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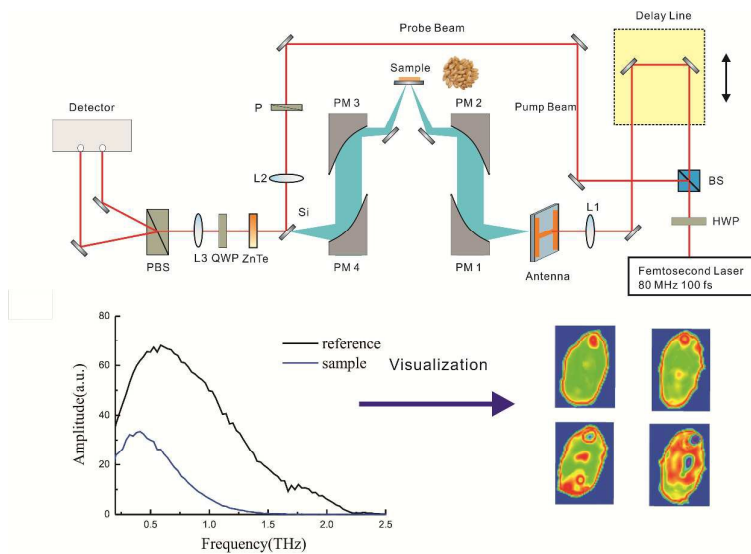
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## Graphical abstract



# Discrimination of Moldy Wheat Using Terahertz Imaging Combined with Multivariate Classification

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13 Terahertz (THz) imaging was employed to develop a novel method for discriminating wheat of  
14 varying states of moldiness. Spectral data, in the range of 0.2–1.6 THz, were extracted from  
15 regions of interest (ROIs) in the THz images. Principal component analysis (PCA) was used to  
16 evaluate the spectral data and determine the cluster trend. Six optimal frequencies were selected  
17 by implementing PCA directly for each image's ROI. Classification models for moldy wheat  
18 identification were established using the support vector machine (SVM) method, a partial  
19 least-squares regression analysis, and the back propagation neural network method. The models  
20 developed from these methods were based on the full and optimal frequencies, using the top  
21 three principal components as input variables. The PCA-SVM method achieved a prediction  
22 accuracy of over 95%, and was implemented at every pixel in the images to visually  
23 demonstrate the moldy wheat classification method. Our results indicate that THz imaging  
24 combined with chemometric algorithms is efficient and practical for the discrimination of  
25 moldy wheat.

26 **Keywords: discriminate analysis, wheat grain, moldy, terahertz imaging, spectral analysis,**

27 **multivariate classification**

28

## 29 1. Introduction

30 Wheat is a primary food crop worldwide, and contains high amounts of carbohydrates,  
31 proteins, fat, and vitamins (Oladunmoye, Akinoso, & Olapade, 2010). Mildew such as  
32 Aflatoxin and *Aspergillus niger* are prevalent throughout all stages of wheat growth and  
33 production. When improperly stored and processed, these mildews pose a potential threat to  
34 humans and fowls (Neethirajan, Karunakaran, Jayas, & White, 2007). Recently, food quality  
35 and safety assessment have increased within the food industry. Conventional moldy grain  
36 detection methods, such as naked-eye observations, microscope inspection, liquid  
37 chromatography, and enzyme-linked immunosorbent assays, are time-consuming and  
38 labor-intensive (Turner, Subrahmanyam, & Piletsky, 2009).

39 To satisfy the demand for high-quality consumer products, extensive studies into grain  
40 quality via nondestructive rapid evaluations have been performed. Wang et al. (Wang, Liu,  
41 Yu, Wu & He, 2011) presented a new approach for non-invasive classification of raisins by  
42 using computer vision techniques. Eifler et al. (Eifler, Martinelli, Santonico, Capuano, Schild,  
43 & Di Natale, 2011) used an electronic nose to differentiate between infected and non-infected  
44 wheat grains. Arngren et al. (Arngren, Hansen, Eriksen, Larsen, & Larsen, 2011) used  
45 near-infrared hyperspectral imaging combined with nonlinear neural networks to identify  
46 early-stage pregermination in barley grains. ElMasry et al. (ElMasry, Wang, ElSayed, Ngadi,  
47 2007) proposed a novel tool for nondestructive determination of moisture content, total soluble  
48 solids, and acidity in strawberry using NIR spectroscopy. However, these measurement  
49 techniques do not probe the far-infrared spectral region, which contains a wealth of physical

50 and chemical information.

