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Exploring the potential of microscopic hyperspectral, Raman, and LIBS for nondestructive quality assessment of diverse rice samples

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Abstract

The enhancement of rice quality stands as a pivotal focus in crop breeding research, with spectral analysisbased non-destructive quality assessment emerging as a widely adopted tool in agriculture. A prevalent trend in this field prioritizes the assessment of effectiveness of individual spectral technologies while overlooking the influence of sample type on spectral quality testing outcomes. Thus, the present study employed Microscopic Hyperspectral Imaging, Raman, and Laser-Induced Breakdown Spectroscopy (LIBS) to acquire spectral data from paddy rice, brown rice, polished rice, and rice flour. The data were then modeled and analyzed with respect to the amylopectin and protein contents of the rice samples via regression methods. Correlation analysis revealed varying degrees of correlation, both positive and negative, among the three spectral techniques and the analytes of interest. LIBS and Raman spectroscopy demonstrated stronger correlations with the analytes compared to microscopic hyperspectral imaging. Based on the selected correlation variables, feature screening and regression modeling were conducted. The modeling results indicated that microscopic hyperspectral data modeling yielded the lowest coefficient of determination of $R^2 = 0.2$, followed by Raman data modeling result was higher than it, which was about 0.5. The modeling effect of polished rice is the best. LIBS data modeling performed best, with a coefficient of determination of 0.6. The influence of different sample types on the modeling results was less than that of Raman spectroscopy, and modeling results of grains were better. The feature matching analysis of Raman and libs spectroscopy techniques showed that there were spectral variables that could match amylopectin and protein in the features obtained by multiple modeling statistics, but some modeling variables failed to match. LIBS matched more variables than Raman. These findings provide valuable insights into the application effectiveness of different spectral techniques in detecting rice contents across diverse sample types.

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Keywords Rice quality detection, Raman, LIBS, Microscopic hyperspectral, Regression analysis

Introduction

Rice stands as one of the paramount food crops globally, supporting nearly half of the world's population [1]. With improvements in living standards, there has been a notable increase in the demand for high quality rice [2]. Rice quality critically influences consumer preferences and varietal breeding strategies, serving as a cornerstone for sustainable global food supply chains [3]. Starch and protein are two essential components that directly affect rice quality. Starch comprises 80-90% of the chemical composition of rice, with amylose and amylopectin being its primary constituents. The crystallinity and thermal stability of starch granules are critical factors influencing rice quality. Protein, the second most abundant component, accounts for approximately 6%~9% of the total rice content, and affects rice quality by regulating the gelatinization characteristics of rice starch. Consequently, the extraction, quantification, and analysis of starch and protein in rice constitute the cornerstone for increasing rice quality.

Spectral technologies have revolutionized crop analysis through non-destructive, rapid detection capabilities. Gámez et al. established hyperspectral reflectance-biomass correlations in alfalfa using full-band field spectroscopy [4], while Wanyu Li and colleagues developed a multispectral-driven "spectral-physiological-protein" model for monitoring rice grain protein dynamics. Concurrently, Zhang linked UAV-acquired vegetation indices to photosynthetic parameters across rice growth stages, enabling diurnal canopy photosynthesis prediction [5]. Hyperspectral imaging has distinguished itself as a prominent method for detecting quality attributes in agricultural products, boasting a plethora of spectral bands alongside high image resolution, providing extensive spectral and spatial information [6]. Microscopic hyperspectral systems synergize the analytical strengths of hyperspectral imaging and optical microscopy, enabling non-destructive characterization of micro-scale material properties. Yaodi Zhu et al. introduced a method for the rapid determination of spore germination utilizing microscopic hyperspectral imaging technology. By integrating spectral variables with imaging data to develop a predictive model, significantly enhanced the accuracy of forecasting spore germination [7].

Raman spectroscopy, a nondestructive technique leveraging inelastic light scattering, is renowned as fingerprint spectroscopy due to the unique Raman shifts dictated by molecular structures and vibrational modes. The intensity of Raman signals is directly proportional to the number of molecules participating in the scattering process, rendering it a suitable tool for the quantitative analysis of substances [8]. Gulce Ogruc Ildiz et al. utilized microscopic Raman spectroscopy in conjunction with principal component analysis to measure starch and protein contents in various maize kernel varieties [9]. while Wang et al. successfully identified rice samples of the same variety but from different producing areas using similar methodologies [10].

Laser-induced breakdown spectroscopy (LIBS) has recently become a significant technique for elemental analysis. It uses a laser pulse to create a plasma from the sample, which emits a characteristic spectrum. This spectrum is then analyzed by a high-resolution spectrometer to determine the elements and concentrations in the sample. It is a spectral technique capable of simultaneous and rapid analysis of multiple elements without the need for sample preparation [11]. Hou et al. proposed an inverse Fourier transform method based on LIBS for batch identification of rice seeds [12]. Milena R. Martelli et al. employed LIBS technology to investigate the cohesion of wheat grain tissue, highlighting the potential of LIBS for expediting structural analysis of plant materials [13].

While spectral techniques have exhibited significant potential for detecting crop quality, the utilization predominantly occurs individually in scenario-specific contexts, with a notable dearth of comparative analyses among distinct spectral methodologies within this domain. Furthermore, these applications generally focus on a particular sample type that undergoes processing, while the attention given to the original state samples and samples at each stage of processing remains limited [14– 17]. It is worthwhile to explore whether these different sample types affect the results of crop quality testing and whether they can provide information for nondestructive testing of crop quality. Therefore, investigating these aspects could hold the promise of exploring broader possibilities for the application of spectral techniques in the field of crop grain quality detection.

