modeling framework is proposed to integrate a new dynamic uniformity measure modeling the evolution of critical current uniformity, a vector autoregression analysis capturing the autocorrelations and the relationships between time-series process parameters and uniformity, and a feature selection technique identifying a set of important process parameters for critical current uniformity modeling, monitoring and control.

3. Related Research

The uniformity of critical current has recently been studied in the literature. Vysotsky et al. reviewed the non-uniform distribution of critical current in multi-strand superconducting cables [4]. Different metrics have been proposed to quantify the I_c uniformity in existing studies [3, 4, 6]. When the deterioration factor is available, one can measure the uniformity of critical current based on the parameters in the power law of the electric field [8]. When dropouts are of concern, the ratio of region is proposed to quantify the region where the critical current is lower than a threshold [3]. The commonly used metrics are the summary statistics of critical current along a tape, including the mean, variance and the coefficient of variation (CV) that is the standard deviation normalized by the mean value of critical current [7]. However, these summary statistics over a whole tape cannot capture the spatial and temporal non-homogeneity in the uniformity along different locations of an HTS tape, especially a long tape with a kilometer length.

Process parameters or growth conditions are various variables involved in the complex MOCVD process of HTS tapes, including voltage, temperature, pressure, and residual oxygen concentration [6]-[10]. Recent studies have identified some process parameters that have noticeable influence on the I_c of the superconductor tape, such as substrate temperature, voltage, and residual oxygen concentration [8, 9]. However, the underlying relationships between these process parameters and the uniformity of I_c have not been well studied using analytical approaches in existing studies. As a time series mode, vector autoregression (VAR) has been proved useful in product quality modeling [11]. We hence consider modeling the relationship between the CV of HTS tapes and the process parameters in the MOCVD process with a VAR model.

4. Methodology

The uniformity of critical current may break down in two ways: low-performance spots where I_c drops below a certain threshold in a short range of the tape (dropouts), and the spatial variability over the long tape [3, 4]. In our research, we focus on the latter one. To identify the process parameters that are associated with tape uniformity, we propose a dynamic uniformity modeling framework shown in **Figure 1**. The framework consists of three steps including the data preprocessing, dynamic uniformity measuring, and uniformity and process parameter modeling. In the data-preprocessing step, the multivariate process parameters collected from the production process of a superconductor tape are preprocessed to mean and coefficient of variation features. In the second step, the uniformity of the superconductor tape is measured dynamically using statistical uniformity metrics and a moving window. Different statistical metrics are compared in the dynamic uniformity measuring and the optimal one is chosen. Finally, the relationships between process parameters and tape uniformity are modeled using a vector autoregression analysis model, and the important process parameters are identified through the feature selection technique.

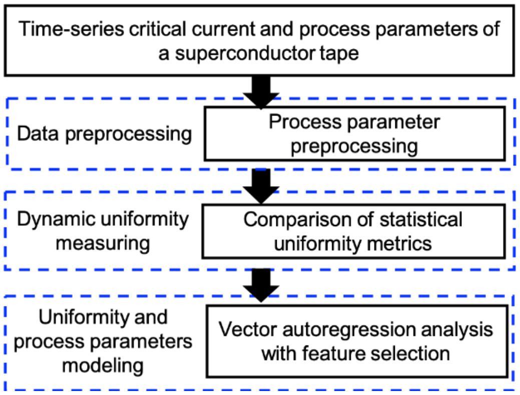

Figure 1: Framework of the proposed dynamic uniformity modeling method.

4.1 Data Description and Processing

The data consists of three tapes produced from a MOCVD process shown in **Figure. 2** at the University of Houston under various process conditions [12]. The MOCVD is a complicated process involving over one hundred real-time monitored process parameters, including the temperature at various locations, and the pressure of the reaction zone where the MOCVD takes place. Based on the domain knowledge, we selected 26 important process parameters including the temperature, pressure, composition and electrical parameters of the process that are most influential to the performance of the tape. The critical current (I_c) of each tape was measured offline using a reel-to-reel scanning Hall probe microscope (SHPM) method, which scans the 2D magnet field distribution on the surface of the tape [9]. The critical current was deconvoluted from the magnet field distribution and integrated over the tape width, resulting in a 1D instrument measured over the tape length.

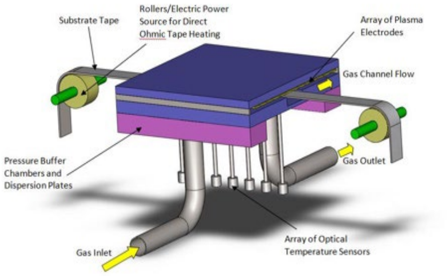

Figure 2. The MOCVD process.