51 Terahertz (THz) radiation (with frequencies from 0.3 to 10 THz and wavelengths from 3.3  
52 to  $333 \text{ cm}^{-1}$ ) occupies the region between the microwave and infrared bands; it can be used for  
53 non-destructive and non-invasive analyses, and possesses attractive features such as extremely  
54 low-energy levels, broad spectral bandwidth, transparency, and good penetration through  
55 various materials (Ferguson, & Zhang, 2002; Tonouchi, 2007). THz spectroscopy and imaging  
56 are rapidly becoming novel techniques in the field of optics research. The new techniques are  
57 widely used as solutions in art conservation (Fukunaga, & Hosako, 2010), security problems  
58 (Melinger, Laman, & Grischkowsky, 2008), biomedical applications (Oh. et. al., 2014; Siegel,  
59 2004), agricultural quality control (Gowen, O'Sullivan, & O'Donnell, 2012; Ge, Jiang, Xu, Lian,  
60 Zhang, & Xia, 2014), and other fields (Guillet. et. al., 2014). THz imaging is performed both by  
61 the transmission and reflection of THz waves. In reflectance imaging, THz waves reflect not  
62 only from the surface of samples, but also from interfaces present in the samples within the  
63 penetration depth of the radiation (Safrai, Ben Ishai, Polsman, Einav, & Feldman, 2014). Thus,  
64 both surface and depth information can be obtained from the timing and amplitude of the  
65 reflected waves. Time- and frequency-domain structural images can be acquired from detected  
66 THz waves associated with various parameters at each pixel in the measured sample area (Reid,  
67 Pickwell-MacPherson, Laufer, Gibson, Hebden, & Wallace, 2010). Owing to the absorption,  
68 reflection, scattering, and phase-shifting of the imaged material, measured parameters can  
69 change due to differing wave delay and attenuation.

70 The aim of this study was to evaluate the validity and feasibility of identifying different

71 moldy states of wheat using THz imaging and multivariate data analysis methods. THz spectra  
72 of wheat grains with different moldy statuses were extracted in the range of 0.2–1.6 THz from  
73 regions of interest (ROIs) in each THz image. Principal component analysis (PCA) was used to  
74 explore features of the spectral data and select the optimal frequencies. Support vector machine  
75 (SVM), partial least-squares regression (PLSR), and back propagation neural network (BPNN)  
76 models were established based on the full frequencies and optimal frequencies for  
77 discriminating between the four stages of moldy wheat. Finally, THz images of wheat with  
78 different moldy states were investigated using the optimal classification method (i.e.,  
79 PCA-SVM).

## 80 **2. Materials and methods**

### 81 *2.1 Experimental setup*

82 A standard THz-TDS laboratory setup, using reflection geometry as developed by Zomega  
83 Terahertz Corporation in USA, was used in our experiment. A schematic of the THz-TDS  
84 reflection imaging system is shown in Fig. 1. The THz imaging system employed an externally  
85 pulsed femtosecond laser Ti-sapphire with a pulse width, central wavelength, and repetition  
86 frequency of 100 fs, 800 nm, and 80 MHz, respectively. The beam produced by the laser was  
87 split into a pump and a probe using a polarizing beam splitter. The pump beam was irradiated  
88 on a photoconductive dipole antenna fabricated on a LT-GaAs wafer for generation of the THz  
89 waves, and the probe beam was focused onto an electro-optic ZnTe crystal for detection of the  
90 THz waves (Taylor. et. al., 2008). The THz pulses emitted by the generator were focused on the

91 sample via two metal parabolic mirrors, and the THz pulses reflected by the sample via two  
92 additional parabolic mirrors were guided to the detection antenna. The system measures  
93 far-infrared spectra between 0.1 THz and 3.0 THz. The sample was scanned by moving the  
94 two-dimensional motorized stage, and the obtained image data were saved and analyzed using a  
95 computer. Details about the principles of the system are explained elsewhere (Kim. et. al.,  
96 2012). The experiment was performed at room temperature, and the humidity was maintained at  
97 approximately zero by purging the system with dry nitrogen to avoid absorption of vapor.

## 98 *2.2 Sample preparation*

99 Wheat used in the experiment was collected from the School of Food Science and  
100 Technology, Henan University of Technology, Zhengzhou, China. The wheat was of the same  
101 variety and produced in 2013. Wheat grains were moistened at a humidity of 28% and were  
102 evenly distributed in a circular Petri dish. The Petri dish was put into an incubator box that was  
103 maintained at a constant temperature of 25°C, where it remained for eight days. Wheat with  
104 different stages of mold growth (none, slight, moderate, and serious) were then selected (as  
105 shown in Fig.2) and individually imaged by the THz imaging system with a spatial resolution of  
106 0.25 mm. For each degree of mold contamination, 50 samples were used without further  
107 processing.

## 108 *2.3 Multivariate Analysis Methods*

### 109 *2.3.1 Principal component analysis*

110 PCA (Lin, Zhao, Sun, Chen, & Zhou, 2011; Noori, Sabahi, Karbassi, Baghvand, & Zadeh,



111 2010) is a multivariate statistical and dimensional reduction method that can be used to reduce  
 112 the complexity of input variables when dealing with large datasets. In this method, a large  
 113 volume of data is transformed into a small number of principal components (PCs). PCs can be  
 114 expressed as:

$$115 \quad Z_i = a_{i1}X_1 + a_{i2}X_2 + \dots + a_{in}X_n \quad (1)$$

116 where  $Z_i$  represents the PCs,  $a_i$  represents the related eigenvectors, and  $X_i$  represents the input  
 117 variables. This information can be acquired by solving following equation.

$$118 \quad |R - I\lambda| = 0 \quad (2)$$

119 where  $R$  is the variance-covariance matrix,  $I$  is the unit matrix, and  $\lambda$  is the eigenvector.