In summary, the study employed three spectral techniques to establish spectral-quality index regression models with four types of rice grain samples, respectively. Aiming to investigate the differences in various spectral methodologies and the influence of sample types on the outcomes of nondestructive rice quality assessment and serves as a valuable reference for the application of spectral technologies in advancing crop quality detection capabilities.

Materials and methods

Sample preparation

The study sourced 533 rice core germplasm resources from the Crop Phenotype Center of the National Key Laboratory of Crop Genetic Improvement at Huazhong Agricultural University. From this pool, 20 diverse rice varieties were randomly selected. For each variety, five seeds were designated as experimental paddy rice samples. Other seeds were then hulled to produce brown rice, from which another five seeds were selected as brown rice experimental samples. The remaining brown rice was milled to obtain polished rice, with five seeds per variety used as polished rice experimental samples. Lastly, the leftover polished rice was ground into flour, and $4 \sim 6$ g of this flour was compressed into round sheets for storage as rice flour experimental material.

Instruments and parameters

In this study, three distinct spectral detection instruments were utilized: the portable Raman spectrometer, the LIBS spectrometer and the microscopic hyperspectral spectrometer. These spectrographs were independently developed by the Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences, the Advanced Spectral Technology and Application Innovation Room.

The portable Raman spectrometer incorporates modular components including a laser, a dispersion unit, and an external optical path. It features a laser wavelength of 785 nm, an adjustable laser power up to 500mW, a spectral range of $200 \sim 2700$ cm-1, with a spectral resolution between 6 cm⁻¹ and 8 cm⁻¹. The integration time of the system is adjustable, ranging from 4 ms to 120 s. Signal-to-noise ratio > 3000:1, spectral stability of o/u < 0.5% (COT 8 h).

The LIBS system consists of a laser, an optical system, a spectrometer, a computer and a mobile power supply. The laser used is a Q-switched Nd: YAG solid-state laser (CFR200,Quantel, Paris, France) with a laser wavelength of 1064 nm, a beam diameter of 7.1 mm, a pulse width of 7.1 ns, a working frequency of 20 Hz, laser pulse energy of 200 mJ. The spectrometer uses a four-channel modular fiber optic spectrometer (LIBS2500+) with channel wavelength ranges of $186 \sim 304$, $300 \sim 402$, $400 \sim 487$, $485 \sim 1000$. The spectral integration time is 1ms.

The microscopic hyperspectral imager (CLH-M-D-1) consists of an integrated push-broom hyperspectral imaging module, a camera, a microscope, a halogen light source, and an externally connected computer. The hyperspectral module operates within a spectral range of $400 \sim 1000$ nm, a spectral resolution > 2.8 nm, a spatial resolution > 1 µm, with a total of 300 spectral channels and 480 spatial channels incorporated. The microscope provides a field of view ranging from 0.22 to 4.4 mm. The

detector employed is a CMOS sensor, and the illumination system utilizes a 12 V/100 W halogen lamp.

The PertenDA7250 near-infrared grain analyzer was employed to quantify the percentages of amylopectin and protein content in rice samples. The instrument features a wavelength rang of $950 \sim 1650$ nm, an adjustable spectral resolution ranging from 0.1 to 10 nm, a scan duration of 15 s per scan, and an analysis time of six seconds.

Technical route of the study

This section outlines the technical approach employed in this research, including sample preparation, spectral acquisition, parameter extraction, rice quality index determination, and model development (Fig. 1). Sample processing involves a series of steps to convert paddy rice into rice flour. The spectral data were acquired via three different spectral systems. Following acquisition, these spectral datasets are analyzed to extract relevant spectral parameters. The rice quality index was quantified using a precise near-infrared grain analyzer. Ultimately, a regression model is developed, with the extracted spectral parameters serving as independent variables and the rice quality index as the dependent variable.

Spectral data collection and quality index measurement *Microscopy hyperspectral spectral data acquisition*

The sample was placed on a glass slide, aligned with the light source and lens, and the appropriate objective lens magnification was adjusted before signal acquisition. Spectral curves and image data were collected at 5X, 10X, 20X, and 50X objective lens magnifications for each sample. For each type of paddy rice, brown rice, and milled rice, 20 sets of replicates were performed, with 5 samples per variety. For rice flour samples, a single sample was utilized for each variety, resulting a total of 5 sets of replicates.

Raman spectral data acquisition

The acquisition instrument was set up with a laser power of 200mW, an integration time of 5 s, and a peak-seeking threshold of 30. It featured automated baseline correction during spectrum acquisition. The samples were placed on a flat surface, and the handheld Raman laser probe was aligned vertically with the target sample for detection. Spectral acquisition was performed at 5 different positions for each sample to ensure comprehensive coverage. For each type of paddy rice, brown rice, and polished rice, 25 sets of replicates were conducted, with 5 samples per variety. For rice flour samples, a single sample was used for each variety, resulting in 5 sets of replicates.

