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SPECIALTY SECTION
This article was submitted to
Chemometrics,
a section of the journal
Frontiers in Analytical Science

RECEIVED 15 September 2022
ACCEPTED 23 January 2023
PUBLISHED 16 February 2023

CITATION
Saito T and Fujiwara K (2023), Causal
analysis of nitrogen oxides emissions
process in coal-fired power plant
with LiNGAM.
Front. Anal. Sci. 3:1045324.
doi: 10.3389/frans.2023.1045324

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Causal analysis of nitrogen oxides emissions process in coal-fired power plant with LiNGAM

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Coal has been an important energy source worldwide; however, it is the largest source of nitrogen oxide (NO_x) emissions because the amount of nitrogen in coal is larger than that of other fossil fuels. Precise control of NO_x emissions is required in operations of coal-fired power plants from the viewpoint of air pollution control. Although theoretical analyses of NO_x generation from a coal-fired power plant have been conducted, it is difficult to precisely predict NO_x generation in an actual plant. NO_x generation is affected by various factors, such as furnace design and operating conditions, and there are complicated relationships among them. Thus, it is necessary to identify important operating factors that affect NO_x generation in actual coal-fired power plants. A linear non-Gaussian acyclic model (LiNGAM) is an exploratory causal analysis method that identifies a causal ordering of variables and their connection strengths without any prior knowledge of causal relationships among variables. In this study, we analyzed real operation data collected from a coal-fired power plant using LiNGAM to identify factors of NO_x generation. The causal relationship between process variables and NO_x generation was estimated by means of LiNGAM, and the connectional strengths of the variables on NO_x generation were derived. The analysis results agreed with previous reports on NO_x generation mechanisms, such as combustion air temperature, steam temperature on a specific side of the furnace, and air flow rate of forced draft fans. In addition, we found the steam flow rate and the furnace pressure as new candidate factors of NO_x generation through causal analysis using LiNGAM, which heretofore has not been suggested. Our analysis result should contribute to reducing NO_x emissions from coal-fired power plants in the future.

KEYWORDS

causal analysis, coal-fired power plant, lingam, NO_x emission, data-driven approach

1 Introduction

A coal-fired power plant must be monitored and controlled well to maintain sustainable and clean emissions despite variations in external factors. In particular, nitrogen oxide (NO_x) emission is one of the most critical matters in the operation of coal-fired power plants because it is the largest source of NO_x emission. The amount of nitrogen in coal is larger than that of other fossil fuels (Gonzalez-Salazar et al. (2018)). To understand deeply the relationship between plant operation and NO_x emissions is critical for process monitoring and control although some factors affecting NO_x emission are known such as coal properties, operation settings, equipment maintenance, and power demand (Strbac (2008); Ampimah et al. (2018)).

Process state estimation and factor identification of NO_x generation in a coal-fired power plant based on first principle models have been attempted; however, these model-based methods remain applicable only to pilot systems (Vo et al. (2019); Ke et al. (2022)). It is

difficult to comprehensively consider influence from external factors on daily operations using first principle models (Kadlec et al. (2009)).

The large amount of historical process data from long-running monitoring may contain rich information about NO_x generation. Thus, data-driven approaches based on process data may be helpful in identifying factors of NO_x generation and assisting optimal process management.

Deep learning models have been successfully applied to predict NO_x emissions from boilers. Adams et al. applied a combination of a deep neural network and a least square support vector machine to predict SO_x-NO_x emissions in a coal-fired power plant (Adams et al. (2020)). They demonstrated the effect of coal properties on SO_x-NO_x emissions by comparing performances of models on NO_x prediction, with and without coal properties. Liukkonen et al. also applied self-organizing maps (SOM) and k-means to estimate process states from combustion process data of a circulating Fluidized Bed (CFB) boiler (Liukkonen et al. (2011)). They individually selected input variables and developed NO_x emission prediction models for multiple states. Wang, et al. developed an NO_x emission prediction model using a Gaussian process (GP) (Wang et al. (2018)). The model confirmed that air-staged combustion, which is a well-known low NO_x combustion technology, has significant impact on NO_x generation.