### 120 2.3.2 Support vector machines

121 SVM is a widely used, supervised statistical learning method for analyzing data and  
 122 recognizing patterns (He, Yang, & Xie, 2013; He, Wu, & Sun, 2014). SVM demonstrates  
 123 advantage over other methods when dealing with small samples, and high-dimensional and  
 124 non-linear data. In the multi-class SVM method,  $k(k-1)/2$  classifiers are constructed, where  
 125  $k$  is the class number of the data. The following two-class classification problem was  
 126 implemented by training the  $i$ th and  $j$ th data classes:

$$127 \quad \min_{w^{ij}, b^{ij}, \xi^{ij}} \frac{1}{2} (w^{ij})^T w^{ij} + c \left( \sum_t (\xi^{ij})_t \right) \quad (3)$$

$$128 \quad \text{subject to} \quad \begin{aligned} & (w^{ij})^T \phi(x_i) + b^{ij} \geq 1 - \xi^{ij}, \text{ if } x_i \text{ in } i\text{th class} \\ & (w^{ij})^T \phi(x_i) + b^{ij} \leq -1 + \xi^{ij}, \text{ if } x_i \text{ in } j\text{th class} \\ & \xi^{ij} \geq 0 \end{aligned} \quad (4)$$

129 where  $w$  and  $b$  define the optimal hyperplane,  $\xi$  represents the slack variable,  $c$  is the  
130 penalty factor, and  $\phi(x)$  is the sample set. Selection of the kernel function in SVM models  
131 significantly affects model performance. In this paper, the commonly used radial bias function  
132 (RBF)  $k(x_i, y_i) = \exp(-\frac{\|x_i - y_i\|^2}{\gamma^2})$  was used. The adjustable kernel function parameter  $C$  controls  
133 the trade-off between the minimum model complexity and minimum training error, while  $\gamma$   
134 represents the degree of generalization and the width of the kernel function. A grid-search  
135 procedure was employed to find the optimal parameters of the model (Maali, & Al-Jumaily,  
136 2013).

137 The root mean square error (RMSE) was used to evaluate the performance of the  
138 established model (Zhang. et. al., 2008). The RMSE is calculated as

$$139 \quad RMSE = \sqrt{\frac{\sum_{i=1}^N (y_i^{pre} - y_i)^2}{N}} \quad (5)$$

140 where  $y_i$  represents actual value of the  $i$ th sample in the data set,  $y_i^{pre}$  is the predicted weight  
141 ratio value of the  $i$ th sample in the developed model, and  $N$  is the sample size.

### 142 2.3.3 Partial least squares regression

143 PLSR is one of most robust and reliable multivariate-data analysis methods, and is  
144 particularly suitable for use in situations where there is a linear relation between the spectra and  
145 properties of the considered objects (Brereton, 2000). A PLSR analysis was performed to  
146 establish a regression model for the prediction of target chemical concentrations (variable  
147 matrix  $Y$ ) based on the corresponding spectra data (variable matrix  $X$ ). The underlying PLSR

148 model is expressed as:

$$\begin{aligned} X &= TP^T + E \\ Y &= UQ^T + F \end{aligned} \quad (6)$$

150 where  $T$  and  $U$  are the feature matrices of the variable matrix of  $X$  and  $Y$  respectively,  $P$   
151 and  $Q$  represent the orthogonal loading matrices, and  $E$  and  $F$  are the error terms.

### 152 2.3.4 Back propagation neural network

153 BPNN is a type of nonlinear multi-layer network, and it has been used extensively to solve a  
154 variety of classification and regression problems (Dubey, Bhagwat, Shouche, & Sainis, 2006).  
155 A BPNN is based on an algorithm that rectifies the weights within each layer in proportion to  
156 the error obtained from the previous layer. In this study, an input layer, a hidden layer, and an  
157 output layer were used. By optimizing the hidden nodes from the input variables by “trial and  
158 error,” BPNN was used to classify samples into predefined varieties, and a new output layer  
159 that provided a more precise discrimination of a sample’s variety was obtained. Details of the  
160 BPNN method are discussed extensively elsewhere (Marengo, Bobba, Robotti, & Lenti, 2004).  
161 The whole experiment procedure by using THz imaging technique, as illustrated in Fig. 3, is  
162 made from three steps to prepare the data structure for mold statuses wheat identification.

