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# Interpretable AI Explores Effective Components of CAD/CAM Resin Composites

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**ABSTRACT**

High flexural strength of computer-aided manufacturing resin composite blocks (CAD/CAM RCBs) are required in clinical scenarios. However, the conventional *in vitro* approach of modifying materials composition by trial and error was not efficient to explore the effective components to contribute on the flexural strength. Machine learning (ML) is a powerful tool to achieve the above goals. Therefore, the aim of this study was to develop ML models to predict the flexural strength of CAD/CAM RCBs and explore the components that affect flexural strength as the first step. The composition of 12 commercially available products and flexural strength were collected from the manufacturers and literature. The initial data consisted of 16 attributes and 12 samples. Considering that the input data for each sample were recognized as a multi-dimensional vector, a fluctuation range of 0.1 was proposed for each vector and the number of samples was augmented to 120. Regression algorithms, that is, random forest (RF), extra trees, gradient boosting decision tree, light gradient boosting machine, and extreme gradient boosting, were used to develop five ML models to predict flexural strength. An exhaustive search and feature importance analysis were conducted to analyze the effective components that affected flexural strength. The $R^2$-values for each model were 0.947, 0.997, 0.998, 0.983, and 0.927, respectively. The relative errors of all the algorithms were within 15%. Among the high predicted flexural strength group in the exhaustive search, UDMA was contained in all compositions. Filler content and TEGDMA were the top two features predicted by all models in the feature importance analysis. $ZrSiO_4$ was the third important feature for all models, except the RF model. The ML models established in this study successfully predicted the flexural strength of CAD/CAM RCBs and identified the effective components that affected flexural strength based on the available dataset.

**KEYWORDS** Artificial Intelligence, CAD-CAM, Composite materials, Deep Learning/Machine Learning, Prosthetic Dentistry/Prosthodontics, Restorative dentistry

## 1. Introduction

In the last 20 years, materials used for dental restoration have changed from alloys and metals to ceramics and resin composites because of the increasing aesthetic demand of patients. Currently, for chairside computer-aided design and computer-aided manufacturing (CAD/CAM) systems, materials that include machinable ceramic and resin composite blocks (RCBs) have been developed (Ruse and Sadoun 2014). CAD/CAM RCBs are attracting much attention because their esthetics are more favorable than metals and their cost is lower than ceramics, meanwhile, it owns preferable mechanical properties such as flexural strength comparing to direct resin composites. However, edge chipping and fracture still occur under clinical service, which results in the limited longevity of restorations (Brandeburski et al. 2020; Yamaguchi et al. 2020). Therefore, how to improve the mechanical properties of restorative materials has always been a topic of great interest. Efforts have been made to improve the mechanical properties, including the flexural strength of CAD/CAM RCBs, by changing the type of fillers and monomers (Lee et al. 2020; Mainjot et al. 2016; Tsujimoto et al. 2017). However, because different compositions result in the varied flexural strength of CAD/CAM RCBs, which specific filler or monomer contributes the most to improving flexural strength remains unknown, and thus forms a convoluted nonlinear phenomenon that requires analysis.

The conventional approach to modifying material compositions to achieve superior properties relies on repetitive *in vitro* experiments, which are often time-consuming and inefficient (Liu et al. 2017), and can barely distinguish the contribution of each composition to the target material properties. In recent years, artificial intelligence (AI) technologies have become widely accepted in society, and preliminarily implemented in dentistry (Shan et al. 2021; Yamaguchi et al. 2019). A

