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Feasibility of near-infrared spectroscopy for online multiple trait assessment of sawn lumber

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Abstract Near-infrared (NIR) spectroscopy coupled with multivariate analysis was applied to estimate multiple traits of sawn lumber. The effects of the lumber conveying speed (LCS) and measurement resolution of spectra (MRS) on the calibrations were examined. NIR spectra ranging from 1300 to 2300 nm were acquired at LCSs of 10, 20, and 30 m/min and at MRSs of 2, 4, and 16 nm. Prediction models of bending strength (F_b), modulus of elasticity in bending tests (E_b), dynamic modulus of elasticity (E_{tr}), and wood density (DEN) were developed using partial least-squares (PLS) analysis. LCS and MRS did not significantly influence the calibration performance for any wood property. The regression coefficients also showed no clear differences for any of the conditions. This indicates that the important explanatory variables included in the models are not greatly influenced by these measurement conditions. PLS2 analysis results, when presented graphically, allowed easy interpretation of the relationships between wood mechanical properties and chemical components, e.g., bending strength and stiffness were mainly related to polysaccharides cellulose and hemicellulose. NIR spectroscopy has considerable potential for online grading of sawn lumber, despite the harsh measurement conditions.

Key words Near-infrared spectroscopy · Mechanical stress grading · Bending strength · Cellulose · Japanese larch

Introduction

Wood products used as construction materials require a high degree of structural performance and reliability, and

hence mechanical stress grading is necessary to ensure structural reliability.^{1,2} Current methods for grading structural lumber include visual stress rating and machine stress rating, but both grading methods have some inherent limitations.^{1,3} Visual grading is less precise and is time-consuming. Machine stress grading can evaluate strength more precisely and efficiently than visual grading, but it can detect only the modulus of elasticity. A device for multiple trait assessment would be useful for evaluation of wood strength properties that are affected by a number of factors.⁴ Hence, increased demand for high-performance lumber has led to greater demand for enhanced grading techniques.

Near-infrared (NIR) spectroscopy, a fast-growing technique for nondestructively evaluating organic materials, has found widespread use in variety of industries.⁵ Previous studies have demonstrated that NIR spectroscopy could be successfully applied to the rapid analysis of various wood characteristics.⁶ With regard to mechanical properties, Thumm and Meder,⁷ Gindl et al.,⁸ Kelley et al.,⁹ and Fujimoto et al.¹⁰ provided reasonable calibration models to predict wood stiffness and strength traits in many species using small clear specimens. Additionally, Meder et al.¹¹ and Fujimoto et al.¹² reported that NIR diffuse reflectance spectra could be used to estimate the stiffness of full-length lumber with large dimensions. Consequently, NIR spectroscopy appears to have considerable potential for online grading of solid wood products.

In our previous report,¹³ we examined the feasibility of NIR spectroscopy for online stress grading using diffuse reflectance spectra from static and moving lumber. Models for the prediction of several wood properties, such as bending strength and modulus of elasticity, were superior in the moving condition than in the static condition because NIR spectra acquired at multiple measurement points along the length of the lumber are more representative of the lumber variability than spectra obtained at only one or two positions. As the next step, it is necessary to confirm the applicability of NIR methods from the viewpoint of practical use in the wood industry. In actual wood manufacturing plants, lumber products are streamed as quickly as possible along the process lines; thus, the inspection of lumber

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quality should be done rapidly. Meglen and Kelley¹⁴ pointed out that for effective process monitoring measurements of solid wood online, very rapid spectral acquisition times are required that are typically between 10 μ s and 1 s. We investigated the effects of the lumber conveying speed and measurement resolution of NIR spectra on the calibration performance.

Materials and methods

Sample materials and measurements of mechanical properties

A total of 102 Japanese larch (*Larix kaempferi*) boards with dimensions of 30 (radial) \times 100 (tangential) \times 1000 (longitudinal) mm were prepared for the mechanical tests and NIR experiments. Detailed information about sample origin and processing procedures was described in our previous article.¹³ After kiln drying, board surfaces (tangential surfaces) were planed by a molder. The average moisture content was 10.6 %. The traits investigated in this study were the bending strength (F_b), modulus of elasticity in bending tests (E_b), dynamic modulus of elasticity (E_{fr}), and air-dried wood density (DEN). The testing procedures for each trait were also the same as in the previous study. In brief, the test span of static four-point bending was set at 630 mm and the load was applied at two points, located equidistant from the midspan. F_b and E_b were calculated according to the provisions of ISO standards.¹⁵ E_{fr} was measured using the longitudinal vibration method.¹⁶