LIB spectral data acquisition

For LIBS data acquisition, the laser output energy focused on the sample was set to 106 mJ, with an output



Fig. 1 Technical route of the study. The comprehensive process encompasses the refinement of raw materials, acquisition of spectral signals, processing of spectral data, correlation analysis between rice quality indices and spectral data, and the development of regression models

pulse frequency of 20 Hz. The integration time of the spectrometer was set to 1 ms, and the integration delay was set to 1 μ s to ensure a stable plasma. The sample was securely positioned at the laser port, and the laser was activated in continuous excitation mode for spectral acquisition. Each sample was subjected to five consecutive laser pulses, resulting in the acquisition of five spectral curves as replicate measurements. In total, there were 25 replicate samples for each category of paddy rice, brown rice, and polished rice across all varieties, as well as 5 replicate samples of rice flour.

Determination of rice quality index

The rice flour samples were dispensed into the detection tanks, filling them to capacity. A total of 3 detection tanks were prepared for each variety to ensure triplicate repetitions. Each filled detection tank was then placed into the near-infrared grain analyzer, and the appropriate model was selected to initiate the quality index detection process.

Data processing and analysis

Spectral data preprocessing and parameter extraction

The microscopic hyperspectral data was analyzed using ENVI5.3 software, with all pixels in the captured images defined as the region of interest (ROI), considering the sample target size. Spectral parameters including reflectivity (R), its first and second derivatives (d(R) and dd(R)), and logarithm (lg(R)) were computed and normalized to unit vectors for subsequent analysis.

Raman spectral data visualization was conducted using RamanTools software. Given the inherent weakness and susceptibility of Raman scattering signals to various influences, a manual screening process excluded anomalous spectral signals [18]. Savitzky-Golay (SG) filtering with a window size of 7 and polynomial order of 3 was applied to enhance the signal-to-noise ratio, smoothing the spectral data and improving its quality.

Raman intensity (I), its derivatives (d(I) and dd(I)), and logarithm (lg(I)) were calculated as spectral indices for regression analysis, providing valuable information about the chemical bonds and molecular structures present in the samples. These indices were then integrated and normalized using the maximum value position in each sample as the benchmark. This normalization accounted for deviations from external factors or intramolecular interactions affecting Raman signal intensity. To amplify intersample differences and facilitate accurate comparison, data scaling was applied across different varieties due to the low signal intensity and crucial intensity variations among them. This step enabled more precise correlation and quantitative analyses, identifying key differences in chemical composition and structure.

In LIBS laser ablation excitation, spectral signals are susceptible to interferences from instrumentation, background, and sample properties, which can cause deviations in results [19]. To address these challenges, outlier removal using triple standard deviation and noise filtering via SG (Savitzky-Golay) smoothing with a window size of 7 and polynomial order of 3 are applied. There is a linear relationship between the intensity of the elemental spectral lines and the concentration of the analyte without self-absorption. Therefore, the spectral intensity (C) is used as the available spectral variable. Additionally, the logarithm of intensity (lg(C)), first derivative of intensity (d(C)), and second derivative of intensity (dd(C)) were calculated as spectral indices for regression analysis.

All spectral indices undergo integration and unit vector normalization to ensure that they were on a comparable scale. Data scaling was also indispensable among different varieties to amplify inter-sample differences and facilitate accurate comparison.

Correlation analysis between spectral data and quality indicators

To efficiently identify pertinent variables, Pearson correlation coefficients were calculated between the spectral characteristics of paddy rice, brown rice, polished rice, and rice flour and the contents of amylopectin and protein. Variables with high correlations, defined by a threshold of 0.2, were retained, while those with lower correlations are filtered out. These retained variables were then utilized in subsequent regression analyses.

Regression modeling of spectral data and quality indicators

Regression modeling were performed separately for amylopectin and protein content of rice, using spectral parameters of distinct spectral types as independent variables. Given the sample size constraint of this study, the selection of modeling techniques is crucial.

These regression methods were employed in this study: Adaptive Boosting (AdaBoost) regression: A sequential ensemble method that leverages machine learning to create a robust predictor by randomly integrating weak learners from the dataset [20]. AdaBoost regression possesses strong applicability and resistance to overfitting, making it ideal for studies with limited sample sizes [21].

Bayesian regression: A machine learning algorithm that integrates Bayesian statistics with linear modeling. It exhibits excellent applicability for scenarios with scarce data and inadequate prior knowledge [22]. Least absolute shrinkage and selection operator (Lasso) regression: This method applies an L1 penalty term to the partial least squares (PLS) model to identify and filter out irrelevant variables, achieving better performance than PLSR [23]. Ridge regression: A biased estimation method for analyzing multicollinearity data, tailored for multicollinearity data, sacrifices some least squares unbiasedness for practicality, enhancing model simplicity and robustness [24].

In addition, linear regression, as the most common regression method, served as a comparison and reference in this study to ensure a comprehensive and objective analysis of the relationship between spectral data and quality indicators of rice. Given the constraints of the sample size in this study, it is imperative to limit the number of independent variables in the model to prevent overfitting. Adhering to the principle that the number of variables should not exceed one-tenth of the sample size, 1–2 modeling variables were selected. These variables were determined through the Competitive Adaptive Reweighted Sampling (CARS) feature selection method. Following the CARS feature screening process, it is often the case that a relatively large number of variables are identified. If the number of filtered variables exceeds two, a subset of 1–2 variables were selected randomly and cyclically for model construction.