## 163 3 Results and Discussion

### 164 3.1 Spectral Analysis

#### 165 3.1.1 Moldy wheat spectra

166 After THz images of wheat with different stages of mold growth were acquired, the only  
167 wheat grain areas are segmented as the ROIs to exclude the interfering information origin from

168 the background in each image. The spectra of each pixel within the ROI were extracted and  
169 averaged at each frequency to generate a mean value, which is then expressed as the ROI  
170 spectrum. The average frequency domain spectra of each degree of mold growth, in the range  
171 of 0.1–2.0 THz, are shown in Fig. 4. It is seen that an intense trough is present at around 1.67  
172 THz, which is related to the absorption of water within the grain. And the spectral curves of  
173 these four mold statuses wheat are quite similar at the beginning. Hence, spectral frequency  
174 range from 0.2-1.6 THz is employed for further identification study. Meanwhile, the general  
175 trends of the four spectral curves show no obvious differences, which indicated that mold  
176 statuses of the wheat could not be identified from spectral curves directly.

177 To solve this problem, more sophisticated computational analysis methods were employed  
178 to differentiate between the mold statuses of the wheat. Therefore, a dataset with 512 spectral  
179 features and 200 wheat samples was selected in order to construct a classification model to  
180 discriminate between the different degrees of moldiness. A dataset consisting of 200 samples  
181 was randomly split into a calibration set (120 samples) and a prediction set (80 samples). The  
182 classification errors would clearly decrease when training more samples. Hence each wheat  
183 sample leaves fewer samples to analyze and obtains higher prediction accuracy. But when more  
184 training number, redundant information (existed in the large number of input variable) would  
185 affect the robust and ability of the classification models. Meanwhile, the less input simplify the  
186 classification models and accelerate the calculated speed.

### 187 *3.1.2 PCA Analysis*

188 PCA was performed on all of the spectral data (with a frequency range of 0.2–1.6 THz)  
189 obtained from the normal, slightly moldy, moderately moldy, and seriously moldy wheat  
190 samples to reduce the high dimensionality of the problem and qualitatively identify the samples.  
191 The explained variance rate for the top four PCs extracted from the original THz spectra data  
192 are 93.22%, 3.61%, 1.24%, and 0.21%, respectively. The top four PCs explain 98.25% of the  
193 total contribution to the original data. It is shown that the cumulative reliabilities of the top four  
194 PCs represent 98% of the total information to the original data. Thus, they contain the  
195 maximum information across all the wheat samples and reduce the dimensions from 512  
196 spectral measurements for classification of different mold statuses of wheat to only three  
197 components. Figure 5 shows the three-dimensional scores plotted for the first three PCs for all  
198 of the samples. As we can see, the different mold statuses are distributed separately in the  
199 three-dimensional area. However, some sample points near the boundaries of normal and  
200 slightly moldy wheat are mixed although their sample points are clustered. Therefore, it is  
201 necessary to employ an adequate classification model based on the PCA process for further  
202 discrimination.

### 203 *3.1.3 Optimal Frequency Selection*

204 A PCA was used for each ROI image to select the optimal frequencies. PC loadings were  
205 employed to identify sensitive frequencies that were highly correlated with each PC. The  
206 x-loading weights of the first four PCs were used to select each frequency in the full spectral

207 range. Strong peaks and troughs for the top four PCs were selected as the optimum frequencies.  
 208 As seen in Fig. 6, six frequencies with the values of 0.32 THz, 0.59 THz, 0.87 THz, 1.0 THz,  
 209 1.29 THz, and 1.58 THz were selected as discriminators of different moldy statuses. The  
 210 reduced number of frequencies decreased the time to acquire and process each image.

### 211 3.2 Multivariate Data Analysis

#### 212 3.2.1 Multivariate Data Analysis Based on Full spectra

213 SVM, PLSR, and BPNN classification models were used to predict the degree of moldiness  
 214 using the entire spectral dataset. Within the SVM models, the optimization values for the  
 215 regularization parameter  $\gamma$  and the RBF kernel function parameter  $C$  were selected when the  
 216 smallest RMSE was obtained. The optimal parameters  $\gamma$  and  $C$  were set at 3.6 and 1.8,  
 217 respectively, which were determined by using the grid search algorithm. For the BPNN model,  
 218 after several attempts to optimize the parameters, the learning rate factor, momentum factor,  
 219 initial weight, permitted training error, and maximal training times were set at 0.1, 0.1, 0.6,  
 220 0.00001, and 1,000, respectively.

221 The SVM, PLSR, and BPNN models were constructed using the top four PCs as inputs.  
 222 The discrimination results of normal, slightly moldy, moderately moldy, and seriously moldy  
 223 wheat in the calibration set and prediction set using these models are presented in Table 1.

224 Table 1 Results of the classification models based on full spectra (Cal. represents the calibration  
 225 set of the samples and Pre. represents the prediction set of the samples.)

Model	Accuracy per type (%)				Overall prediction
	Normal	Slightly moldy	Moderately	Seriously	

					moldy		moldy		accuracy (%)
	Cal.	Pre.	Cal.	Pre.	Cal.	Pre.	Cal.	Pre.	
PCA-SVM	100%	100%	100%	86.67%	100%	84%	100%	100%	96.5%
PCA-PLSR	100%	95%	91.43%	86.67%	88%	84%	100%	95%	93%
PCA-BPNN	93.33%	90%	88.57%	80%	84%	76%	93.33%	90%	87%

226 As the table shows, the performance of the SVM model was, in general, better than those of  
 227 the PLSR and BPNN models, and achieved a prediction accuracy of 96.5%. The SVM model  
 228 achieved a classification rate of the normal and serious moldy statuses of 100% in both the  
 229 calibration and prediction sets; however, the classification rates of the prediction sets of slightly  
 230 moldy and seriously moldy wheat were relatively lower. Moreover, the PLSR and BPNN  
 231 models misclassified some statuses, with an overall prediction accuracy of 93% and 87%,  
 232 respectively. The results indicate that PLSR and SVM models can be used as effective methods  
 233 for moldy wheat identification, with the SVM model considered the optimum method.