promising approach that combines traditional experimental methods with intelligent data analysis grew out of the quest for AI, and is known as machine learning (ML). ML is a powerful tool for finding meaningful regularities in high-dimensional data, which allows for predictions of unknown data. It uses algorithms by which a computer can learn from empirical data by modeling the linear or nonlinear relationships between material properties and related factors (Liu et al. 2017; Schwendicke et al. 2020). It has successfully resolved the difficulties of modeling the relationships between material properties and complex physical factors (Butler et al. 2018). Compared with using only experimental measurement, ML quickly assesses and analyzes the collected data with extraction of various relevant features, which saves a great amount of time and cost for scientists and manufacturers (Chen and Gu 2019). Moreover, for many AI users in both the dental and medical fields, a high level of accountability is required; thus, it is highly possible that directly interpretable and tractable AI techniques will be adopted as assistants for decision-making (Arrieta et al. 2020; Gunning et al. 2019). In explainable AI (XAI), a set of ML algorithms are proposed that can produce models with high prediction accuracy, while allowing users to understand, trust, and effectively manage these new AI partners (Gunning et al. 2019). Unlike the opaque explainability of deep neural networks, the output of ML algorithms can be verified mathematically (Hu et al. 2020).

For the purpose of predicting material properties, ML models should contain three parts: training data, descriptors, and algorithms that can map the descriptors to the property of interest (Ward et al. 2016). The descriptors are a set of attributes that require selection to be capable of both uniquely defining each of the materials in the dataset and relating to the targeted property (Ward et al. 2016) . Compositional information has been commonly used as descriptors for developing ML models for materials (Hu et al.

2020). Hyperparameters are parameters of ML algorithms that must be pre-set and tuned to control how an algorithm learns from the training data (Tso et al. 2020). The development of an effective model also relies on the optimization of hyperparameters (Yang and Shami 2020).

To date, the dental applications of ML, such as computer-aided diagnosis, treatment, and disease prediction, have mainly focused on classification problems for which the outputs are discrete values (Hung et al. 2019; Shan et al. 2021; Yamaguchi et al. 2019). The correlation between the composition and mechanical behavior of aging enamel (Yan et al. 2021) was considered in only one study. There have been no studies in which ML has been applied to predicting dental material properties. However, this data-driven informatic approach has already been applied to classical materials science to predict the mechanical properties (e.g., toughness, strength, and stiffness) of composite materials, and densities and elastic modulus of $SiO_2$-based glass using regression models with only the chemical composition or with the chemical or physical quantities as descriptors (Bishnoi et al. 2019; Marani and Nehdi 2020; Ramprasad et al. 2017; Xiong et al. 2020).

The aim of this study was to predict, for the first time, the flexural strength of CAD/CAM RCBs using ML methods and identify the effective components that affect flexural strength based on the available dataset, which contains information about the chemical composition and corresponding flexural strength of CAD/CAM RCBs.

## 2. Materials and Methods

### 2.1 CAD/CAM RCBs

Twelve commercially available CAD/CAM RCBs were considered in this study: Cerasmart (CS; GC, Tokyo, Japan), Katana Avencia Block (KA; Kuraray Noritake Dental, Tokyo, Japan), Katana Avencia P Block (AP; Kuraray Noritake Dental), Shofu Block HC (HC; Shofu, Kyoto, Japan), Shofu Block HC Hard (HC; Shofu), KZR-CAD HR2 (HR2; Yamakin, Osaka, Japan), Estelite Block (EB; Tokuyama Dental, Tsukuba, Japan), Estelite P Block (EP; Tokuyama Dental), Brilliant Crios (BC; Coltene, Switzerland), Lava Ultimate (LU; 3M ESPE, St. Paul, MN, USA), Paradigm MZ 100 (MZ100; 3M ESPE), and Tetric CAD (TC; Ivoclar Vivadent, Schaan Liechtenstein). The details of the composition of each block are summarized in Table 1.

### 2.2 Data collection

The detailed compositional information and flexural strength of each commercial product were collected from the manufacturers and literature (Abdou et al. 2021; Alamoush et al. 2018; Ducke and Ilie 2021; Lauvahutanon et al. 2014; Lawson et al. 2016; Niem et al. 2020; Zhi et al. 2016). The flexural strengths of the products were selected from the literature that contained the following information in the Materials and Methods section: (1) the specimens were immersed in water for 24 hours at 37℃; and (2) the three-point bending test was conducted for these specimens, with a crosshead speed of 1.0 mm/min (Lawson et al. 2016; Niem et al. 2020).