For regression modeling, a five-fold cross-validation approach was adopted. The dataset was divided into five equal groups, each containing four samples, where four groups were used as training data and the remaining group as testing data. This procedure was repeated five times, ensuring that each group served as the test set once, and the average value was taken as the final modeling result. Performance metrics, including the coefficient of determination (\mathbb{R}^2), root mean square error ($\mathbb{R}MSE$), and relative prediction deviation ($\mathbb{R}PD$), were computed for both the training and test sets based on the predicted and actual values.

All analyses were carried out in a Python 3.7 environment, utilizing libraries such as Scikit-learn, NumPy, and Pandas to ensure computational efficiency and facilitate data manipulation.

Results and discussion

Microscopic hyperspectral original curve

The microscopic hyperspectral reflectance curves of 20 varieties of paddy rice, brown rice, polished rice, and rice flour samples exhibited a consistent trend across different treatments but vary in peak reflectance (Fig. 2). Specifically, paddy rice displayed lower reflectance due to the rough surface texture. Conversely, rice flour, with a smooth surface, enhanced reflectance peaks. Brown and polished rice show only minor differences in their reflectance curves. There are noticeable disparities in the spectral curves among different varieties of the same type of samples, particularly within the 500~700 nm range. These distinct reflectance and radiation characteristics of various materials could be attributed to molecular, atomic, and ionic lattice vibrations. Even within the same biological tissue, structural and compositional differences lead to unique reflectance spectra [25]. Therefore, the variations observed in the reflectance curves reflect the intricate differences in the structure and composition of various rice types and varieties.



Fig. 2 Reflectance curves of microscopic hyperspectral data across 20 rice varieties. (a) paddy rice, (b) brown rice, (c) polished rice, (d) rice flour. Different colors in the figure represent different rice varieties

Raman data analysis

Raman spectrum original curve

The Raman spectra of the 20 varieties of paddy rice, brown rice, polished rice, and rice flour samples exhibited distinct features (Fig. 3). The curve for paddy rice displayed a pronounced peak within the 200–500 cm⁻¹ range, accompanied by a densely oscillating waveform in the 1500–2500 cm⁻¹ range. This phenomenon could be attributed to the dense vibrational activity of polysaccharide molecules within the samples. Additionally, the irregular grooves on the paddy rice surface might influence the morphology of the spectral curve. The spectra of brown and polished rice shared similar characteristics but differ in intensity, which might be due to the differences in surface properties between brown rice and polished rice [2]. Rice flour, derived from polished rice, maintains the same composition but exhibited a distinct spectral profile, particularly a prominent and broadened peak within the 200–500 cm⁻¹ range. Furthermore, the spectral curves of different varieties of rice flour were not identical in shape. Research highlights that grinding polished rice into flour generates heat and mechanical energy, leading to disruptions in the starch crystal structures, increased starch damage, and uneven particle size distribution. A significant amount of mechanical heat also accelerates fatty acid oxidation [26]. Raman, which is sensitive to molecular structure and state, could detect these alterations [27].

A comparative analysis was conducted on the average Raman spectral curves of paddy rice, brown rice,



Fig. 3 Raman spectral curves of 20 rice varieties. (a) paddy rice, (b) brown rice, (c) polished rice, (d) rice flour. Different colors in the figure represent different rice varieties

polished rice, and rice flour (Fig. 4). The spectral curve of paddy rice exhibited minimal overlap with those of the other three categories, underscoring the distinct compositional differences among them. Inspecting the overlap of spectral curves of brown rice, polished rice and rice flour, it is revealed that the characteristic peak positions of the these sample were consistent in the region of $550 \sim 2000 \text{ cm}^{-1}$, which indicated that the data of this study were in line with the real situation and were effective.

Raman curve band analysis and material attribution

The Raman shift acts as an indicator of the motion of specific molecules, making the analysis of characteristic peaks within the Raman curve vital for understanding molecular composition. To assign these characteristic peaks in the Raman spectral curves of the four forms (Fig. 5), the NGSLabSpe software was employed. For optimal peak detection, the parameters were set as follows: the peak finding function was GaussLoren, the peak level was set to 2, the size was set to 6, and the number of iterations was set to 20. For detailed information on specific peaks and their attributions, please refer to Table 1.

Rice husk is composed mainly of cellulose, hemicellulose, and pectin. The complex vibrational modes of natural cellulose closely mirror those of hemicellulose, encompassing CCC, COC, OCC, and OCO skeleton bending, as well as methane bending (CCH and OCH), and CC and CO stretching. The spectral characteristics of natural cellulose are relatively subtle. In the range of 250 to 500 cm⁻¹, nearly all molecules participate in these motion modes, resulting in the formation of numerous characteristic peaks. Between 500~850 cm⁻¹, bands are observed that correspond to COC glycosidic bond vibrations, CCH bending, and COC plane symmetry at specific frequencies such as 496, 520, 596, 641, and 820 cm⁻¹ [28]. From 950 to 1500 cm⁻¹, densely packed bands arise





Fig. 4 Average Raman spectral signatures of four sample types, including paddy rice(green), brown rice(orange), polished rice(red) and rice flour(blue). The grey prominent part corresponds to the consistent characteristic peak position of brown rice, polished rice and rice flour

due to skeletal stretching and atomic bending [29]. Lignin, which is evident between 1500 and 1700 cm⁻¹, displays characteristic bands attributed to aromatic ring symmetric stretching [30]. The structural variations in lignin and hemicellulose across lignocellulosic materials lead to alterations in aromatic ring stretching modes, contributing to the observed spectral differences. The corresponding Raman shifts do not align precisely due to the inherent structural diversity of lignin and hemicellulose molecules within these materials [31].