### 234 3.2.2 Multivariate Data Analysis Based on Optimal frequencies

235 Although the classification models have good moldy wheat prediction performances, the  
 236 large number of frequency variables resulted in complicated and time-consuming data  
 237 processing. Instead, the use of optimal-frequency selection can reduce the complexity and time  
 238 required for model establishment. As a consequence of optimal frequency selection, the top four  
 239 PCs and the selected six frequencies (0.32 THz, 0.59 THz, 0.87 THz, 1.0 THz, 1.29 THz, and  
 240 1.58 THz) were used as inputs to the SVM, PLSR, and BPNN models. The performance of the

241 optimized models based only on the optimal frequencies is presented in Table 2.

242 Table 2 Results of the classification models based on their optimal spectra (Cal. represents the  
243 calibration set of the samples and Pre. represents the prediction set of the samples.)

Model	Accuracy per type (%)								Overall prediction accuracy (%)
	Normal		Slightly moldy		Moderately moldy		Seriously moldy		
	Cal.	Pre.	Cal.	Pre.	Cal.	Pre.	Cal.	Pre.	
PCA-SVM	100%	100%	97.14%	86.67%	92%	84%	100%	95%	95%
PCA-PLSR	100%	95%	91.43%	80%	92%	84%	96.67%	95%	92.5%
PCA-BPNN	93.33%	85%	88.57%	73.33%	84%	76%	93.33%	90%	86%

244 As shown in Table 2, the BPNN model had the worst prediction result, with a classification  
245 accuracy of 86%. The classification rates of the SVM and PLSR models in both the calibration  
246 and the prediction sets were all over 80%. The SVM model obtained the highest overall  
247 prediction accuracy, 95%, and a classification accuracy of 100% for normal and seriously  
248 moldy wheat in the calibration set. The slightly moldy and moderately moldy wheat showed  
249 poorer prediction accuracy in all models, compare with the normal wheat and seriously moldy  
250 wheat.

251 The plots of the actual values compared to the predicted values using the PCA-SVM  
252 models based on the full spectra and selected optimal frequencies are shown Fig. 7. A threshold  
253 value (dummy variable  $\pm 0.5$ ) was set to define the class limits. Subintervals from 0.5–1.5, 1.5–  
254 2.5, 2.5–3.5, and 3.5–4.5 represent normal, slightly moldy, moderately moldy, and seriously



255 moldy wheat samples, respectively. It can be seen in Figs. 6 (a) and (b) that a similar  
256 distribution of points between the full spectrum and the optimal frequencies was obtained. The  
257 experimental results demonstrate the feasibility of using selected optimal frequencies for the  
258 discrimination of wheat grains with different mold statuses.

### 259 *3.3 THz Images of Moldy Wheat*

260 The implementation of a visualization process is helpful for determining the degree of  
261 moldiness of a wheat grain, which can be difficult when observed by just the naked eye. In this  
262 study, the PCA-SVM model acquired the best classification accuracy and therefore was used to  
263 generate THz moldy wheat images. Training of the SVM model was done using the optimal  
264 frequencies selected by the PCA. The reduced spectral data were then used as input to the SVM  
265 model. The output value of the model was the reflectivity of each pixel, which corresponds to a  
266 different component within each wheat grain. When the values of all pixels within the wheat  
267 grain were calculated, an image was generated based on the spatial positions of each pixel.

268 Figure 8 shows the THz images of normal, slightly moldy, moderately moldy, and seriously  
269 moldy wheat. Regions (1), (2), and (3) represent the embryo of each wheat grain. Except for the  
270 embryo structure, the inner structures of the wheat sample in Fig. 7(a) and 7(b) are evenly  
271 distributed. However, in Fig. 7(b) the embryo and edge structure have changed, indicating that  
272 the wheat is in its moldy infancy, while it is seen that the wheat in Fig. 7(a) is not contaminated  
273 with mold. In Fig. 7(c), the embryo area and small range of inner structures are damaged,  
274 indicating that the sample has a moderate degree of mold growth. Finally, in 7(d), the red area

275 (5) indicates that the inner structures of this wheat sample are totally damaged, and the  
276 embryonic area is absent.