### 2.3 Training dataset construction

The initial data consisted of 16 attributes (15 input compositional descriptors and 1 label) and 12 samples. There were two types of compositional descriptors: fillers and monomers. The fillers were $SiO_2$, $ZrO_2$, $ZrSiO_4$, micro-fumed silica, barium glass, $Al_2O_3$, methacrylate mixed filler, $SiO_2$-$ZrO_2$ filler, and filler content, and the monomers were urethane dimethacrylate (UDMA), 2,2-Bis(4-methacryloxypolyethoxyphenyl)propane (Bis-MEPP), triethylene glycol dimethacrylate (TEGDMA), neopentyl glycol dimethacrylate (NPGDMA), bisphenol A glycidyl methacrylate (Bis-GMA), and ethoxylated bisphenol A-glycol dimethacrylate (Bis-EMA). Each product had a unique composition; therefore, 1 and 0 were used to represent whether the sample contained the specific descriptor or not, respectively. For the descriptor filler content, it was set to be in the range from 62 to 85(wt%). Considering that the input data for each sample were recognized as a multi-dimensional vector, a fluctuation range of 0.1 was defined for each vector, specifically, [0, 0.1] and [0.95, 1.05] for 0 and 1, respectively. Then, new samples ($n$ = 9) were created according to the data of the original sample. Specifically, for each original sample, new samples were constructed by generating random numbers to two decimal places using a random number generator (Jupyter Notebook, version 6.0.1) within the range [0, 0.1] for 0 and [0.95, 1.05] for 1. The same labels were used for the original samples and created samples. Consequently, the training dataset was increased to 16 attributes and 120 samples.

### 2.4 Model development

The learning model was developed and run in Jupyter Notebook (version 6.0.1) on a laptop (Surface Laptop 2: Core i5-8250U CPU and 8 GB RAM, Microsoft, Redmond,

Washington, USA). Regression algorithms, that is, random forest (RF), extra trees (ET), gradient boosting decision tree (GBDT), light gradient boosting machine (LightGBM), and extreme gradient boosting (XGBoost), were implemented using the scikit-learn package in Python. The whole dataset was imported and randomly split into two groups: 80% of the data was used for training the model and 20% was used for testing. The variable "random_state" was set to a fixed value to ensure the same split of the data for each model. The function "GridSearchCV" in scikit-learn's model selection package was applied to search for the optimal combination of hyperparameters for each model. This function evaluated the model's performance for each combination of hyperparameters using 10-fold cross-validation, in which the model fitted the training data 10 times. For each iteration, the training data were split into 10 subsets: 9 subsets were used for training the model and the $10^{th}$ subset was used as test data. The combination of hyperparameters that exhibited the best performance during the cross-validation process was selected.

### 2.6 Model evaluation

The coefficient of determination ($R^2$-value), root mean square error (*RMSE*), and mean absolute error (*MAE*) were calculated to assess the regression accuracy of each model, and the values were compared. The metrics are expressed as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^{m}\left(\hat{y}^{(i)} - y^{(i)}\right)^2}{\sum_{i=1}^{m}\left(\bar{y} - y^{(i)}\right)^2} \quad (1)$$

$$RMSE = \frac{1}{m}\sum_{i=1}^{m}\left(y^{(i)} - \hat{y}^{(i)}\right)^2 \quad (2)$$

$$MAE = \frac{1}{m}\sum_{i=1}^{m}\left|y^{(i)} - \hat{y}^{(i)}\right|, \quad (3)$$

where $m$ is the total specimen number. Additionally, to further assess the performance of the models, the relative error was defined as (Hu et al. 2020)

$$Relative\ error = \frac{|\hat{y}^{(i)} - y^{(i)}|}{y^{(i)}}, \quad (4)$$

where $y^{(i)}$ is the flexural strength calculated from *in vitro* experiments, $\hat{y}^{(i)}$ is the predicted flexural strength from the above five algorithms, and $m$ is the number of test samples.