Long short-term memory (LSTM), a kind of neural network, is a model suitable for processing time series data. Many studies have applied LSTM and reported good performance in dynamic NO_x prediction (Tan et al. (2019); Yang et al. (2020); Song et al. (2022); Xie et al. (2020); Wang et al. (2022); Tuttle et al. (2021)). Some studies have reported that convolutional neural networks (CNN) accurately predicted emissions of NO_x from coal-fired boilers (Li and Hu (2020); Saif-Ul-Allah et al. (2022,?)). In addition, deep hybrid neural networks also have been applied to CFB gas emission prediction (Hu et al. (2020)). The computational complexity thereof was almost the same as CNN and LSTM, and the prediction performance was approximately five times better than that of CNN and 7.5 times better than LSTM.

Most machine-learning (ML) models are black-boxes, and it is difficult for us to interpret the relationships between process variables and NO_x generation. Attention mechanisms (AM) may help interpretation of ML models. In an analysis of gasoline engines, quantitative impact of each process variable on NO_x emission was investigated using graph neural networks with AM (Chen et al. (2023)). Several studies have also applied AM to develop NO_x emission models in coal-fired power plants; however, they did not always obtain good-interpretable models (Wan et al. (2022); Wang et al. (2022); Li et al. (2023)).

Path analysis or the structural equation modeling (SEM) approach is useful for process interpretation because it estimates the structural relationships between process variables. PLS-SEM (Hair et al. (2011)) and process PLS (van Kollenburg et al. (2021)) have been applied to structural modeling of industrial production processes (van Kollenburg et al. (2020); Offermans et al. (2021)). However, the relationship of process variables must be manually determined before constructing a model with these structural methods. Prior knowledge about causal relationships between process variables is only sometimes fully known in large and complex processes, including coal-fired power plants. Thus, we should adopt a method that does not require prior knowledge about processes.

Causal discovery methods are gaining popularity in industrial process analysis (Chen et al. (2018); Sun et al. (2022); Menegozzo et al. (2022)). Linear non-gaussian acyclic model (LiNGAM) is a useful causal discovery method for estimating a causal structure among variables based only on

data without any prior knowledge of the structure (Shimizu et al. (2006; Shimizu et al. (2011)). LiNGAM has been widely adopted in various fields, such as the social sciences (Feringstad et al. (2011); Lai and Bessler (2015)) and neuroscience (Smith et al. (2011); Bielczyk et al. (2019)), and has been applied to fault diagnosis and causal discovery in industrial processes in recent years (Uchida et al. (2022); Cao et al. (2022)). The analysis results using LiNGAM provide better insight into the process operation to process operators and engineers.

In this study, we applied LiNGAM to real process data of an actual coal-fired power plant in order to identify significant factors of NO_x emission based on causality between process variables. By utilizing LiNGAM, we did not need prior knowledge of the process, which is not the case with other structural methods. We discuss the significant factors of NO_x emission identified by LiNGAM based on the physicochemical knowledge of the coal-fired power plant. It was confirmed that some identified factors were consistent with previous studies; however, we found two new factors of NO_x emission—steam flow rate and furnace pressure—that have not been mentioned in previous studies.

2 Materials and methods

2.1 Coal-fired power plant

This study focuses on a coal-fired power plant with a 700 MW supercritical tangential firing boiler built in the Kansai region of Japan and is operated using mixtures of various types of coal in consideration of economic efficiency. Figure 1 shows a schematic diagram of the overall system configuration (Zhang. (2013)).