### 277 *3.4 Discussion*

278 The excellent discrimination results demonstrate that the THz reflection imaging technique  
279 combined with PCA feature extraction and a SVM classification model can be used to identify  
280 wheat grains with different mold statuses. Six optical frequencies (0.32 THz, 0.59 THz, 0.87  
281 THz, 1.0 THz, 1.29 THz, and 1.58 THz) were selected according to the top four PC loading  
282 weights. The overall prediction accuracy of the PCA-SVM model based on the selected optimal  
283 frequencies was 95%, which is higher than that achieved with the PCA-PLS and PCA-BPNN  
284 models. The optimal frequency-based models used six frequencies instead of 159 frequencies,  
285 indicating a decrease of 96.49%. The performance of each classification model showed only a  
286 slight decline from full spectra to optimal frequencies, implying that the optimal frequencies  
287 were effective, and as such, we encourage further study of them. Furthermore, the fewer input  
288 variables accelerated the data calculation speed and simplified the model complexity. In further  
289 studies, different frequency selection methods and different classification models will be  
290 applied to improve the prediction accuracy and explore the optimal frequency for moldy wheat  
291 identification.

292 Additionally, the PCA-SVM model was used to classify the THz image data and determine  
293 the degree of mold contamination as normal, slightly moldy, moderately moldy, and seriously  
294 moldy. The THz images provided information regarding the spatial distribution of different

295 components within the wheat grain, and were helpful for detecting changes in a grain's inner  
296 structure due to varying mold status. Our results show that THz imaging can be used to  
297 recognize the wheat when it is in its early moldy stage, which cannot be done with conventional  
298 imaging and spectroscopy, and thus provides an early warning technique for mold  
299 contamination. The THz imaging technique has the potential to be an effective tool for  
300 agriculture quality and safety control. Therefore, it is essential to expand the sample variety  
301 number and optimize the image classification algorithm in further studies to assist  
302 in discriminating the multiple statuses of wheat mold en masse and for practical applications.

#### 303 **4 Conclusion**

304 THz imaging combined with multivariate data analyses was employed to discriminate  
305 wheat grains with different mold statuses. Spectral information was extracted from the THz  
306 images, in the range of 0.2–1.6 THz, for each wheat sample. The feature data of each spectrum  
307 were analyzed and six optimal frequencies were selected using PCA. In addition, the SVM,  
308 PLSR, and BPNN models were constructed based on the full spectra and optimal frequencies to  
309 help discriminate between different moldy wheat samples. The prediction accuracies of the full  
310 spectra were similar to those obtained using only the optimal frequencies. The PCA-SVM  
311 model was considered to be the optimal model, and the prediction accuracies reached 95%. The  
312 PCA-SVM model was also used on THz images as a visual demonstration of the classification  
313 technique. Our experimental results demonstrate that THz imaging is a potential tool for the  
314 classification of moldy wheat.

315 **ACKNOWLEDGMENTS**

316 This work is supported by the National High-tech R&D Program of China (863 Program)  
317 (Grant No. 2012AA101608), the National Natural Science Foundation of China (Grant No.  
318 61071197), the Key Project of Educational Committee of Henan Province of China (Grant No.  
319 14B413011), the Key Science and Technology Program of Henan Province of China (Grant No.  
320 122102210217), the Plan of Nature Science Fundamental Research in Henan University of  
321 Technology (11JCY07), and the High-Level Personnel Funds (2012BS047) in Henan  
322 University of Technology. Finally, the authors are grateful to the reviewers for their helpful  
323 comments and constructive suggestions.

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401 **Figure captions**

402 Fig.1 THz reflectance imaging experimental setup.

403 Fig.2 Wheat samples with different stages of mold contamination: (a) normal; (b) slightly; (c)  
404 moderately; (d) seriously.

405 Fig. 3 Flowchart of the procedure of discrimination moldy wheat by using THz imaging: (a)  
406 Imaging pre-processing; (b) Spectral analysis; (c) Imaging visualization.

407 Fig. 4 Frequency-domain THz spectra of the moldy wheat samples

408 Fig.5 Scores scatter plot of PC1, PC2, and PC3 for each moldy wheat sample

409 Fig.6 Loading weights of the top four PCs used for selecting the optimal frequencies

410 Fig.7 Scatter plots of the actual value versus the predicted value using the PCA-SVM model  
411 based on (a) the full spectrum and (b) the optimal frequencies for different moldy wheat samples.

412 Fig. 8 THz images of four wheat grains with different mold statuses: (a) normal; (b) slightly  
413 moldy; (c) moderately moldy; (d) seriously moldy.