**2.7 Exhaustive search**

The first 14 descriptors were set to 0 or 1, and the 15$^{th}$ descriptor (filler content) was set to be in the range from 62 to 85 in Jupyter Notebook (version 6.0.1). An exhaustive search was performed by five finely tuned models to iterate all $2^{14} \times 24$ (393,216) combinations of the descriptors and predict 393,216 values of the corresponding flexural strengths. The combinations were then screened and the impossible combinations were deleted: the fillers were all 0, the monomers were all 0, $SiO_2$ was 0, and only $SiO_2$ was contained in the fillers. The combinations of descriptors with the highest and lowest flexural strengths were selected and compared.

### 2.8 Feature importance

Feature importance was calculated and compared within the five tuned models. Feature importance analysis determined the contribution of each feature to the targeted properties by assigning a score for each feature.

## 3. Results

The prediction performance of each model is shown in Table 2. The $R^2$-values were 0.947, 0.997, 0.998, 0.983, and 0.927, respectively. The relative errors of all the algorithms were within 15%. The flexural strength predictions using the ML models beyond the training set are plotted versus the observed values in Figure 1. The tuned hyperparameters were shown in the Appendix Table 1.

Figure 2 shows the results of an exhaustive search using each ML model. The plot of the ET and GBDT models mainly contains three groups of predictions, the top group and the bottom group are indicated by red arrows. In Figure 2b, the predictions of the bottom group ranged from 132.0 MPa to 180.1 MPa, those of the middle group ranged from 180.1 MPa to 263.7 MPa, and those of the top group ranged from 263.7 MPa to 270.0 MPa. For the GBDT model, the bottom group of Figure 2c shows four high-density areas of points, where the predictions varied from 132.2 MPa to 180.1 MPa. By contrast, the highest predictions in the top group ranged from 256.6 MPa to 269.5 MPa. A detailed illustration of Figure 2 was in the supplemental (Appendix Figure 2 and 3).

The feature importance analysis results are shown in Figure 3. The filler content and TEGDMA were the top two features that had a relatively high importance value among all the developed models. Although micro-fumed silica was the next important feature according to the RF model, according to the other four models, $ZrSiO_4$ was the third high importance feature that contributed to flexural strength.

## 4. DISSCUSSION

Data size is of great importance in the ML process (Ramprasad et al. 2017). It is likely that relatively little attention has been paid to the application of ML methods to dental materials, particularly CAD/CAM RCBs, because of the limitation of compositional information. Therefore, to avoid the negative effect of a small dataset, ensembles (Marani and Nehdi 2020) were used in this study. In an ensemble, a set of base learners are trained to act together as a strong learner, thereby providing more accurate predictions (Marani and Nehdi 2020). Bagging and boosting are the two most frequently used approaches for constructing ensemble models (Dietterich 2000). Among these two approaches, algorithms that involve bagging, such as RF, and algorithms that use boosting, such as GBDT and XGBoost, have demonstrated robust performance in predicting material properties in recent studies (Kern et al. 2019; Marani and Nehdi 2020; Song et al. 2020; Zhang et al. 2020). The detailed demonstration of each algorithm is in supplemental (Appendix Algorithm basis). In the present study, the five selected ensemble algorithms all achieved acceptable $R^2$-values of over 0.9 in terms of prediction accuracy. The RMSE and MAE values indicated the superior predictive ability of the developed models for the flexural strength of CAD/CAM RCBs. GBDT was the best-performing model. This was followed closely by the ET model. These results imply that for the available dataset applied in this study, the algorithms performed similarly when bagging or boosting techniques were used.

Because the ML models were only trained on limited data, it was crucial for the models to provide reliable predictions beyond the training set. The prediction results using the test data suggested that the ET, GBDT, and LightGBM models had a promising ability to reliably predict the flexural strength values of CAD/CAM RCBs, provided the chemical compositions were given. However, several predictions of the

XGBoost and RF models deviated from the observed values, and their relative errors were within 15%. Moreover, the RMSE values for the RF and XGBoost models were 5.643 MPa and 6.639 MPa, respectively, which were much larger than those for the other three models. These results suggest that the RF and XGBoost models yielded uncertainties during the extrapolation process.