NIR measurements

Figure 1 shows the NIR measurement setup. Diffuse reflectance spectra were acquired with a MATRIX-F spectrometer (Bruker Optics) equipped with a contact-free NIR illumination and detection head. The working distance was 170 mm. The NIR spectra were obtained over the wavelength range 1300 to 2300 nm. Sample boards were placed on a belt conveyer and average spectra were acquired along the entire length of the sample. Spectral measurements were conducted at various conditions; the outline of each condition is shown in Table 1. From 4 to 16 scans were collected and averaged into a single average spectrum. For TEST_1, the lumber conveying speed (LCS) was set at 10,

20, and 30 m/min. Reduction of spectral resolution will lead to a shortened acquisition time.^{13,17} Thus, we examined the effect of resolution on the calibrations by setting the measurement resolution of spectra (MRS) at 2, 4, and 16 nm in TEST_2. In these experiments, LCS was fixed at 20 m/min.

Statistical analysis

All spectral data were split randomly into the calibration or validation sets, which consisted of 68 and 34 samples, respectively. Sample set parameter values are summarized in Table 2. In previous research, we found that there was no clear evidence for improvement of the prediction accuracy for models with spectra preprocessing.¹³ It is well known that the second derivative treatment can remove both baseline offset and slope from a spectrum and can help resolve nearby peaks and sharpen spectral features. To discuss how calibration models predict wood mechanical traits in relation to the spectral features, only the second-derivative spectra were used in the following analyses. Second-derivative spectra were obtained using the Savitzky-Golay algorithm¹⁸ with a 21-point window and a second-order polynomial. However, the smoothing points were reduced to 11 and 3 points in the case of MRS at 4 and 16 nm, respectively, because using these conditions, the number of data points was low.

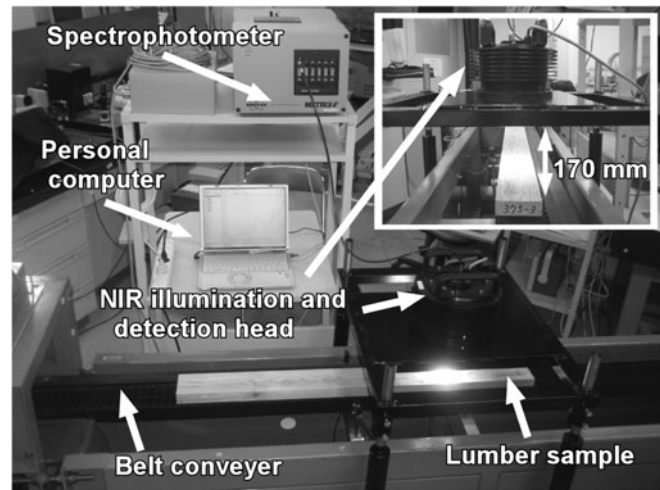


Fig. 1. Experimental setup for measurements of near-infrared (NIR) diffuse reflectance spectra

Table 1. Outline of the measurement conditions

	Lumber conveying speed (LCS) (m/min)	Measurement resolution of spectra (MRS) (nm)	Number of scans	Acquisition time (s)
TEST_1	10	2	16	6.0
	20	2	8	3.0
	30	2	4	2.0
TEST_2	20	2	8	3.0
	20	4	12	3.0
	20	16	16	3.0

Table 2. Summary of wood properties of lumber samples for calibration and prediction sets

Wood property	Calibration set ($n = 68$)				Prediction set ($n = 34$)			
	Mean	Min	Max	SD	Mean	Min	Max	SD
F_b (MPa)	84.4	31.8	131.3	23.9	82.8	35.1	130.6	22.9
E_b (GPa)	12.75	4.88	20.14	3.35	12.77	5.63	19.40	3.36
E_{fr} (GPa)	13.56	5.12	21.23	3.68	13.37	5.98	20.16	3.49
DEN (kg m^{-3})	556	382	721	67	549	412	684	61

Sample number of prediction set for E_{fr} was 33

F_b , bending strength; E_b , modulus of elasticity in bending; E_{fr} , dynamic modulus of elasticity; DEN, air-dry wood density; SD, standard deviation

Table 3. Correlation coefficients among wood properties

	F_b	E_b	E_{fr}	DEN
F_b	1.00			
E_b	0.92	1.00		
E_{fr}	0.90	0.99	1.00	
DEN	0.83	0.87	0.87	1.00