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## Figures

Fig. 1

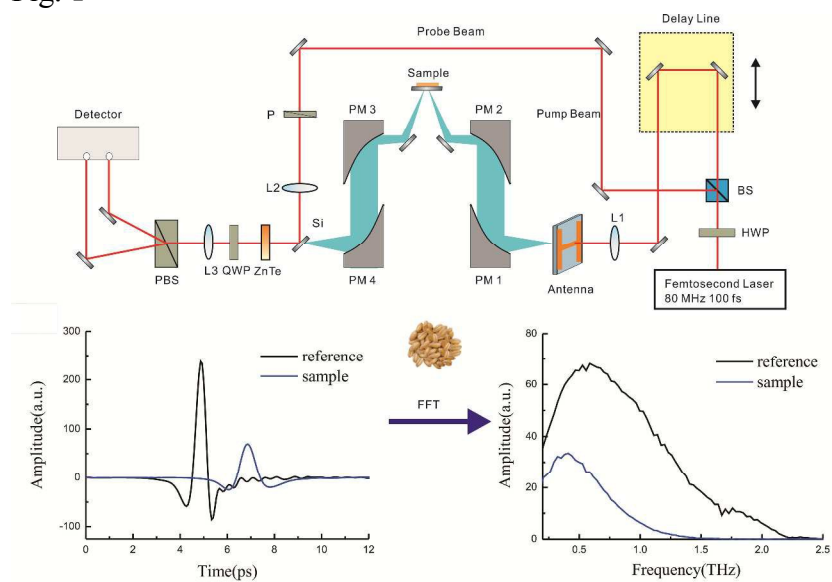


Fig. 2

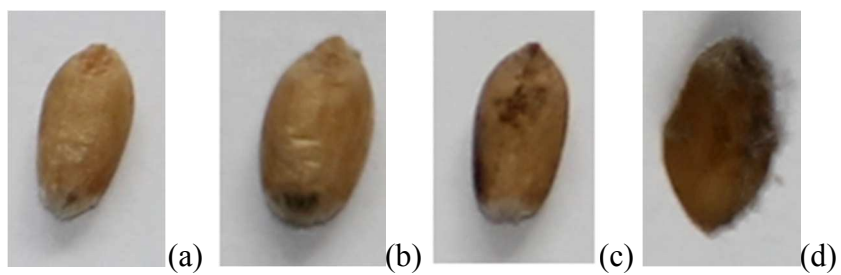


Fig. 3

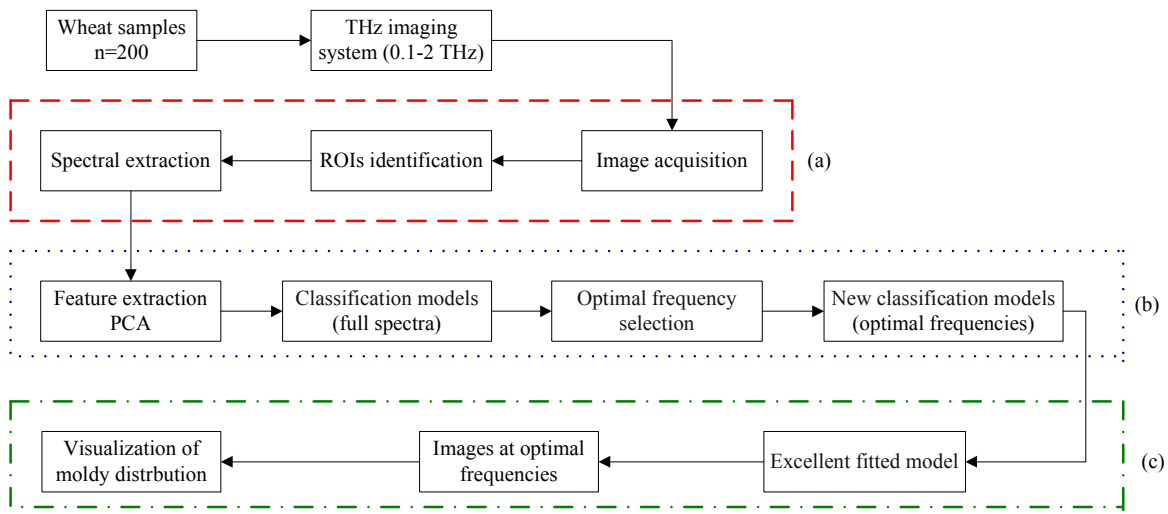