The exhaustive search results of the ET and GBDT models were analyzed because of their promising prediction performance. In the bottom group of predictions from the GBDT model (Figure 2c), the filler content in the combinations ranged from 62 (wt%) to 69 (wt%), whereas in the top group, it ranged from 82 (wt%) to 85(wt%), which yielded higher predicted flexural strength values. It has been proved that high filler content improves flexural strength (Yao et al. 2014), which is in agreement with the finding in the present study. The same tendency was also identified in the results predicted using the ET model (Figure 2b). However, exceptions to this rule were observed for MZ 100, which obtained a relatively low strength value compared with the other materials listed in this study, despite its relatively high filler fraction (85 wt%). Furthermore, the same predictions were made by the ML models using compositions that varied only in filler content. This result suggests that, for CAD/CAM RCBs, the filler content and flexural strengths did not always positively correlate. Flexural strength tended to decrease when the filler content exceeded 60 vol% (Mainjot et al. 2016; Nguyen et al. 2013). Our results suggest that, instead of a fixed percentage of filler content affecting flexural strength, within a specific range, simply increasing/decreasing the content of fillers does not necessarily improve/decrease the flexural strength.

For the monomers in the lower predictions group, TEGDMA was found to be contained in over 99.9% of the combinations predicted by the ET model (Figure 2b).

UDMA, Bis-MEPP, Bis-GMA, and Bis-EMA were contained in a similar ratio of 50.6%. In the predictions of the GBDT model (Figure 2c), the results also showed the same tendency predicted by the ET model, with TEGDMA sharing the highest ratio. These results suggest that TEGDMA could be an essential component that affects the predicted flexural strength. This finding is in agreement with *in vitro* results (Asmussen and Peutzfeldt 1998), where increasing the content of TEGDMA in the experimental RCBs slightly reduced the flexural strength.

In the higher predictions group for the ET and GBDT models, none of the combinations contained TEGDMA or Bis-GMA; instead, UDMA was the most frequently contained monomer. Moreover, the results demonstrated that among all the combinations that contained UDMA, half also contained Bis-EMA. UDMA has a lower molecular weight and exhibits lower viscosity, and simultaneously demonstrates higher cross linking and polymerization activity with light curing than Bis-GMA (Mainjot et al. 2016; Sideridou et al. 2002). UDMA can be used alone or with other monomers, such as TEGDMA and Bis-GMA, in a matrix. For an *in vitro* experiment, it was reported that when fillers were fixed, UDMA used alone exhibited the highest flexural strength compared with the mixture of different ratios of UDMA and TEGDMA (Nguyen et al. 2013), which is consistent with the finding in the present study.

In the case of fillers, the results demonstrated that $ZrSiO_4$ had a relatively high frequency in the lower prediction group for the ET (67.6%) and GBDT (59.2%) models' predictions, whereas it halved in the higher prediction group. $ZrSiO_4$ is an important component in the ceramic industry because of its high chemical stability and excellent coloring performance at high firing temperatures (Schabbach et al. 2013). These results suggest that $ZrSiO_4$ may have some effect on the flexural strength of CAD/CAM RCBs, which needs to be explored.

It is noteworthy that the maximum flexural strengths predicted by the ET and GBDT models were 270 MPa and 269.5 MPa, respectively. For the GBDT model's prediction, the related chemical composition for the maximum flexural strength was $SiO_2$, barium glass, methacrylate mixed filler, with or without $Al_2O_3$ for fillers, and UDMA alone for monomers. Simultaneously, the filler content was from 82 (wt%) to 85 (wt%). For the ET model's prediction, the combination that resulted in the largest flexural strength was nearly the same as the result for the GBDT model, except $ZrO_2$ was added. None of these combinations were shown in Table 1; therefore, they could be considered for use in the future.