Partial least-squares (PLS) regression was used to develop all prediction models.^{19,20} There are two types of PLS algorithm, namely PLS1 and PLS2. The former deals with only one response variable at a time and the latter handles several responses simultaneously.¹⁹ First, the models for each trait were built through the PLS1 algorithm. Highly significant correlations were found among all the traits (Table 3). Thus, the PLS2 analysis was also performed by putting all traits into the Y-matrix. When the PLS2 models were constructed, weighting the Y-matrix values by the inverse of their standard deviations compensated for the large differences in the magnitude of each trait value. The final number of factors selected for incorporation into the model was chosen to minimize the residual variance when using full cross-validation. All data analyses were performed using Unscrambler software version 9.6 (CAMO AS, Norway).

Results and discussion

Near-infrared spectra

Figure 2 shows NIR diffuse reflectance raw spectra (Fig. 2a,c) and their second-derivatives (Fig. 2b,d) obtained from Japanese larch lumber samples. All spectral lines indicate the average of all samples. Assignments related to specific wood components have been reported by a number of authors.^{21–27} Wood-specific absorption bands are labelled in Fig. 2, and their assignments are summarized in Table 4.

Trends of the raw and second-derivative spectra were quite similar and were independent of LCS, and thus, typical absorption bands associated with chemical components of wood were stable for each condition (Fig. 2a,b). This fact strongly suggests that the intrinsic information about wood substances can be detected by NIR spectroscopy even when the sample lumbars move at “high” speed in a lumber production line. As mentioned above, another

possible solution for the issue of shortening the inspection time may be to reduce the resolution of spectra acquisition. Although a few weak absorption bands were unable to be clearly observed at an MRS of 16 nm, the main absorption bands still could be seen (Fig. 2c,d). Schimleck et al.¹⁷ measured NIR spectra changing the spectral sampling interval (SSI) from 2 to 64 nm and reported that differences between NIR spectra were small for SSIs of 2, 4, 8, and 16 nm.

PLS1 modeling for each wood property and their regression coefficients

Calibration models for each wood property were developed for various conditions using PLS1 analyses. Statistical results are summarized in Tables 5 and 6. Figure 3 shows the relationship between laboratory-measured and NIR-predicted values for each property for an LCS of 20 m/min.

Calibration performance for all traits showed no clear dependence on LCS or MRS (Tables 5 and 6). The calibrations of all wood properties had relatively strong relationships between laboratory-measured and NIR-predicted values, with coefficients of determination (r^2) ranging from 0.62 to 0.77. The calibration equations were applied to the prediction set of 34 specimens and it was found that predictions of the respective wood properties were also well fitted, with coefficients of determination (r_p^2) ranging from 0.54 to 0.83. The error terms, i.e., standard error of cross-validation (SECV) and standard error of prediction (SEP), showed similar values to those found in previous reports.¹³ Models of each trait were well fitted over a wide range of variation (Fig. 3). The ratio of performance to deviation (RPD), calculated as the ratio of the standard deviation of the reference data to SEP, was good enough in the practical sense, ranging from 1.70 to 2.36. An RPD of greater than 2.5 is considered satisfactory for screening;²⁸ however, it has been shown that with an RPD of approximately 1.5, NIR spectroscopy can be used as an initial screening tool.²⁹ The calibrations presented in this study demonstrate that NIR spectroscopy can meet the demands of rapid inspection in wood product manufacturing.

Meglen and Kelley¹⁴ examined the effect of decreased spectral resolution on calibrations developed for the stiffness and modulus of rupture. Sampling intervals up to 32 nm did not have a large negative effect on the coefficient of determination. This fact supports our results. Schimleck