Fig. 4

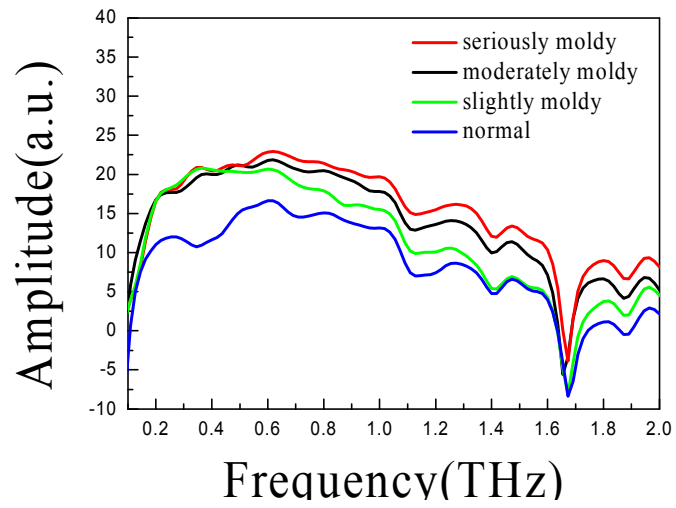


Fig. 5

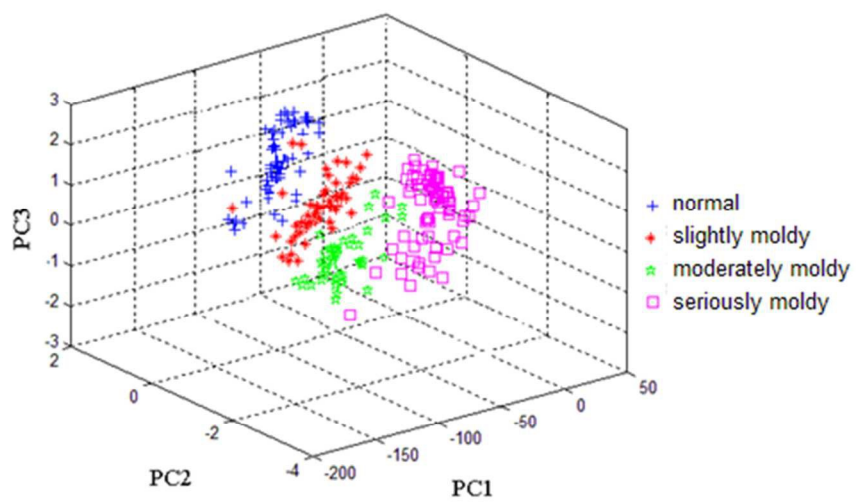


Fig. 6

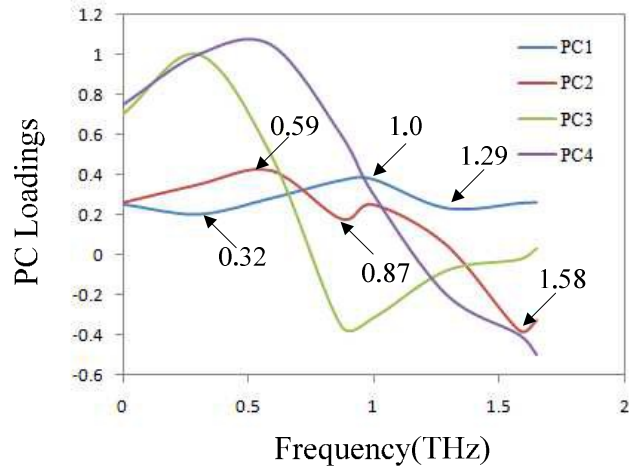


Fig. 7

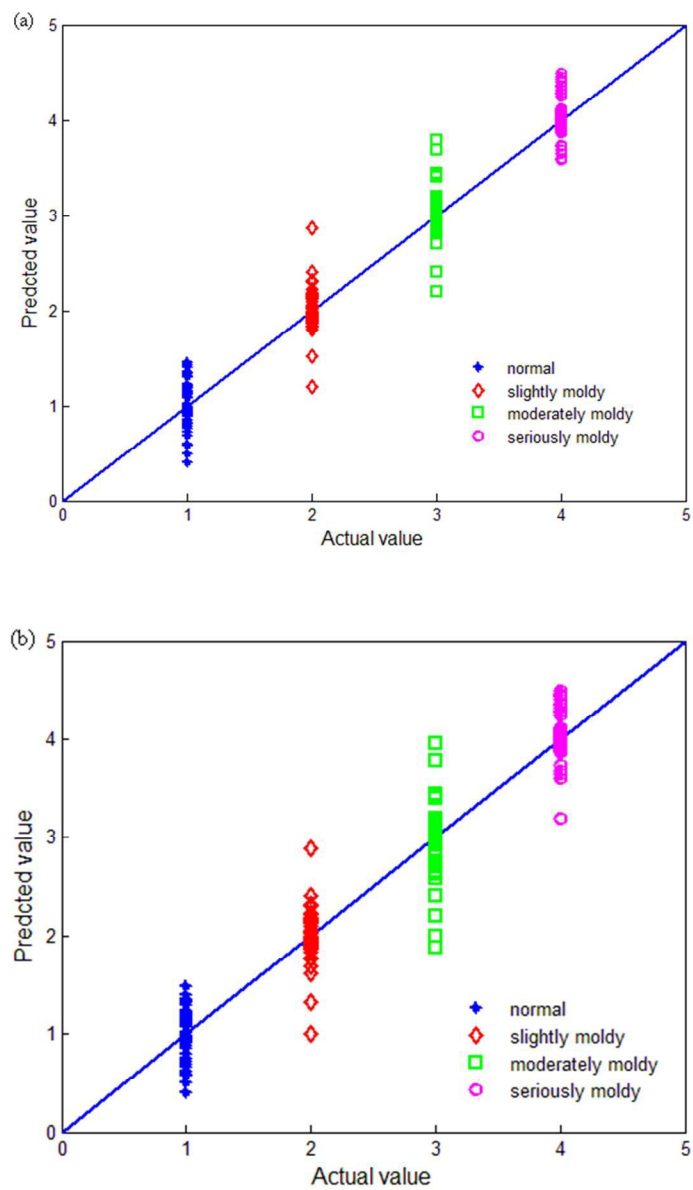




Fig. 8

