Automatic classification of metal alloys from their LIBS spectra and its robustness against spectrometer decalibration

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In metal scrap sorting industry, an online identification system would enable automatic sorting based on value, recycling requirements, presence of hazardous materials ... LIBS has probed a suitable technique. However, simultaneous identification of some elements (Phosphor, Sulfur...) is not easy and instrumentation cost is an issue. If low-cost spectrometers are used, long-term decalibration due to thermal drift, shocks or ageing could drastically impact the classification performance.

In this work, we propose the use of deep-learning algorithms for automatic classification using raw LIBS spectra in a wide spectral window with low resolution, avoiding the preprocessing or the peaks/elements identification step. This approach enables the use of low cost spectrometers and simplify the processing software in operation once the deep network has been trained. However, it could be very sensitive to the long-term decalibration of the spectrometer.

A deep network of stacked autoencoders has been implemented in Matlab®, with 1020 neurons in the input layer, and 3 internal layers of 256, 128 and 32 neurons. A soft-max classifier with 20 outputs gives the predicted class.

The network has been trained with 5,000 raw spectra from each ingot, preserving the intrinsic shot-to-shot intensity variations. The classification performance with new spectra not used for training shows a 0.3% classification error.

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However, the expected long-term wavelength decalibration of the spectrometer should affect the classification performance (+/- 0.25nm deviation for a 10ºC temperature change has been reported). The measured spectra have been artificially decalibrated and the robustness of classification has been obtained. But … training the network with randomly and purposely decalibrated data reduce the classification error in the long term.

Deep ANN networks provide an almost black-box classification tool from raw LIBS spectra, but it is very sensitive to the small wavelength decalibration that is expected from long-term operation in industrial environments. This effect can be reduced if the ANN network is trained with artificially decalibrated spectral data. We are working now with real multi-element scrap samples to check the classification performance.

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