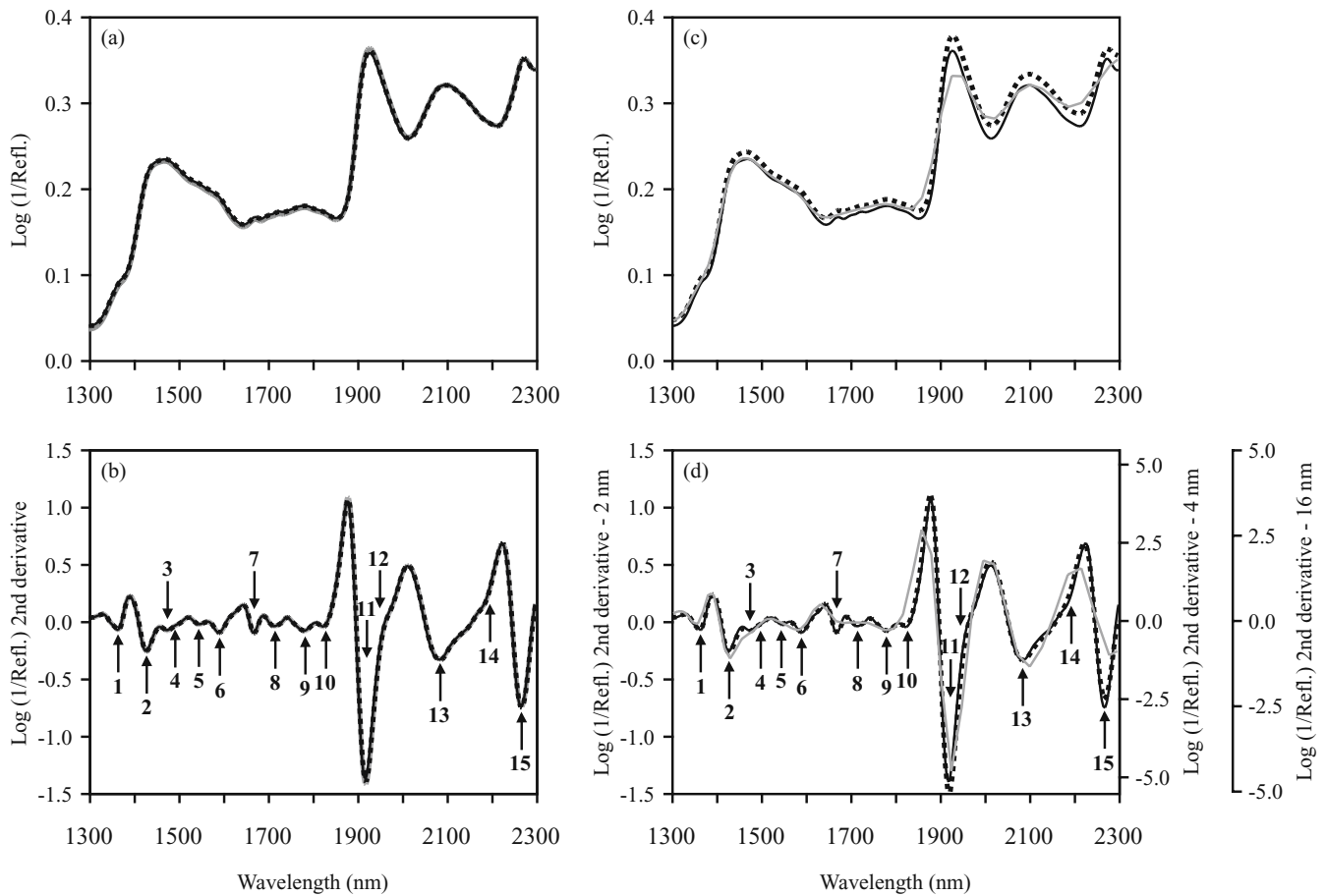


Fig. 2. NIR diffuse reflectance (*Refl*) raw spectra (**a** and **c**) and their second-derivative spectra (**b** and **d**). In **a** and **b**, the *solid*, *dashed*, and *gray* lines indicate lumber conveying speeds (LCSs) of 10, 20, and 30 m/min, respectively, with measurement resolution of spectra (MRS) of

2 nm. In **c** and **d**, the *solid*, *dashed*, and *gray* lines indicate MRSs of 2, 4, and 16 nm, respectively, with an LCS of 20 m/min. All spectral lines indicate the average of all samples. Important absorption bands are labeled and are described in Table 4

Table 4. Assignment of the near-infrared absorption bands from Japanese larch lumber

	Wavelength (nm)	Assignment	Reference
1	1366	2×CH str. + CH def., cellulose	19
2	1428	OH str. first overtone, amorphous regions in cellulose and H ₂ O	20
3	1450	OH str. first overtone, CH str. + CH def., lignin	21
4	1489	OH str. first overtone, crystalline regions in cellulose	19
5	1548	OH str. first overtone, crystalline regions in cellulose	20
6	1592	OH str. first overtone, crystalline regions in cellulose	20
7	1672	CH str. first overtone, aromatic groups in lignin	22
8	1724	CH str. first overtone, furanose/pyranose due to hemicellulose	22
9	1780	CH str. first overtone, semi-crystalline or crystalline regions in cellulose	23
10	1830	OH str. + 2×CO str., semi-crystalline or crystalline regions in cellulose	22
11	1916	OH str. + OH def., H ₂ O	24
12	1940	OH str. + OH def., H ₂ O	24
13	2080	OH str. + CH def., semi-crystalline or crystalline regions in cellulose	25
14	2200	CH str. + C = O str., -CHO	25
15	2270	CH str. + OH str., cellulose	23