In terms of the feature importance analysis, the high importance of the top three features (filler content, TEGDMA, and $ZrSiO_4$) was also proved by the exhaustive search results, as discussed above. According to the ranking, the filler content and the use of monomers should be adjusted as a priority when modifying the composition of CAD/CAM RCBs to improve flexural strength.

Regarding the limitation of this study, the data used for training the ML models were not sufficiently comprehensive to contain all factors that affected the target material property. Even though an approach was established to increase the dataset, the information it contained was still limited; hence, the models developed in this study may not have excellent extrapolating ability. However, this study is the first step in introducing interpretable AI technology into the field of dental materials.

In conclusion, the ML models established in this study successfully predicted the flexural strength of CAD/CAM RCBs and identified the effective components that affected the flexural strength based on the available dataset. This technology has great potential as an important tool to help modify various targeting properties for different

dental materials, provided an adequate dataset is available, which will save a great amount of time and cost for both manufacturers and scientists.

## AUTHOR CONTRIBUTIONS

H. Li contributed to data acquisition, analysis, and interpretation, and drafted and critically revised the manuscript. T. Sakai, A. Tanaka, and M. Ogura contributed to data acquisition, analysis, and interpretation, and critically revised the manuscript. C. Lee and S. Yamaguchi contributed to conception, design, data acquisition, analysis, and interpretation, and drafted and critically revised the manuscript. S. Imazato contributed to conception, design, data analysis, and interpretation, and drafted and critically revised the manuscript. All authors gave their final approval and agree to be accountable for all aspects of the work.

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**Table legends**

**Table 1**. Detailed information of the computer-aided design/computer-aided manufacturing resin composite blocks used in this study. UDMA: urethane dimethacrylate, Bis-MEPP: 2,2-Bis(4-methacryloxypolyethoxyphenyl)propane, TEGDMA: triethylene glycol dimethacrylate, NPGDMA: neopentyl glycol dimethacrylate, Bis-GMA: bisphenol A glycidyl methacrylate, and Bis-EMA: ethoxylated bisphenol A-glycol dimethacrylate

**Table 2**. Prediction errors for the five machine learning models. RF: random forest, ET: extra tree, GBDT: gradient boosting decision tree, LightGBM: light gradient boosting machine, XGBoost: extreme gradient boosting, RMSE: root mean square error, MAE: mean absolute error

**Figure legends**

**Fig. 1**. Prediction performance of the ML models on the test set. The predicted flexural strengths from the five ML models are plotted versus the *in vitro* three-point bending test result (observed value). **a** RF model; **b** ET model; **c** GBDT model; **d** LightGBM model; **e** XGBoost model. The data points within the region of two black dashed lines have relative errors less than 5%.

**Fig. 2**. Flexural strengths of $2^{14} \times 24$ (393,217) combinations of descriptors predicted by the ML models using an exhaustive search after permutation and combination of 15 features. For each dot on the figure, the horizontal axis indicates the number of combinations. Each number refers to a specific combination of 15 features, that is, a unique composition of CAD/CAM RCBs. The vertical axis is the flexural strength predicted by ML model corresponding to the specific composition. **a** RF model; **b** ET model; **c** GBDT model; **d** LightGBM model; **e** XGBoost model. For ET model, in Figure 2b, the predictions of the bottom group shown by red dotted circle ranged from 132.0 MPa to 180.1 MPa, and those of the top group shown in red circle ranged from 263.7 MPa to 270.0 MPa. For figure 2c, the predictions of the bottom group varied from 132.2 MPa to 180.1 MPa. By contrast, the high prediction group ranged from 256.6 MPa to 269.5 MPa, as shown in red circle. The component in both lower and higher prediction group was analyzed and compared in the discussion section. The highest predicted flexural strength and its corresponding composition was illustrated in the discussion section.

**Fig. 3**. Feature importance for each composition calculated by the implemented models. **a** RF model; **b** ET model; **c** GBDT model; **d** LightGBM model; **e** XGBoost model.

**References**


Abdou A, Takagaki T, Alghamdi A, Tichy A, Nikaido T, Tagami J. 2021. Bonding performance of dispersed filler resin composite cad/cam blocks with different surface treatment protocols. Dent Mater J. 40(1):209-219.

