Vision Based Metal Spectral Analysis using Multi-label Classification

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   - Background
2. Experimental Setup
   - Simulation Setup
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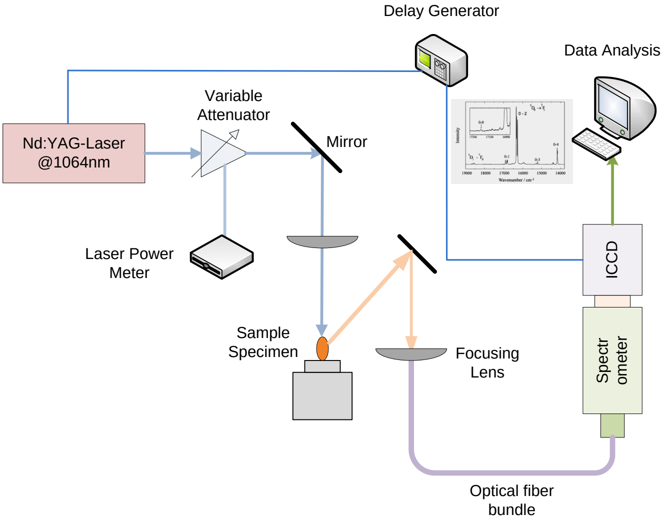
   - Contributions and Future Work

What is Laser Induced Breakdown Spectroscopy (LIBS)?

- An atomic emission spectroscopic method
- Spectral composition of emission depends on the constituent atomic species of the ablated material
- A simple identification of elements to a determination of relative concentrations

Schematic Diagram of a LIBS Setup



Machine Vision System for Automated Spectroscopy

- A fully automatic, real-time technique for detecting constituent elements using machine vision and machine learning techniques on LIBS spectra
- Developed within a commercially available camera
- Two dimensional analysis of spectra
- Developed for detecting contaminants in machine lubricants

Detection Algorithms in the Background

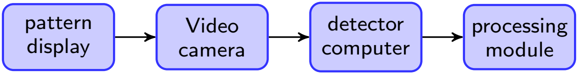
Task:
Identify an unknown sample by correlating its spectrum with a library of spectra

Algorithms:

- Linear correlation [Lentjes. *et al.* 07]
- Rank correlation [Gornushkin *et al.* 99]
- Peak detection [Barbini *et al.* 00]
- Method of normalized coordinates [Ferrero *et al.* 08]
- Principle Component Analysis [Samek *et al.* 01]
- Neural networks [Sirven *et al.* 06]

Our Simulation Setup

- A simulation setup for verifying proposed detection algorithms
- Our setup consists of four main blocks: a random pattern display, a video camera, detector computer and a processing module



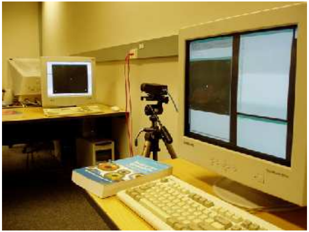


Figure: Camera-computer setup

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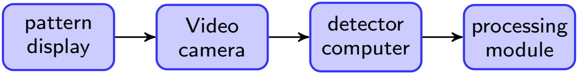

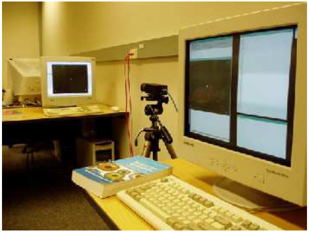

Figure: Camera-computer setup

Registration Using Homographies

- Image plane and the scene plane are not parallel in general
- The observed image and canonical point locations in the repository need to be registered
- Pattern alignment is obtained using markers and computing homographies [Hartley & Zisserman, 03]

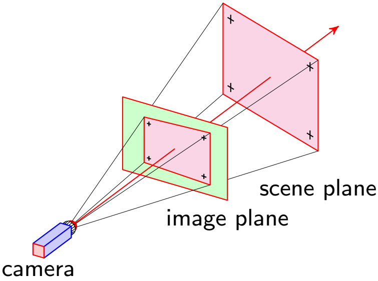

Figure: Necessity for plane alignment

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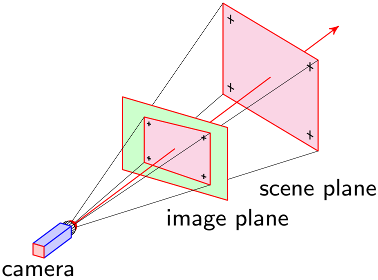


Figure: Necessity for plane alignment

Screenshots of Pattern Display

(a) Ag

(b) Cr

(c) Cu

(d) Fe

(e) Ni

(f) Pb

Experimental Apparatus

- Possess complete access to the camera internals
- Algorithms are developed in C language and cross compiled for the embedded processor of the camera