Numbers in the first column correspond to those in Figs. 2, 4, and 5
str., stretching; def., deformation

et al.¹⁷ investigated the same trials and reported that the quality of the calibrations associated with the various wood properties was affected to different degrees as the resolution decreased: the microfibril angle calibration was the most affected, whereas the air-dry density was the least

affected. Such a tendency was not found in our study. Since general trends of the regression coefficients showed the same pattern for all traits, results for E_b are shown in Fig. 4. Important absorption bands are labeled and are described in Table 4.

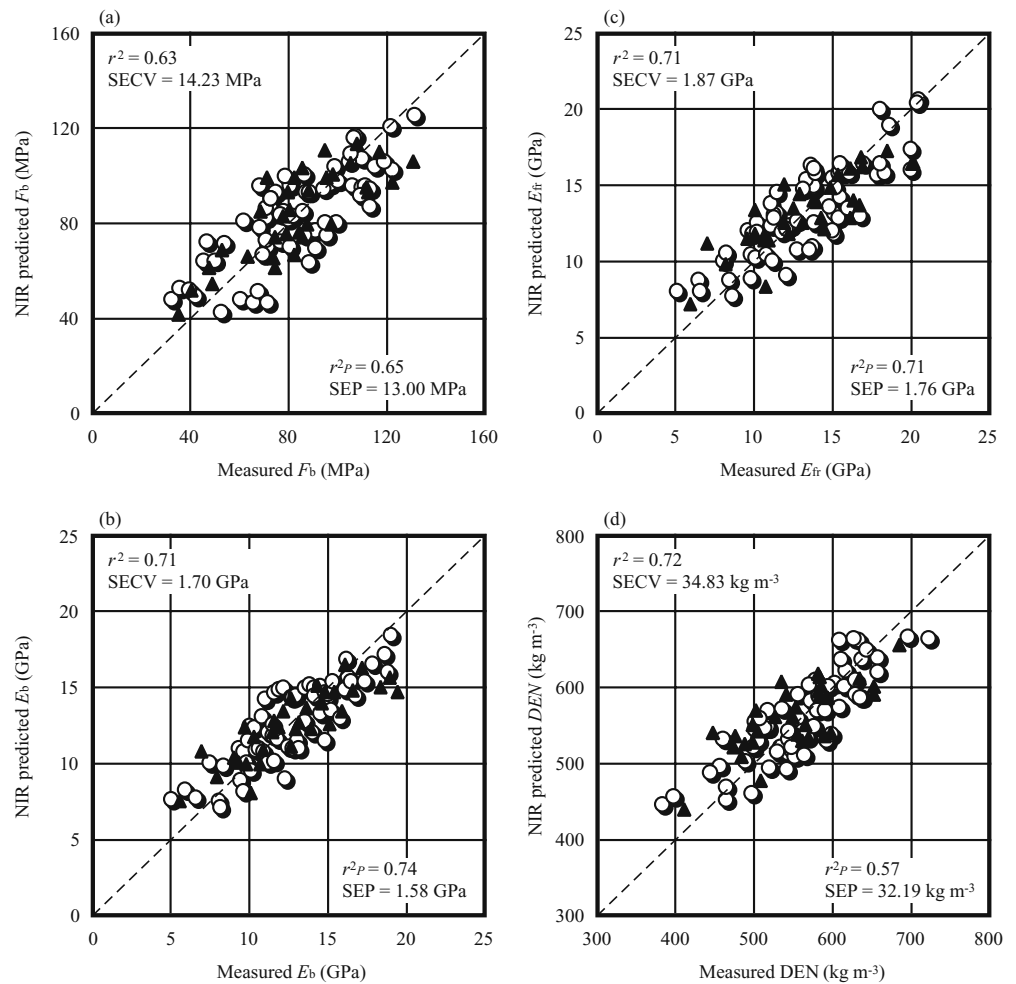
Table 5. Results of PLS1 modeling for each wood property for various lumber conveying speeds