Alamoush RA, Silikas N, Salim NA, Al-Nasrawi S, Satterthwaite JD. 2018. Effect of the composition of cad/cam composite blocks on mechanical properties. Biomed Res Int. 2018:4893143.

Arrieta AB, Diaz-Rodriguez N, Del Ser J, Bennetot A, Tabik S, Barbado A, Garcia S, Gil-Lopez S, Molina D, Benjamins R et al. 2020. Explainable artificial intelligence (xai): Concepts, taxonomies, opportunities and challenges toward responsible ai. Inform Fusion. 58:82-115.

Asmussen E, Peutzfeldt A. 1998. Influence of uedma bisgma and tegdma on selected mechanical properties of experimental resin composites. Dent Mater. 14(1):51-56.

Bishnoi S, Singh S, Ravinder R, Bauchy M, Gosvami NN, Kodamana H, Krishnan NMA. 2019. Predicting young's modulus of oxide glasses with sparse datasets using machine learning. J Non-Cryst Solids. 524.

Brandeburski SBN, Vidal ML, Collares K, Zhang Y, Della Bona A. 2020. Edge chipping test in dentistry: A comprehensive review. Dent Mater. 36(3):e74-e84.

Butler KT, Davies DW, Cartwright H, Isayev O, Walsh A. 2018. Machine learning for molecular and materials science. Nature. 559(7715):547-555.

Chen CT, Gu GX. 2019. Machine learning for composite materials. Mrs Commun. 9(2):556-566.

Dietterich TG. 2000. An experimental comparison of three methods for constructing

ensembles of decision trees: Bagging, boosting, and randomization. Mach Learn. 40(2):139-157.

Ducke VM, Ilie N. 2021. Aging behavior of high-translucent cad/cam resin-based composite blocks. J Mech Behav Biomed Mater. 115:104269.

Gunning D, Stefik M, Choi J, Miller T, Stumpf S, Yang GZ. 2019. Xai-explainable artificial intelligence. Sci Robot. 4(37).

Hu YJ, Zhao G, Zhang MF, Bin B, Del Rose T, Zhao Q, Zu Q, Chen Y, Sun XK, de Jong M et al. 2020. Predicting densities and elastic moduli of sio2-based glasses by machine learning. Npj Comput Mater. 6(1).

Hung M, Voss MW, Rosales MN, Li W, Su WC, Xu J, Bounsanga J, Ruiz-Negron B, Lauren E, Licari FW. 2019. Application of machine learning for diagnostic prediction of root caries. Gerodontology. 36(4):395-404.

Kern C, Klausch T, Kreuter F. 2019. Tree-based machine learning methods for survey research. Surv Res Methods. 13(1):73-93.

Lauvahutanon S, Takahashi H, Shiozawa M, Iwasaki N, Asakawa Y, Oki M, Finger WJ, Arksornnukit M. 2014. Mechanical properties of composite resin blocks for cad/cam. Dent Mater J. 33(5):705-710.

Lawson NC, Bansal R, Burgess JO. 2016. Wear, strength, modulus and hardness of cad/cam restorative materials. Dent Mater. 32(11):E275-E283.

Lee C, Kashima K, Ichikawa A, Yamaguchi S, Imazato S. 2020. Influence of hydrolysis degradation of silane coupling agents on mechanical performance of cad/cam resin composites: In silico multi-scale analysis. Dent Mater J. 39(5):803-807.

Liu Y, Zhao TL, Ju WW, Shi SQ. 2017. Materials discovery and design using machine learning. J Materiomics. 3(3):159-177.

Mainjot AK, Dupont NM, Oudkerk JC, Dewael TY, Sadoun MJ. 2016. From artisanal

to cad-cam blocks: State of the art of indirect composites. J Dent Res. 95(5):487-495.

Marani A, Nehdi ML. 2020. Machine learning prediction of compressive strength for phase change materials integrated cementitious composites. Constr Build Mater. 265.