Brown rice, polished rice, and rice flour primarily consist of starch and protein. The Raman scattering signals of starch exhibit distinct regional distributions, with each region corresponding to specific molecular vibrations. In the spectral range of 400 to 800 cm⁻¹, the characteristic peaks primarily arise from the vibrational modes of the CCC and CCO glycosidic ring backbone. Within 800 to 1200 cm⁻¹, the peaks were attributed to the stretching vibrations of CC, CO, and COC groups within glycosidic bonds, as well as ring breathing motions. The region spanning 1200 to 1500 cm⁻¹ primarily exhibits peaks originating from the vibrations of hydrogen-bonded carbon-containing groups, including CH, CH₂, COH, and CCH [30]. At 479 cm⁻¹, the Raman spectrum displays a prominent peak attributed to the respiratory vibration of the pyran ring skeleton in glucose. In the 500 to 700 cm⁻¹ region, weaker peaks emerge, stemming from the bending vibrations of the CCO bond in dextran. The broader range of 800 to 1500 cm⁻¹ hosts multiple characteristic peaks, primarily reflecting vibrations of hydrocarbons, alcohols, esters, as well as CC and CO bonds within ring structures. Specifically, peaks at 867, 942, 1083, and 1382 cm⁻¹ are attributed to stretching, bending,

and deformation vibrations of CH, CO, COH, and COC bonds in starch and sugar rings [32].

The assignment of Raman spectral bands for protein vibrations is a complex process that often relies on model compounds such as amino acids and short peptides for reference [32]. The constituent amino acids of proteins share common groups and bonds, such as CC and CH. The Raman vibration peaks of these bonds are primarily clustered within the range of 360 to 1500 cm^{-1} [33, 35]. The amide I band, which appears in the range of 1600 to 1700 cm⁻¹, primarily involves stretching of the CO bond, stretching of the CN bond within the peptide group, and in-plane bending of N-H and C α CN within the peptide group. Vibrations in the amide II and III regions encompass N-H in-plane bending and CN stretching motions. These vibrations appear in the range of 1210 to 1506 cm⁻¹ [34].CCN skeleton deformation vibrations typically occur within the range of 360 to 400 cm⁻¹. NH₂ or CH₂ Rocking Vibrations: Rocking vibrations of NH₂ or CH₂ contribute to spectral peaks near 1115 and 1385 cm⁻¹. OCO Vibrations: Stretching, rocking, and in-plane bending vibrations of OCO result in characteristic peaks within the range of 430 to 620 cm⁻¹ and at 1470 cm⁻¹ [35].

LIBS data analysis

LIBS spectrum original curve

The analysis of LIBS spectral curves for different types of rice samples (paddy rice, brown rice, polished rice, and rice flour) reveals several observations (Fig. 6). All sample types exhibited a prominent peak within the 700 ~ 800 nm range. This peak is likely related to the presence of certain elements that are commonly found in rice, such as potassium or calcium. Multiple weaker peaks and minor peaks are observed in the 300-600 nm region. These peaks may represent various elements, or the same element can appear at distinct peak positions due to different plasma conditions or interactions with other elements in the sample. The maximum peak intensity of paddy rice is significantly lower than that of brown rice, polished rice, and rice flour. This difference may be attributed to the presence of the rice husk in paddy rice, which can affect the laser-induced plasma and subsequently the spectral intensity. Spectral analysis reveals two distinct and prominent peak clusters within the wavelength range of 300 to 600 nm, and weaker peak clusters in the 800 to 1000 nm region, similar to rice flour.

The LIBS data of brown rice exhibits two prominent features in the spectral, indicating the presence of specific elements or compounds that are more pronounced in brown rice.

The spectral profiles of polished rice demonstrate a relatively high degree of overall stability, with no discernible deviation observed between different rice varieties. This



Fig. 5 Characteristic Raman spectral peaks assigned to four sample types. (a) paddy rice, (b) brown rice, (c) polished rice, (d) rice flour. The dotted line represents the average spectral profile across 20 varieties of each sample type, the solid lines depict individual characteristic peaks post-peak identification. The numbers accompanying the peaks indicate the Raman shifts. Different colors represent the characteristic peaks at different positions obtained after peak searching operation of the NGSLabSpe software