	LCS (m/min)	Calibration set			Prediction set		
		Factor	r^2	SECV	r_p^2	SEP	RPD
F_b (MPa)	10	6	0.63	14.6	0.61	14.0	1.71
	20	6	0.63	14.2	0.65	13.0	1.84
	30	5	0.63	14.2	0.64	14.1	1.70
E_b (GPa)	10	4	0.74	1.62	0.64	1.64	2.05
	20	3	0.71	1.70	0.74	1.58	2.13
	30	5	0.72	1.63	0.65	1.62	2.07
E_{tr} (GPa)	10	4	0.75	1.80	0.69	1.89	1.95
	20	3	0.71	1.87	0.71	1.76	2.10
	30	6	0.76	1.77	0.74	1.76	2.09
DEN (kg m^{-3})	10	3	0.67	36.4	0.54	37.5	1.78
	20	3	0.72	34.8	0.57	32.2	2.08
	30	5	0.67	34.9	0.61	34.9	1.91

The measurement resolution of spectra was fixed at 2 nm in all cases

LCS, lumber conveying speed; r^2 , coefficient of determination from cross-validation; SECV, standard error of cross-validation; r_p^2 , coefficient of determination for prediction set; SEP, standard error of prediction; RPD, ratio of performance to standard deviation

Fig. 3. Measured versus NIR-predicted value plots for **a** bending strength (F_b), **b** modulus of elasticity in bending (E_b), **c** dynamic modulus of elasticity (E_{tr}), and **d** wood density (DEN) for an LCS of 20 m/min. The *open circles* indicate the calibration set and *filled triangles* indicate the prediction set. SECV, standard error of cross-validation; SEP, standard error of prediction



There were also no clear differences in regression coefficients for any measurement condition. Substantial NIR absorptions could be found even at a resolution of 16 nm, which was the worst-case measurement scenario. These results are consistent with Fig. 2 and indicate that important

explanatory variables included in the models are not strongly influenced by the measurement conditions. There were significant negative regression coefficients at wavelengths related to cellulose, which is the skeletal substance of the cell wall (1, 4–6, 9, 10, 13, and 15). This fact explains

Table 6. Results of PLS1 modeling for each wood property in the various measurement resolutions of spectra

	MRS (nm)	Calibration set			Prediction set		
		Factor	r^2	SECV	r_p^2	SEP	RPD
F_b (MPa)	2	6	0.63	14.2	0.65	13.0	1.84
	4	5	0.62	14.5	0.73	12.5	1.92
	16	6	0.64	13.9	0.72	12.3	1.94
E_b (GPa)	2	3	0.71	1.70	0.74	1.58	2.13
	4	3	0.73	1.67	0.73	1.70	1.98
	16	3	0.70	1.82	0.79	1.52	2.21
E_{fr} (GPa)	2	3	0.71	1.87	0.71	1.76	2.10
	4	3	0.76	1.75	0.69	1.75	2.11
	16	6	0.77	1.68	0.83	1.55	2.37
DEN (kg m^{-3})	2	3	0.72	34.8	0.57	32.2	2.08
	4	3	0.70	36.3	0.58	37.1	1.80
	16	3	0.70	36.5	0.63	32.1	2.08

The lumber conveying speed was 20 m/min in all cases
MRS, measurement resolution of spectra