As the data collected at the start and end of MOCVD process are highly unstable, they were removed from the analysis. The process parameters from the in-line sensing system and the I_c quantified offline were measured under different sampling frequencies. Therefore, the first step of our data preprocessing was to align the process parameters and I_c to same frequency. Specifically, the process parameters were down sampled by aggregating the time-series measurements, collected when a moving window of HTS tape passing through the reaction zone, to their mean and coefficient of variation (CV). Thus, each process parameter was down sampled and transformed to two time-series features.

4.2 Dynamic Uniformity Measuring

After the data preprocessing, we measured the dynamic uniformity of I_c along the tape length based on a moving window with a width of w cm. That is, the uniformity of I_c at a position x is quantified by the uniformity metrics on

I_c between x and $x + w$. Different uniformity metrics, including the standard deviation, variance, range, interquartile range (IQR), mean average deviation (MAD), and coefficient of variation (CV) are considered in this study [2]. We also considered $\Delta(\alpha)$, which measures the percentage of the tape that lies below $\alpha\bar{I}_c$ where $\bar{I}_c$ denotes the average I_c of the tape. All of these metrics were applied to the critical current within each window. For example, the CV metric at position x was calculated as the standard deviation of I_c between position x and position $x + w$ divided by the mean of I_c of the same segment. The width of the moving window was determined as the smallest window size that gives us a smooth curve of the uniformity.

4.3 Uniformity and Process Parameters Modeling

After preprocessing the process parameters and measuring the dynamic uniformity of critical current, we modeled their relationships and autocorrelations using a vector-autoregression (VAR) model. The VAR model is a multivariate linear regression model where the multivariate time series at time *t* is the dependent variable and the previous values of the same time series are the independent variables. It is widely used in time series modeling and prediction. Specifically, denote the uniformity of critical current in the t^{th} moving window as $y(t)$ and the process parameters in the corresponding window as $x_1(t), \dots, x_p(t)$, where *p* represents the number of process parameters. The VAR model predicts the critical current uniformity in each window as a linear regressor of the corresponding process parameters and the uniformity in the previous window [13], which is denoted as

$$y(t) = c + ay(t-1) + \sum_{k=1}^{p} b_k x_k(t) + \varepsilon(t) \tag{1}$$

where c, α, and b_k are the modeling parameters representing the effects of intercept, autocorrelation, and process parameters, respectively. They can be estimated from the training data using the least square estimator [13]. $\varepsilon(t)$ represents a normally distributed random noise in the uniformity measurement of the t^{th} window.

In order to identify the most significant process parameters, we used the forward feature selection algorithm [14], which starts from an empty set and adds process parameters one by one to the optimal feature set until the performance of the model stops improving. The performance of the model is evaluated by out-of-sample R-square [15], denoted as R_{OS}^2, which represents the percentage of variance explained by the model and is defined as:

$$R_{OS}^2 = 1 - \frac{SS_{res,OS}}{SS_{tot,OS}} = 1 - \frac{\sum_{t\in\mathcal{T}_{OS}}\left(I_{c,cv}(t) - \hat{I}_{c,cv}\right)^2}{\sum_{t\in\mathcal{T}_{OS}}\left(I_{c,cv}(t) - \bar{I}_{c,cv}\right)^2} \tag{2}$$

where $\mathcal{T}_{OS}$ is the set of sample points that are not used for estimating the model, $\hat{I}_{c,cv}$ is the CV at point t estimated by the model and $\bar{I}_{c,cv}$ is the mean of $I_{c,cv}$ samples in $\mathcal{T}_{OS}$. This feature selection approach is efficient and straightforward to implement, while being able to give us a relatively good R_{OS}^2 with the selected features.

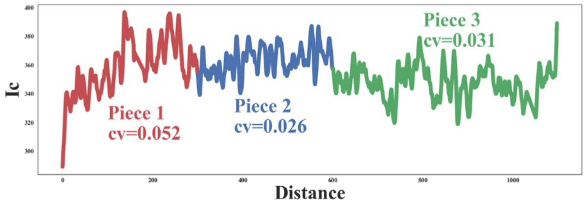

Figure 3. The critical current of a HTS tape and the CV of critical current in three segments.