Table: Experimental conditions and apparatus

Laser	Microchip
Frequency	1KHz free mode
Optical fiber	
Numerical Aperture, core diameter	0.11, 50 μm
Spectrometer	
Minimum Spectral range	250 nm to 600 nm
Spectral resolution	1 nm
Detector	CMOS image Sensor
Active pixels	1280 $\times$ 1024
Image Area	6.66 mm $\times$ 5.32 mm
Pixel Size	5.2μm $\times$ 5.2μm
Camera	Elphel 353 series
Processor	Axis ETRAX FS
Embedded OS	Linux 2.6
Grating	Diffraction Grating Array
Size	12.5 mm $\times$ 12.5 mm
lines	four 12.5 $\times$ 2.8 mm titled gratings

Point Spread Function (PSF)

- A spatial response of an imaging system to a point light source
- Blobs are spread largely across dispersion lines
- Rough approximation for PSF

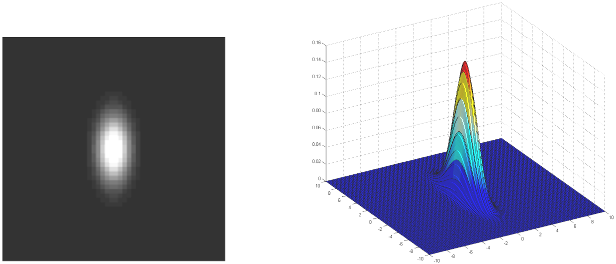


Figure: An anisotropic Gaussian kernel used in our LIBS experiment

Quantum Efficiency (QE) of the Sensor

- Percentage of photons hitting the photo detector that will produce electron-hole pair
- Limit the detection of metals whose emissions lie at wavelengths of lower QE
- Use of inverse gain characteristic curve to compensate for blobs corresponding to lower QE

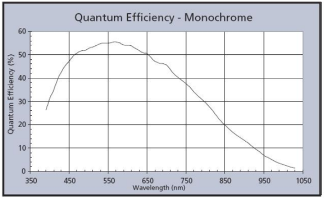


Figure: QE of the monochrome sensor: MT9T001. Figure is reproduced here from the datasheet

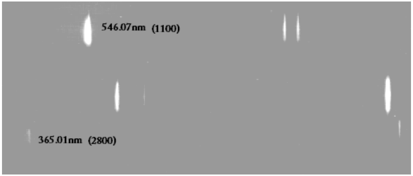


Figure: Effect of quantum efficiency on blob patterns

Wavelength profile

Sensor and Laser Control

- Laser operators at a significantly higher speed (1KHz). The camera frame rate is 30 frames/second
- This creates a much stronger signal, although it makes the detection more challenging

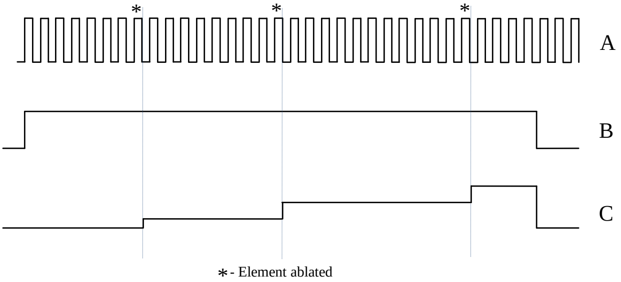


Figure: Laser pulses and exposure time
(a) 1 KHz laser pulses (b) camera exposure (c) signal of a given pixel of the sensor.

Spectral Patterns from Experiments

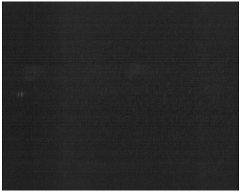
(g) Mercury

(h) Helium

(i) Neon

(j) Sodium

(k) Copper



(l) Aluminum

Multi-label Classification for Spectral Analysis

- A spectrum could contain emissions from multiple elements
- Cast the metal detection problem as a multi-label classification and enable detection of multiple elements
- Used in applications such as text classification, scene classification and protein function classification [Tsoumakas and Katakis, 07]

  e.g: A scene could belong to more than one conceptual class, such as *beaches* and *sunsets* [Boutell *et al.* 04]

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Methods for Multi-label Classification

Support Vector Machines

- Most widely used technique in multi-label classification [Boutell *et al.* 04]
- Use of one-vs-rest approach
- Decompose the problem into a set of binary classification problems and develop a classifier for each class
- Classifiers consider each sample to which it belongs as positive and considers other samples as negative

Artificial Neural Networks

- Use of a neural network with one output node per class
- Use of back propagation algorithm for training

Multi-label Classification Algorithm

Algorithm 1 Multi-label classification algorithm

Ensure: image exists ▷ image is a frame from video stream

Detect markers.
Compute H.
Extract the *regions of interest*
for $k \leftarrow 0, K-1$ patterns **do**
    for $i \leftarrow 0, n_k$ points **do**
        Calculate similarity $score$ between thresholded image region and blob
    end for
    $score \leftarrow$ average similarity.
end for
Form the feature vector
Train L binary classifier
for $j \leftarrow 0, |L|$ classes **do**
    Match the new instance against all
end for
Take the union and Print k of matched patterns