Wave number/cm ⁻¹	Approximate assignment of vibrational mode	Assignment
254~260	(COH) vibration	Fibers
283~299	(CCC) ring torsion	
	(CCC) ring bend vibration	
356~378	(CCC) ring symmetric	
	(CCC) ring bend vibration	
406~410	(CCO) bending vibration (CCC) bend vibration	Amylopectin
434~436	(CCC) ring vibration	Fibers
438~441	(CCO) bending vibration (CCC) bend vibration (CO) torsion vibration	Amylopectin
476~479	Glucose skeleton vibration	Starch
520~521	(COC) glycosidic stretching vibration	Fibers
580	(CCO) bending vibration	Glucan
594	skeletal deformation of aromatic rings, substituent groups and side chains	Lignin
641	(COC) in plane symmetric stretching vibration	Fibers
716–718	(CCO) bending vibration	Amylopectin
724	skeletal deformation of aromatic rings, substituent groups and side chains	Lignin
768~769	(CCO) bending vibration	Amylopectin
820	(COC) in plane symmetric stretching vibration	Fibers
852~867	(CO) ring vibration (CH) deformation vibration	Saccharide ring Amylopectin
941~943	(COC) symmetric stretching vibration	Glycogen Amylopectin
1001~1006	(CH ₂) vibration	Phenylalanine (breathing mode) Fibers
1033~1050	(CC) extensional vibration (COH) bending vibration (CO) extensional vibration	Fat/Amylopectin
1042	CH and CN deformation vibrations	Protein
1083~1084	(COH) bending vibration	Starch
1128~1132	(COH) bending deformation vibration (CC) stretching vibration (CO) extensional vibration	Glucose
1199~1203	(CO) extensional vibration (CC) extensional vibration	Starch
1251~1266	CN stretching vibration of amide band III	Protein
1341~1342	(CC) extensional vibration (COH) bending vibration	Amino acid/Fatty acid
1383~1398	(CC) extensional vibration	Starch
1462~1463	CH in-plane bending vibration	Glucose
1519	(C = C) stretching vibration	Fibers
1522	Amide I/II	Protein
1599~1603	Amide I/II	Protein
1605	(C=C) stretching vibration	Fibers

Table 1 Raman characteristic peak attribution and molecular motion information in rice

suggests that the polishing process may result in a more smooth surface and more consistent spectral signals.

The LIBS data of rice flour exhibits a higher density of peak clusters within the wavelength range of 300 to 700 nm compared to other rice sample types. This may be due to the increased surface area and exposure of different compounds during the milling process.

The diversity of these spectral data may be attributed to external factors such as instrument parameters, fluctuations in laser energy, sample inhomogeneity, and matrix effects. These factors can influence the shape and intensity of the LIBS spectral signals.

The research highlights the complexity of LIBS spectral analysis and the need to consider various factors that can affect the spectral signals. Understanding these factors is crucial for accurately interpreting the spectral data and deriving meaningful information about the composition and properties of rice samples [36].



Fig. 6 LIBS Spectrum curves of 20 rice varieties. (a) paddy rice, (b) brown rice, (c) polished rice, (d) rice flour. Different colors in the figure represent different rice varieties

LIBS curve band analysis and material attribution

Utilizing the NIST atomic spectrum and molecular spectrum identification database (https://physics.nist.gov/P hysRefData/ASD/lines_form.html), elemental analysis was performed on the obtained LIBS curves of paddy rice, brown rice, polished rice and rice flour (Fig. 7). The elements with obvious peaks at the corresponding wavelengths are found, as shown in Table 2. The results are almost identical to the corresponding elements and corresponding wavelengths provided by other literatures, so the reliability of the data results can be explained [37].

Correlation analysis between spectral data and real values

A comprehensive correlation analysis was performed on the LIBS, Raman, and microscopic hyperspectral data obtained from paddy rice, brown rice, milled rice, and rice flour, focusing on their relationship with amylopectin and protein content (Fig. 8).

Correlation analysis with amylopectin

After excluding non-pertinent variables (-0.2 to 0.2), the absolute correlation values between the three spectral variable types and amylopectin content primarily fell within the range of 0.2 to 0.4. A subset of these variables exhibited a stronger association, with correlations ranging from 0.4 to 0.8. Notably, the highest correlations among LIBS and Raman spectral variables were observed in the 0.6 to 0.8 range, while those of microscopic hyperspectral variables were relatively lower, within 0.4 to 0.6. Across the different sample types, LIBS and Raman spectroscopic correlations displayed both positive and negative associations. However, microscopic hyperspectral correlations revealed distinct trends: rice flour variables predominantly showed negative correlations, while polished rice variables displayed positive correlations.

Correlation analysis with protein

Similarly, excluding non-pertinent variables (-0.2 to 0.2), the absolute correlation values between the three spectral



Fig. 7 Peak analysis of LIBS spectral for four sample types. (a) paddy rice, (b) brown rice, (c) polished rice(c), (d) rice flour. The grey prominent part corresponds to the obvious peak that assigned, and the number corresponding to each peak represents the assigned band

elemental attribution		
Element	Spectral emission lines (nm)	
C	247.86	
CN	387.2, 388.4	
Ca II	393.5, 397, 854.0, 865.9	
Cal	422.7, 616.2, 644.0	
Mg I	285.21, 516.7, 517.1, 518.2	
Na I	588.8,744.0, 746.0	
H _α	656.2	
KI	766.5, 769.9	
Fel	379.8, 431.3, 433.1, 657.5	
01	777.1	

Table 2 LIBS characteristic spectral lines and corresponding

variable types and protein content primarily ranged from 0.2 to 0.4. A subset of these variables exhibited a stronger association, with correlations within the 0.4 to 0.6 range. Compared to amylopectin, the peak correlation between these spectral variables and protein content was marginally lower. Across the different sample types, LIBS and Raman spectroscopic correlations again displayed both positive and negative associations. The microscopic hyperspectral correlation analysis revealed a consistent positive correlation trend between grain and brown rice data. For rice flour and milled rice, the analysis indicated the presence of both positively and negatively correlated variables.