5. Results

5.1. Dynamic Uniformity Measuring

The critical current of an exemplary tape with three segments is shown in **Figure 3**, where the first segment has the lowest uniformity with a highest CV of 0.052, and the second segment has the highest uniformity with a lowest CV of 0.026. As the non-uniformity of critical current varies over different parts of a superconductor tape, it demonstrates the necessity to develop a dynamic uniformity measuring method. We applied the proposed dynamic uniformity measuring approach to capture the dynamic changes in critical current uniformity. The moving window size was set at 45cm, which best captures the dynamic and smooth uniformity changes. We compared the performance of different uniformity metrics. The metrics, $\Delta(\alpha)$, range and IQR, provide a stepwise uniformity curve that poses difficulties for modeling. Although the variance, standard deviation and mean absolute deviation (MAD) metrics offer relatively smooth uniformity curses, none of them considers the mean shift of critical current. The coefficient of variation (CV) is robust to the mean shift in critical current, while providing a smooth uniformity curve. Therefore, the CV over moving windows was chosen as the uniformity metric for dynamic modeling.

5.2. Uniformity and Process Parameter Modeling

The extracted uniformity of critical current and preprocessed process parameters were fitted to the VAR model described in Section 4.3 to model their relationships. An autoregression model of critical current uniformity itself without process parameters was chosen as a baseline model for comparison. In this experiment of three sample tapes, the first 80% measurements of each tape were taken as the training set to train the models, while the last 20% data of each tape was taken as the test set to evaluate the model prediction accuracy.

The dataset includes 52 features representing the mean and coefficient of variance of each process parameter. First of all, the process parameter features (mean of cv) that gives worse R_{OS}^2 were discarded. Then a forward feature selection was applied to the remaining features to come up with a VAR model with multiple process parameters. In the end, the selected process parameters were used for building the final VAR models. The performance of uniformity models was evaluated using the R_{OS}^2 given in (2) on the test set. The performance of three uniformity models and baseline models are compared in **Table 1**. It can be observed that by incorporating the process parameters, the accuracy of uniformity prediction is greatly improved on all tapes. The improvement on tape PM5-72-2 is most significant as the proposed model can explain 61.2% of the variance in the critical current uniformity ($R_{OS}^2 = 0.612$).

Table 1: Performance (R_{OS}^2) of the proposed uniformity model on different tapes

Tape Name	Uniformity model with process parameters	Baseline model
PM5-71-3	0.529	0.361
PM5-71-4	0.491	-0.166
PM5-72-2	0.612	0.089

The selected process parameters and their coefficients on one tape (PM5-71-3) are summarized in **Table 2**. The tensions, substrate temperatures, evaporator temperature, reaction zone temperature and oxygen flow, are selected as important process parameters for the uniformity modeling. The CV of tension, substrate temperature and oxygen flow have positive correlations with the CV of critical current, which indicates that the larger fluctuations in these process parameters will lead to lower uniform performance of critical current and need to be controlled. Among these features, the substrate temperatures and tensions are also selected in the other two tapes and positively correlated with the CV of critical current. The process parameters such as deposition voltage and reaction zone pressure were identified in the other tapes. In the literature, deposition temperature has also been identified as an important process parameter to control in the MOCVD process [16]. Sufficient high deposition temperature is needed to sinter the deposited material, but too high temperature, on the other hand, can cause distortions of the substrate tube. Therefore, the substrate temperatures need to be carefully monitored and controlled in real-time to achieve uniform performance of the HTS tapes.

Table 2: The features selected for PM5-71-3 and their coefficients

Process Parameter	Coefficient
Tension_1_cv	0.15
Tension_3_mean	0.015
Tension_1_mean	0.00088
Tension 4_mean	0.013
Oxygen_Flow_mean	0.029
Oxygen_Flow__cv	4.1
Evaporator_Temperature_mean	-0.0025
Reaction_Zone_Temperature _cv	-0.4
Substrate_Temperature_1_cv	1.2
Substrate_Temperature_5_cv	1.2

6. Conclusions

This paper proposed a new measure of the uniformity of the critical current that captures the variability of uniformity along a HTS tape. Based on the new uniformity measure that systematically models the uniformity of the critical current, we used machine-learning techniques to investigate the underlying relationships between the process parameters and the uniformity of tapes. By applying the proposed methods to three long HTS tapes, this paper demonstrated the advantages of the proposed dynamic uniformity measuring. It also discovered an optimal set of process parameters that can explain more than 50% of variance in the uniformity of critical current. The fluctuations in substrate temperature and tension are identified as important factors causing the non-uniform performance of critical current that need to be monitored and prevented. This research attempts to advance the understanding of process parameters on the uniformity performance of HTS tapes. Through optimally controlling the identified process parameters, the outcome of this research will ultimately enhance the quality of long HTS tapes by improving the uniformity of the critical current. In the future, we will apply the proposed method to more HTS tapes for validation and test the relationships between the critical current uniformity and process parameters under different experimental settings. We will also develop the uniformity-based real-time monitoring and control techniques to improve the performance of HTS tapes with large scale and high yield.

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