Simulation Results

- Use of single emission spectra of Ag,Cu,Pb,Cr, Fe and Ni for experiments
- Experiments conducted using:
  - A camera resolution of 800×600 pixels
  - A frame rate of 22.3 frames/second
  - change of pattern display every two seconds
- Use of *Accuracy* as the basis for evaluating the performance of the algorithms

$$\text{Accuracy} = \frac{TP + TN}{TP + FP + FN + TN} \quad (1)$$

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Performance of template matching algorithm for a varying threshold

- Ten experiments for each threshold value (each, 1200 samples)
- Performance is fairly sensitive to threshold

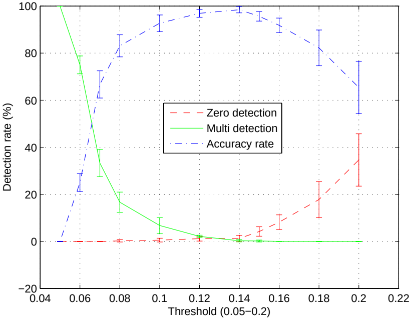


Figure: Detection rates of the pattern matching technique against varying threshold

Training the Classifiers

- Ag, Cu, Pb, Cr, Fe, and Ni metal spectra are considered as single emissions. Ag+Pb, Ag+Cu, Pb+Cu and Ag+Pb+Cu as composite emissions
- Use of similarity score with Ag, similarity score with Cu etc... as features
- SVM employ six binary classifiers
- ANN has six output nodes

Table: Training and Testing Data

Metal	Ag	Pb	Cu	Fe	Cr	Ni	Ag,Pb	Pb,Cu	Ag,Cu	Ag,Pb,Cu	Total samples
Training	220	210	260	160	180	170	150	140	210	200	1900
Testing	450	350	300	350	400	350	400	450	500	250	3800

Results of SVM

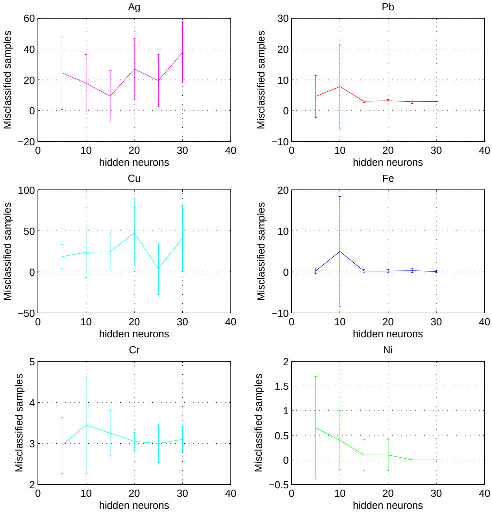
Experimental conditions

- 800×600 resolution, 22.3 frames/second and patterns display every $2s$

Table: Performance of SVM on our synthetic data set

Element	Single metal	Multiple metals	Misclassified samples	Standard deviation	Accuracy rate (%)
Ag	450	1150	7.2	2.82	99.81
Pb	350	1100	4.3	2.26	99.89
Cu	300	1200	8.2	2.57	99.78
Fe	350	–	0.8	0.42	99.98
Cr	400	–	1.2	1.03	99.97
Ni	350	–	0.4	0.51	99.99

Results of ANN against for varying number of hidden Neurons



Actual Experimental Results

- Use of single emission spectra of Hg, Na, Ne, He, Al, Zr, Ag, Pb, Cu and Ni
- Use of ten binary classifiers for SVM and a single ANN with 10 output nodes (10 hidden neurons)
- Higher level of noise present in actual images, e.g. broadband spectra

Table: Results of experiments using real data from the prototype spectrometer

The summary of performance data obtained from the correlation method, SVM and ANN on the actual experimental data. Learning methods show promising results on testing data.

Metal	Training samples	Testing samples	Accuracy (Correlation)	Accuracy (SVM)	Accuracy (ANN)
Hg	30	30	96.12	100.00	100.00
Na	30	30	97.09	99.69	99.69
Ne	50	50	98.34	100.00	100.00
He	20	20	95.31	100.00	99.43
Al	20	20	85.43	98.12	98.00
Zr	40	40	86.65	99.06	98.58
Ag	30	30	89.21	98.83	98.41
Pb	50	50	83.75	99.62	98.94
Cu	20	20	91.47	99.71	98.13
Ni	30	30	88.93	99.81	98.58

Conclusion

- Fully automatic, rapid element detection on LIBS spectra is feasible on a commercial camera
- Able to obtain accuracy rates exceeding 99%
- Useful in instances in which a qualitative analysis of elements is sufficient

Contributions

- Automatic identification of a single element, as well as identifying multiple elements with overlapping spectral peaks
- Use of multi-label classification approach to metal spectroscopy
- A simulation setup for testing detection algorithms

Future Work

- Investigate the ability to estimate relative composition of elements
- Developing the proposed techniques at an FPGA level in the embedded processor of the camera

Thank you

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Questions!