In summary, the correlation analyses with amylopectin and protein content across LIBS, Raman, and microscopic hyperspectral variables revealed varying degrees of association. LIBS and Raman variables generally demonstrated a broader range of correlations, while microscopic hyperspectral correlations exhibited slight differences in trends between sample types. These correlation variables will serve as crucial inputs for the subsequent regression modeling process.

Regression modeling of spectral data and quality index

The R² curves illustrate the performance of models predicting amylopectin and protein content using microscopic hyperspectral, Raman, and LIBS techniques across various rice samples, including paddy rice, brown rice, polished rice, and rice flour (Fig. 9).

Results analysis of microscopic hyperspectral regression modeling

The microscopic hyperspectral analysis for predicting amylopectin and protein contents is illustrated in Fig. 9(a)and (b). The findings show the maximum R²curve is



Fig. 8 Correlation analysis of LIBS, Raman and microscopic hyperspectral data with amylopectin and protein contents in rice varieties. (A) The results of correlation analysis with amylopectin. (B) The results of correlation analysis with protein. The figure employs numerical labels to distinguish sample types (paddy rice(I), brown rice(II), polished rice(III) and rice flour(IV)), and dashed lines to segregate the spectral imaging types (LIBS, Raman, microscopic hyperspectral). The data in the grid represents the proportion of variables within the current correlation interval, relative to the total number of variables analyzed

greatly affected by the regression methods used. The average R^2 curve provided greater stability, with amylopectin modeling averaging 0.19 and protein modeling 0.18. Modeling performance across four samples types did not vary significantly and with low R^2 . Microscopic hyperspectral imaging captures spectral and image data from small regions, but rice grain compound distribution is often non-uniform. Thus, limited spectral information from these areas may inadequately characterize overall amylopectin and protein content.

Results analysis of raman regression modeling

The modeling outcomes using Raman spectral data for predicting amylopectin and protein content were presented in Fig. 9 (c) and (d). The average R^2 curve for amylopectin modeling is stable, revealing a clear hierarchy, the maximum average R^2 was 0.52. In contrast, the average R^2 curve for protein modeling fluctuates, with an overall lower value than that of amylopectin, with a maximum average R^2 of 0.47. Polished rice provided the best results for amylopectin modeling compared to other rice types. For protein modeling results, despite a noticeable decline at the extremes of the rice flour curve, the influence of these four sample types on the modeling results is basically the same as that of amylopectin.

Raman spectroscopy data exhibited promising results in regression modeling for predicting amylopectin and protein content, with performance trends across various sample types. Among these, polished rice yielded the optimal modeling outcomes, likely attributed to its smooth surface and stable molecular configuration. Conversely, paddy rice's outer husk interfered with spectral information, introducing signal instability due to husk grooves. Brown rice, despite being husk-free, still has an outer film slightly affecting Raman signal acquisition. Rice flour may undergo structural alterations and damage from mechanical or thermal processes that can influence the stability of the spectral data obtained.

Results analysis of libs regression modeling

The LIBS spectral data modeling results for amylopectin and protein content are shown in Fig. 9 (e) and (f). Both maximum and average R2 curves exhibit limited variability. A clear hierarchical structure emerges among the diverse sample types. For amylopectin, with maximum and average R2 values of 0.81 and 0.62. Paddy rice leads in stability and effectiveness for modeling, followed by polished rice, brown rice, and rice flour. In terms of protein content modeling, with a similar maximum R2 of 0.81 and an average R2 of 0.6. Polished rice outperforms the others, with paddy rice, rice flour, and brown rice trailing in that sequence. LIBS spectral data effectively characterizes amylopectin and protein content in rice, capturing variations across sample types. Spectral data from grain and polished rice yield superior modeling results. Continuous laser pulse ablation in paddy rice penetrates the husk for better interior spectral signals. Minor burning occurs in brown rice, milled rice, and rice



Fig. 9 Modeled R2 curves of spectral data for four rice sample types with amylopectin and protein content. The colors represent sample types, paddy rice (blue), brown rice (red), polished rice (brown), rice flour (gray). (a)&(b) show R2 results for microscopic hyperspectral data, modeling amylopectin and protein, respectively. (c)&(d) present R2 results for Raman spectral data, for amylopectin and protein modeling. (e)&(f) are LIBS data regression models for amylopectin and protein. The solid line represents the maximum R2 curve, the dotted line indicating the average R2 from multiple modeling iterations

flour during analysis. Rice material heterogeneity may contribute to spectral signal variations, but all sample types demonstrate some proficiency in characterizing amylopectin and protein content.

Feature selection and analysis in modeling The screened common features of raman regression

Statistical analysis was performed on the independent variables derived from Raman spectral data encompassing four distinct sample types, aiming to pinpoint common characteristic variables that consistently emerged across various regression techniques. These identified variables were subsequently correlated with Raman spectral peaks specific to amylopectin and protein, as depicted in Figs. 10 and 11.

Irrespective of the focus being on amylopectin or protein, a portion of the screened common independent variables could be aligned with Raman characteristic variables corresponding to the respective substances, albeit in relatively modest proportions. It is noteworthy that a significant number of these screened variables fell within the spectral range of 1700 to 2500 cm⁻¹, a region devoid of prominent peaks in the sample spectra and characterized by low intensity values. The modeling of polished rice spectral data revealed a higher concentration of characteristic variables, which correlates well with the R2 curve observed in Fig. 9.