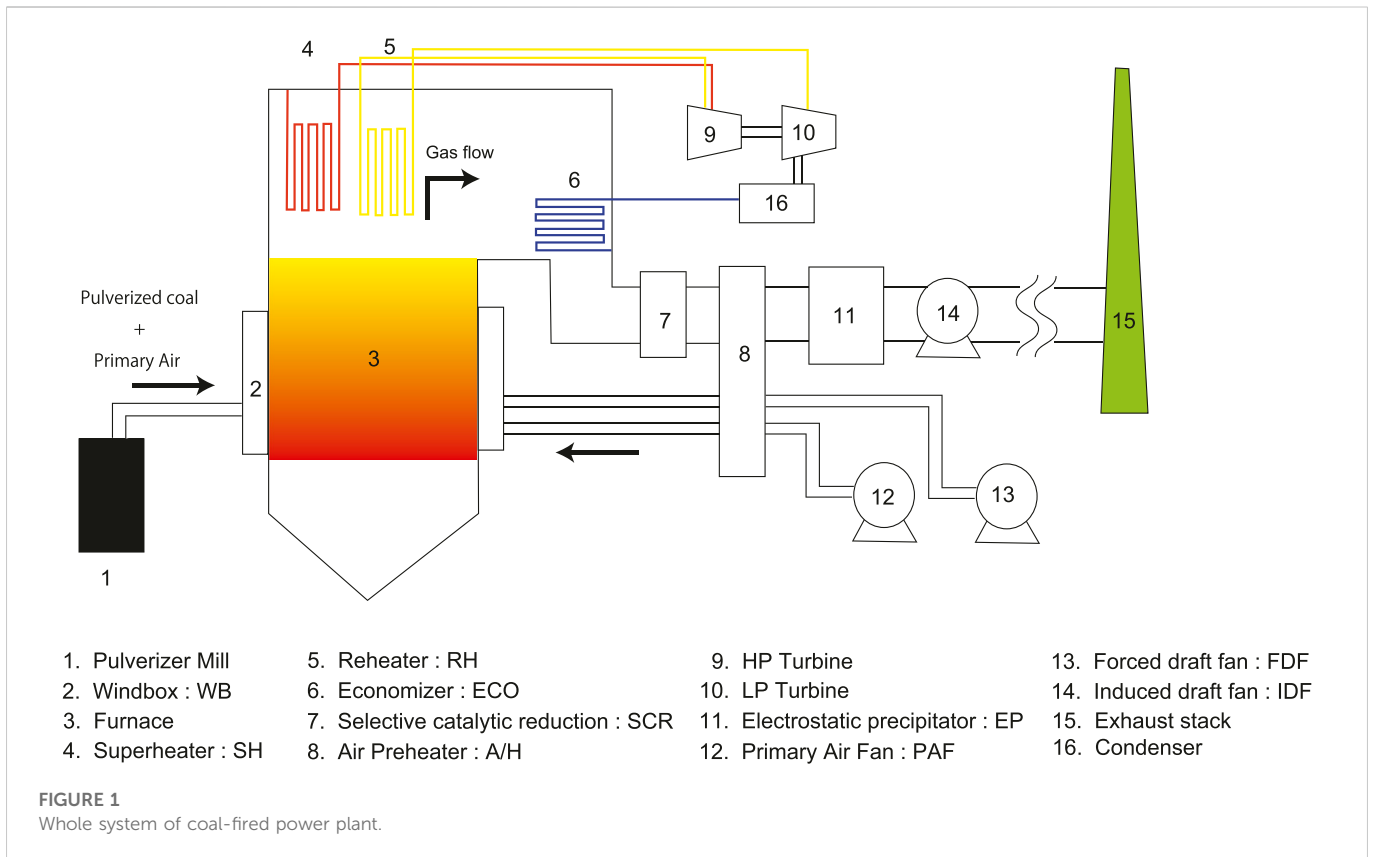
Combustion air is classified into primary air, secondary air, and over-fire air (OFA), and is fed from a primary air fan and a forced draft fan, as indicated by (12) and (13), after being heated by an air preheater (8) before entering a furnace (3) in Figure 1.

The operation data of the coal-fired power plant consist of momentary values measured every hour, collected over approximately 6 years. NO_x emission was measured at the inlet of the denitration equipment and represented as the dry gas basis at 6% O₂. We clipped them only when the boiler load was over 680 MW because only then can it be regarded as a steady-state operation. The unsteady-state operation data, such as data obtained during coal brand changes, were removed. Outliers and noisy data were also eliminated by means of visual observation. In addition, some manipulated variables that did not change throughout the entire period were omitted from the analysis since these variables did not contain any information. Finally, the total number of analyzed samples was 10,763. Table 1 summarizes the process variables used for analysis. Each variable was standardized with zero mean and a standard deviation of one before analysis.

2.2 LiNGAM

LiNGAM is a model expressing the causal structure among variables from data containing confounders (Shimizu et al. (2006)). An example of a causal structure is shown in Figure 2. The vertices represent variables, and the directed edges express causal dependencies among the variables. For example, there is a directed edge from vertex x_1 to x_2 , which means x_1 has a causal effect on x_2 .