Nguyen JF, Migonney V, Ruse ND, Sadoun M. 2013. Properties of experimental urethane dimethacrylate-based dental resin composite blocks obtained via thermo-polymerization under high pressure. Dent Mater. 29(5):535-541.

Niem T, Youssef N, Wostmann B. 2020. Influence of accelerated ageing on the physical properties of cad/cam restorative materials. Clin Oral Invest. 24(7):2415-2425.

Ramprasad R, Batra R, Pilania G, Mannodi-Kanakkithodi A, Kim C. 2017. Machine learning in materials informatics: Recent applications and prospects. Npj Comput Mater. 3.

Ruse ND, Sadoun MJ. 2014. Resin-composite blocks for dental cad/cam applications. J Dent Res. 93(12):1232-1234.

Schabbach LM, Bondioli F, Fredel MC. 2013. Color prediction with simplified kubelka-munk model in glazes containing fe2o3-zrsio4 coral pink pigments. Dyes Pigments. 99(3):1029-1035.

Schwendicke F, Samek W, Krois J. 2020. Artificial intelligence in dentistry: Chances and challenges. J Dent Res. 99(7):769-774.

Shan T, Tay FR, Gu L. 2021. Application of artificial intelligence in dentistry. J Dent Res. 100(3):232-244.

Sideridou I, Tserki V, Papanastasiou G. 2002. Effect of chemical structure on degree of conversion in light-cured dimethacrylate-based dental resins. Biomaterials. 23(8):1819-1829.

Song YQ, Lindsay J, Zhao Y, Nasiri A, Louis SY, Ling J, Hu M, Hu JJ. 2020. Machine learning based prediction of noncentrosymmetric crystal materials. Comp Mater Sci. 183.

Tso WW, Burnak B, Pistikopoulos EN. 2020. Hy-pop: Hyperparameter optimization of machine learning models through parametric programming. Comput Chem Eng. 139.

Tsujimoto A, Barkmeier WW, Takamizawa T, Latta MA, Miyazaki M. 2017. Influence of thermal cycling on flexural properties and simulated wear of computer-aided design/computer-aided manufacturing resin composites. Oper Dent. 42(1):101-110.

Ward L, Agrawal A, Choudhary A, Wolverton C. 2016. A general-purpose machine learning framework for predicting properties of inorganic materials. Npj Comput Mater. 2.

Xiong J, Shi SQ, Zhang TY. 2020. A machine-learning approach to predicting and understanding the properties of amorphous metallic alloys (vol 187, 108378, 2020). Mater Design. 191.

Yamaguchi S, Katsumoto Y, Hayashi K, Aoki M, Kunikata M, Nakase Y, Lee C, Imazato S. 2020. Fracture origin and crack propagation of cad/cam composite crowns by combining of in vitro and in silico approaches. J Mech Behav Biomed Mater. 112:104083.

Yamaguchi S, Lee C, Karaer O, Ban S, Mine A, Imazato S. 2019. Predicting the debonding of cad/cam composite resin crowns with ai. J Dent Res. 98(11):1234-1238.

Yan W, Renteria C, Huang Y, Arola DD. 2021. A machine learning approach to investigate the materials science of enamel aging. Dent Mater.

Yang L, Shami A. 2020. On hyperparameter optimization of machine learning algorithms: Theory and practice. Neurocomputing. 415:295-316.

Yao J, Li J, Wang Y, Huang H. 2014. Comparison of the flexural strength and marginal accuracy of traditional and cad/cam interim materials before and after thermal cycling. J Prosthet Dent. 112(3):649-657.

Zhang ZY, Shi JC, Yu TY, Santomauro A, Gordon A, Gou JH, Wu DZ. 2020. Predicting flexural strength of additively manufactured continuous carbon fiber-reinforced polymer composites using machine learning. J Comput Inf Sci Eng. 20(6).

Zhi L, Bortolotto T, Krejci I. 2016. Comparative in vitro wear resistance of cad/cam composite resin and ceramic materials. J Prosthet Dent. 115(2):199-202.