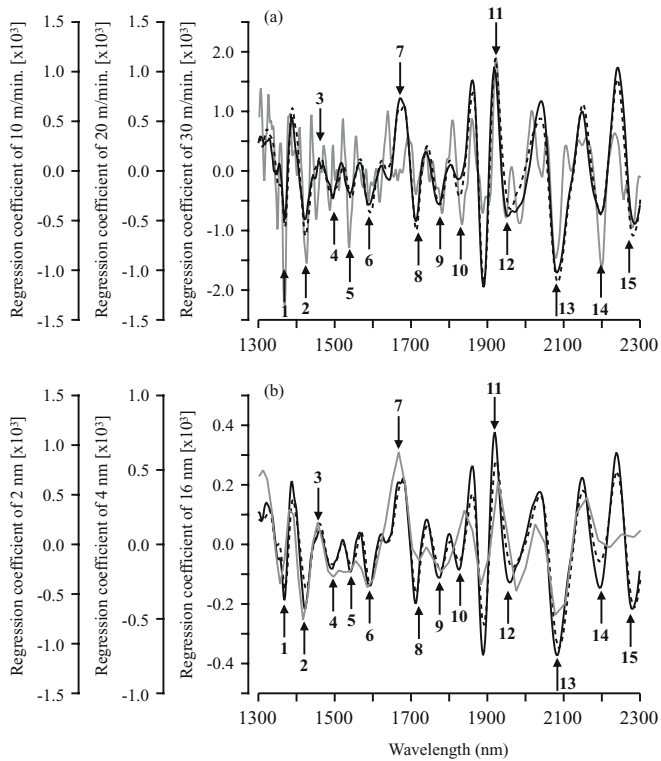


Fig. 4. Regression coefficients for the partial least-squares (PLS) models predicting the modulus of elasticity (E_b). In panel **a**, the *solid*, *dashed*, and *gray* lines indicate LCSs of 10, 20, and 30 m/min, respectively. In panel **b**, the *solid*, *dashed*, and *gray* lines indicate MRSs of 2, 4, and 16 nm, respectively. Important absorption bands are labeled and are described in Table 4

that increases in cellulose are related to increased wood stiffness.^{10,12} The matrix substance of the cell wall, i.e., lignin and hemicelluloses, showed significant regression coefficients at 3, 7, and 8. High negative and positive regression coefficients were observed at the OH absorption bands due to water (2, 11, and 12).

Table 7. Results of PLS2 modeling for each wood property

	Calibration set			Prediction set		
	Factor	r^2	SECV	r_p^2	SEP	RPD
F_b (MPa)	3	0.54	16.0	0.57	14.8	1.62
E_b (GPa)	3	0.71	1.80	0.74	1.66	2.02
E_{fr} (GPa)	3	0.73	1.93	0.73	1.79	2.05
DEN (kg m^{-3})	3	0.66	38.7	0.57	35.7	1.87

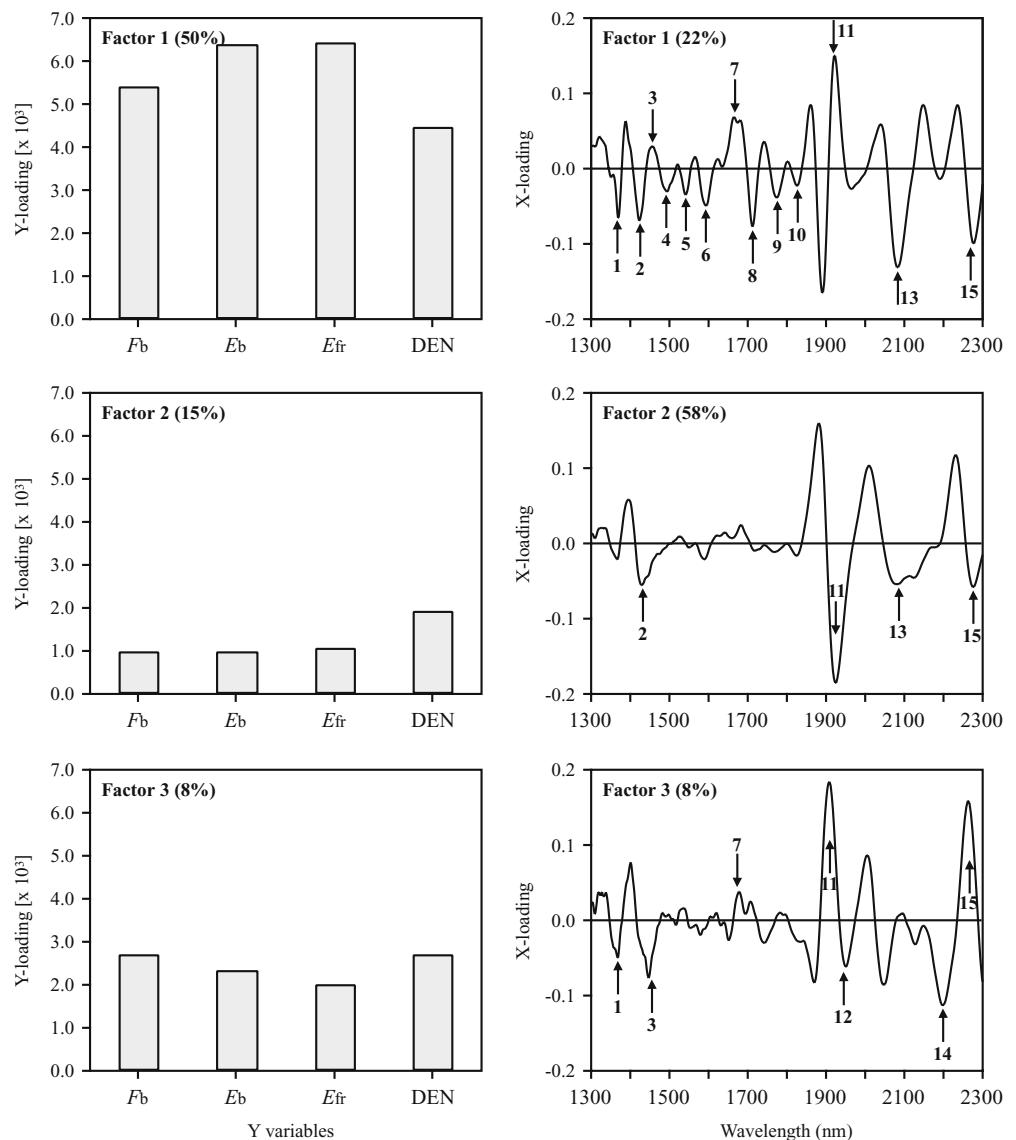
The lumber conveying speed was 20 m/min and the measurement resolution of spectra was 2 nm