LiNGAM assumes that each variable is generated as the linear combination of the causal antecedent variables and an exogenous



variable. In the LiNGAM assumption, the causal structure is expressed as a directed acyclic graph (DAG) that is a directed graph without a cycle. An example of a LiNGAM model in Figure 2 is as shown by 1 and (2); Eq. (3).

$$\begin{aligned}
 x_1 &= e_1 & (1) \\
 x_2 &= b_{21}x_1 + e_1 & (2) \\
 x_3 &= b_{31}x_1 + b_{32}x_2 + e_3 & (3)
 \end{aligned}$$

Where x_i and e_i ($i = 1, 2, 3$) are observed variables and exogenous noise, respectively. b_{21} , b_{31} , and b_{32} are coefficients.

When the data include p variables, the LiNGAM model is expressed as a linear Equation 4:

$$\mathbf{x} = \mathbf{B}\mathbf{x} + \mathbf{e} \quad (4)$$

where $\mathbf{x} \in \mathbb{R}^p$ is the variable vector, $\mathbf{e} \in \mathbb{R}^p$ is the exogenous noise vector, and $\mathbf{B} \in \mathbb{R}^{p \times p}$ is the coefficient matrix of the LiNGAM model, which must be a lower triangular matrix whose diagonal components are zero due to the causal assumption.

The goal of causal discovery with LiNGAM is to estimate the coefficient matrix \mathbf{B} , which describes the causal relationships among the variables. Although there are some assumptions in the LiNGAM model, the most important assumption is that all variables in the data need to be continuous.

The LiNGAM coefficients on a row vector in \mathbf{B} that are associated with NOx emissions express the causal effects of the factors on NOx emissions. Their absolute values and positive/negative signs indicate the strength and the direction of the causal effects. Thus, focus should be placed on a specific row vector β in \mathbf{B} in this analysis. The absolute values and positive/

negative signs of the extracted LiNGAM coefficients were compared to estimate the causal effects on NOx emissions.

Although several LiNGAM algorithms have been proposed, such as ICA-based LiNGAM (Shimizu et al. (2006)), Direct LiNGAM (Shimizu et al. (2011)), and Pairwise LiNGAM (Hyvärinen and Smith. (2013)), we adopted DirectLiNGAM for its ease of practical use.

3 Results

Figure 3 shows the causal effects of each variable on NOx emissions estimated by means of LiNGAM. The bars indicate the strengths and directions of the causal effects. The variables with positive values may increase NOx emission, and those with negative values may decrease NOx emission. The absolute values indicate the strength of the causal effects.

The steam flow rate (SFR) and the furnace pressure (FP) had the first and the second largest positive effects on NOx emission. The combustion air temperature (CAT) has a positive effect, which is a factor of thermal NOx. The steam temperature right wall of the furnace (STR) has a strong negative effect, and the steam temperature left wall of the furnace (STL) has a weak positive effect on NOx emissions. The forced draft fan-air flow rate (FDF-AFR) has a negative effect on NOx, which is understandable because FDF-AFR is associated with Fuel NOx.

4 Discussion

In this section, we discuss the significant factors of NOx emission identified with LiNGAM: the combustion air temperature (CAT), the

TABLE 1 Process variables.

Variable name	Abbreviation
Furnace pressure	FP
Steam temperature front wall of furnace	STF
Steam temperature back wall of furnace	STB
Steam temperature right wall of furnace	STR
Steam temperature left wall of furnace	STL
Pulverized coal flow rate	PCFR
Primary Air temperature	PAT
Primary Air flow rate	PAFR
Secondary air flow rate	SAFR
Combustion air temperature	CAT
Excess air ratio	EAR
Theoretical air flow rate	TAFR
Forced draft fan-air flow rate	FDF-AFR
Flue gas pressure	FGP
NOx emission	NOx
Steam flow rate	SFR
Steam temperature	ST
Steam pressure	SP
SH Metal temperature	SH-MT
RH Metal temperature	RH-MT
ECO Oxygen concentration	ECO-OC
Carbon content	CC
Hydrogen content	HC
Oxygen content	OC
Sulfur content	SC
Nitrogen content	NC
Volatile content	VC
Ash content	AC
Fixed carbon content	FCC
Fuel ratio	FR

steam temperature near the walls of the furnace (STR and STL), the forced draft fan-air flow rate (FDF-AFR), and the steam flow rate (SFR) and the furnace pressure (FP).