The modeling and screening process successfully uncovered Raman characteristic variables associated with both amylopectin and protein. Although the proportion of these matched variables may not be substantial, their frequent appearance in modeling iterations and consistent alignment with R2 curve trends across various model types underscore the feasibility of our research approach. The inherent fluorescence properties of the tested samples and various experimental uncertainties may result in the selected eigenvalues not always perfectly correlating with distinct characteristic peaks. This phenomenon is in line with the findings of Zhang et al. [38] who reported that the optimal spectral features used by SVM for dairy classification did not strictly align with the prominent



Fig. 10 The characteristic variables screened of Raman spectroscopic regression modeling of amylopectin content with various rice samples. (a) paddy rice, (b) brown rice, (c) polished rice, (d) rice flour. The blue represents variables exhibiting deviations in Raman characteristic shifts from the established profile of rice amylopectin. The red signifies variables that align closely with the known Raman characteristic shifts of rice amylopectin. The intensity of color correlates with the frequency of variable



Fig. 11 Variables screened of Raman spectroscopic regression model for protein content across rice samples. (a)paddy rice, (b)brown rice, (c)polished rice, (d)rice flour. The blue represents variables exhibiting deviations in Raman characteristic shifts from the established profile of rice amylopectin. The red signifies variables that align closely with the known Raman characteristic shifts of rice amylopectin. The intensity of color correlates with the frequency of variable

peaks in the original Raman spectra of dairy products. This is consistent with the results obtained in this study.

The screened common features of LIBS regression

A statistical analysis was conducted on the results of regression modeling between LIBS spectral data and the amylopectin and protein content of rice, identifying the common characteristic independent variables across different regression methodologies. The selected variables underwent elemental analysis, with the NIST atomic and molecular spectrum identification databases serving as references.

To address discrepancies between ideal and actual conditions, a tolerance of ± 0.1 (the lowest spectral resolution) was allowed during the variable backtracking process. Given that amylopectin primarily consists of *C*, *H*, and O, the analysis of its associated variables focused on these elements (Fig. 12). Conversely, proteins encompass

a diverse array of elements due to their amino acid composition, with a particular focus on C, H, O, N, P, S, K, and Mg during variable analysis for proteins (Fig. 13). The detailed analysis results indicated that the majority of selected variables, both for amylopectin and protein, correspond to the elements of interest. This highlights the rationality of the information utilized in regression modeling when leveraging LIBS data alongside rice quality indicators. Furthermore, compared to Raman spectroscopy data, LIBS spectral variables exhibit richer information content and demonstrate better regression outcomes with respect to rice quality indicators.

Conclusions

This study focused on assessing the applicability of three spectral methodologies for non-destructive rice quality evaluation, considering the impact of various rice samples on inspection results. Direct modeling and



Fig. 12 Variables screened of LIBS spectroscopic regression model for amylopectin content across rice samples. (a)paddy rice, (b)brown rice, (c)polished rice, (d)rice flour. The blue indicates that there are no matching element(C/H/O) for the variables. The red represents the element(C/H/O) that can be matched within a certain range (±0.1). The intensity of color correlates with the frequency of variable

analysis of LIBS data from paddy rice achieved a higher R2, enhancing detection efficiency compared to general spectral-metabolite research. The same is true for brown rice, polished rice and rice flour data modeling results. LIBS facilitates rapid content analysis across scenarios but consumes slight samples due to high-energy laser ablation.

Raman spectroscopy, using adjustable low-power lasers, showed potential in rice quality detection, particularly for smooth-surfaced and molecularly stable samples due to its sensitivity to weak scattering. It preserves sample integrity and offers stable, reliable spectral signals, ensuring accurate results. Raman spectroscopy exhibits compromised detection efficacy for brown rice and whole grains due to surface heterogeneity and external material coverage. Furthermore, molecular structural alterations induced by mechanical processing of rice flour samples adversely impact spectral modeling accuracy. Consequently, while maintaining non-destructive nature, Raman spectroscopic analysis necessitates stringent experimental conditions and sample standardization.

Conversely, microscopic hyperspectral imaging faced limitations in detecting rice contents due to sample size constraints, hindering comprehensive information capture and limiting its application. In conclusion, this study employed various spectral techniques to assess their applicability in non-destructive rice quality evaluation, aiming to provide valuable insights for crop grain quality detection.



Fig. 13 Variables screened of LIBS spectroscopic regression model for amylopectin content across rice samples. (a) paddy rice, (b) brown rice, (c) polished rice, (d) rice flour. The blue indicates that there are no matching element (C/H/O/N/P/S/K/Mg) for the variables. The red represents the element (C/H/O/N/P/S/K/Mg) that can be matched within a certain range (±0.1). The intensity of color correlates with the frequency of variable

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Author contributions

J.G and S.J conducted experiments, performed comprehensive data analysis, and was the primary contributor to the manuscript. W.Z participated in experiments and data analysis. B.L assisted with experimental work and provided critical reading and revisions of the manuscript. Y.Z and X.H and W.Y both made contributions through the critical reading and editing of the manuscript. F.H and L.X supervised the research, coordinated author contributions, and managed journal communications.All authors reviewed the manuscript.

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Data availability

No datasets were generated or analysed during the current study.

Declarations

Ethics approval and consent to participate Not applicable.

Consent for publication

Not applicable.

Competing interests

The authors declare no competing interests.

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