PLS2 modeling for each wood property

All mechanical stress grading systems are based on the use of predictors to estimate strength (F_b) properties.³ The most common predictor for grading lumber is the modulus of elasticity, i.e., the stiffness (E_b and E_{fr}), because there are very close relationships between stiffness and strength in general (see also Table 3). Additionally, stiffness is the only structural property of wood that can be practically determined by a nondestructive method. However, NIR spectroscopy may be able to directly estimate strength by combining all kinds of predictors. A PLS2 analysis that can operate on all property data simultaneously was performed.

Table 7 shows the results of PLS2 modeling for each property. PLS2 analysis was conducted at an LCS of 20 m/min and an MRS of 2 nm. The results were similar to those of the PLS1, except for the F_b , which showed a slight decline of calibration performance (see Tables 5 and 7). There is no consensus on whether multiresponse modeling (PLS2) can achieve better predictive performance than independent modelling (PLS1).³⁰ Actually, PLS1 usually gives more precise models.^{19,31,32} Nevertheless, PLS2 gives models with similar predictive abilities to PLS1 when the dependent variables are strongly correlated, as was found in this study.^{19,33}

Fig. 5. X- and Y-loading plots for the first three PLS factors resulting from the PLS2 analysis. Important absorption bands are labeled and are described in Table 4



Although PLS2 analysis could not improve the calibration performances for all traits, it is easy to graphically reveal the relationship among X variables (NIR spectra) and Y variables (wood properties).³⁴ Figure 5 shows the X- and Y-loading plots for the first three factors from PLS2 analysis. The first factor explains the large amount of variance in both X (22%) and Y (50%) matrices and was mainly related to mechanical properties (F_b , E_b , and E_{fr}) rather than to wood density (DEN). There were many absorption bands related to wood components in the X-loading of factor 1. Absorptions due to cellulose and hemicellulose (1, 2, 4–6, 8–10, 13, and 15) showed constant negative loading, and absorptions due to lignin (3 and 7) and water (11) showed positive loading. These findings could clearly explain that polysaccharides are positively related to wood mechanical properties. The second factor also explains a considerable amount of variance in both X (58%) and Y (15%) matrices, but this factor was mainly related to wood density. The X-loading of factor 2 indicated that wood density is positively related to water content (2 and 11), which is in agree-

ment with a previous article.¹⁰ The third factor could not add significant further explanation of variance in either X (8%) or Y (8%) matrices. The X-loadings of factor 3 show absorptions due to cellulose (1 and 15) and lignin (3 and 7), but these were not uniform, showing both positive and negative values.

Conclusions

This study examined the effect of lumber conveying speed and measurement resolution of spectra on NIR calibration accuracy. Intrinsic information with regard to wood substances could be detected by NIR spectroscopy even at high speed and low resolution. Reasonable calibration models for predicting wood properties could be obtained under any of the conditions used. There were also no clear differences in regression coefficients for any measurement conditions, indicating that important explanatory variables included in

the models were not greatly influenced by restricted measurement conditions. PLS2 analysis might help to more easily understand the relationships between wood mechanical properties and the chemical components, although it could not achieve better predictive performance than PLS1. It was concluded that NIR spectroscopy could be applied to online grading of lumber quality.

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