4.1 Combustion air temperature

The positive causal effect of CAT estimated with LiNGAM is supported by a previous research which showed that thermal NOx strongly depends on the combustion temperature. The Extended Zeldovich mechanism, analyzed by Bowman and Seery (Fenimore and Jones, 1957), describes the generation process of thermal NOx as follows:



In a conventional combustion of pulverized coal, fuel NOx and thermal NOx contribute to the majority of the total NOx emissions, while prompt NOx makes negligible contribution (Choi and Kim, 2009; Zhao et al. 2017; Ma et al. 2019). Since cracking of stable N₂-binding shown in the first reaction in Eq. 5 requires high activation energy (Hill and Douglas Smoot, 2000), most of the thermal NOx is generated in the areas around flames from the

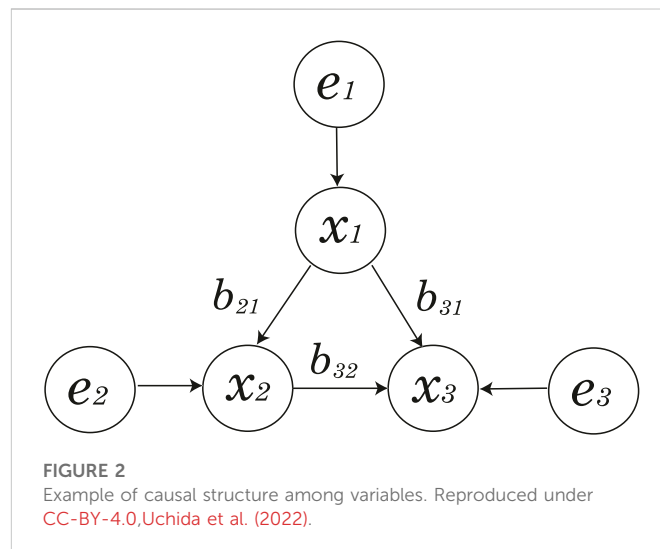


FIGURE 2 Example of causal structure among variables. Reproduced under CC-BY-4.0, Uchida et al. (2022).

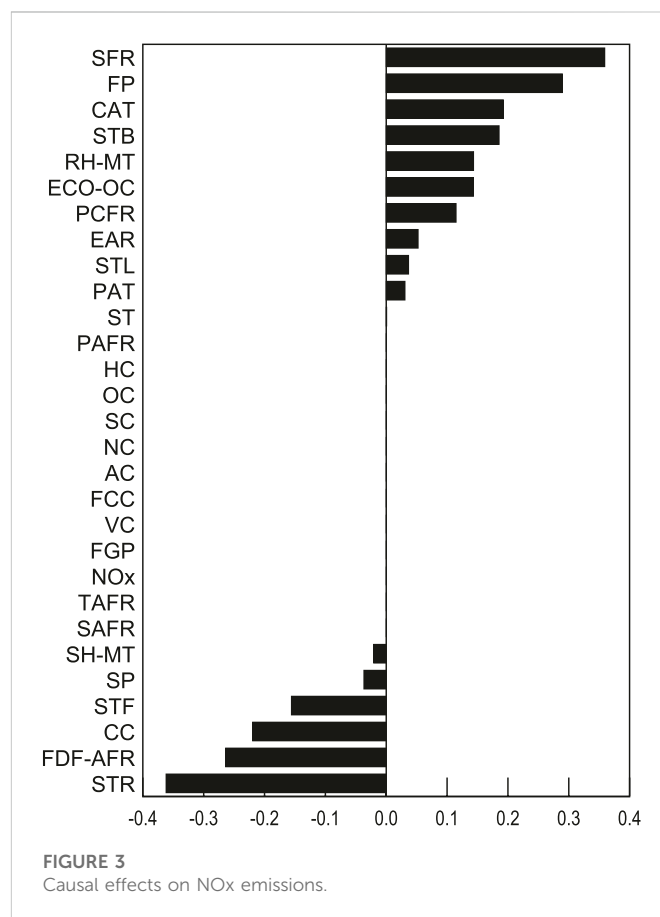


FIGURE 3 Causal effects on NOx emissions.

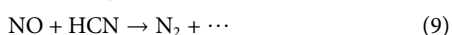
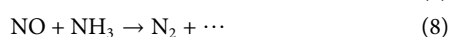
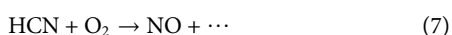
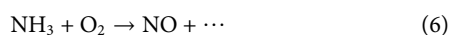
burners. Accordingly, NO_x emissions exponentially decrease as the flame temperature decreases. Hence, CAT affects NO_x emissions, which is consistent with our analysis.

4.2 Steam temperatures near walls of furnace

Our results also showed that steam temperature on a specific side of the furnace wall (STR and STL) was another factor in the NO_x generation. Previous researchers have indicated that the furnace design, such as the angles of the OFA nozzles and the burner nozzles, affect the characteristics of the combustion and NO_x emission, on the basis of computational fluid dynamics (CFD) simulations (Wang et al. (2018); Choi and Kim. (2009); Li et al. (2009)). When the burner nozzle angle increases, the temperature distribution and the turbulent mixing in the furnace change significantly, which then alters NO_x emissions (Tan et al. (2017)). Thus, the furnace design may cause uneven combustion and differences in STR and STL, thereby affecting NO_x generation.

4.3 Air flow rate of forced draft fan

The combustion air fed from the forced draft fan (FDF) is divided into secondary air and over fire air (OFA) related to the Fuel NO_x. Fuel NO_x is generated from the nitrogen bound in the fuel through either the homogenous gas phase reaction or the heterogeneous reaction on the coal char surface as follows (Miller and Bowman. (1989); Molina et al. (2000)).



The N₂-bonding is cracked during the devolatilization process, and a portion of the nitrogen is rapidly converted to HCN, while the remaining fuel nitrogen forms NH₃. These two reactions forming either NO or N₂ depend on the local conditions of the fuel. In fuel-rich regions, HCN and NH₃ will typically be reduced to N₂ as shown in Eqs. 8–9, while they are oxidized to form NO in fuel-lean regions as shown in Eqs. 6–7 (Eaton et al. (1999)).

Air staging with OFA makes a fuel-rich zone near the burners by supplying the combustion air into the secondary burnout zone. The increase in FDF air flow rate may form a hypoxic environment near the burners in the primary combustion zone and allow most of the coal nitrogen to be released into a fuel-rich region. This mechanism suggests a rapid formation of N₂ from NO_x. Thus, it is concluded that FDF-AFR has causality with NO_x emission. Previous research has shown that the rate of OFA has a significant impact on NO_x emissions (Wang et al. (2018)), which is consistent with the results of this study.

4.4 Steam flow rate and furnace pressure

The discussion above indicates the feasibility of causal analysis using LiNGAM in NO_x emissions in a coal-fired power plant, since the identified factors were consistent with previous studies.

However, SFR and FP have not been mentioned in previous research, although they had the first and second largest effects on

NO_x emissions, as shown in Figure 3. FP is the pressure inside the furnace during coal combustion, and there exists a physical causal relationship with it and NO_x emission. FP is a factor of NO_x emissions newly identified in this study, which should be confirmed through experiments and additional data, to thereby generate a new hypothesis that explains how FP affects NO_x generation.

4.5 Limitation

Limitations of this work include the operation data; the data did not contain properties of the coals that were used and their mixtures. Thus, the effects of the coals that were used on NO_x emission was taken into account in this study. We need to collect data on the utilized coal for further analysis.

5 Conclusion

This study analyzed real operation data collected from a coal-fired power plant to identify the factors of NO_x emissions with LiNGAM. As a result, some of the known NO_x emission factors were correctly identified by LiNGAM, while new and spurious factors, the steam flow rate, and the furnace pressure were also estimated.

In future works, we will confirm whether unknown factors also affect NO_x emissions, and discuss the challenges of applying causal discovery algorithms to estimate causal relationships in the context of complex industrial processes.

Data availability statement

Due to commercial restrictions of the operation data of the coal-fired power plant, the authors do not agree for their data to be shared publicly, so supporting data is not readily available. Requests to access the datasets should be directed to Koichi Fujiwara, fujiiwara.koichi@hps.material.nagoya-u.ac.jp.

Author contributions

TS and KF analyzed the data and composed the manuscript. All authors contributed to the article and approved the submitted version.

Funding

This study was partially supported by the Kobe Steel Inc. The funder was not involved in the study design, collection, analysis, interpretation of data, the writing of this article, or the decision to submit it for publication.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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