Supporting Information

Rapid nondestructive assessment of degrees of sensitization of 5456 aluminum alloys using laser-induced breakdown spectroscopy (LIBS) with multivariate analysis

Lei Liu, [#,a] Xi Huang, [#,*,a] Haoyu Dong, [a] Aofei Mao, [a] Peizi Li, [a] Bai Cui, [b] Jean-Francois Silvain, [c] and Yongfeng Lu[*,a]

[a] Department of Electrical and Computer Engineering, University of Nebraska, Lincoln, NE 68588, USA.

[b] Department of Mechanical and Materials Engineering, University of Nebraska, Lincoln, NE 68588, USA.

[c] CNRS, University of Bordeaux; Bordeaux I.N.P., ICMCB, UMR 5026, F-33608 Pessac, France.

# Lei Liu and Xi Huang contributed equally to this work.

* *Corresponding authors: Xi Huang, huangxi.1989.u.s@gmail.com; Yongfeng Lu, ylu2@unl.edu*

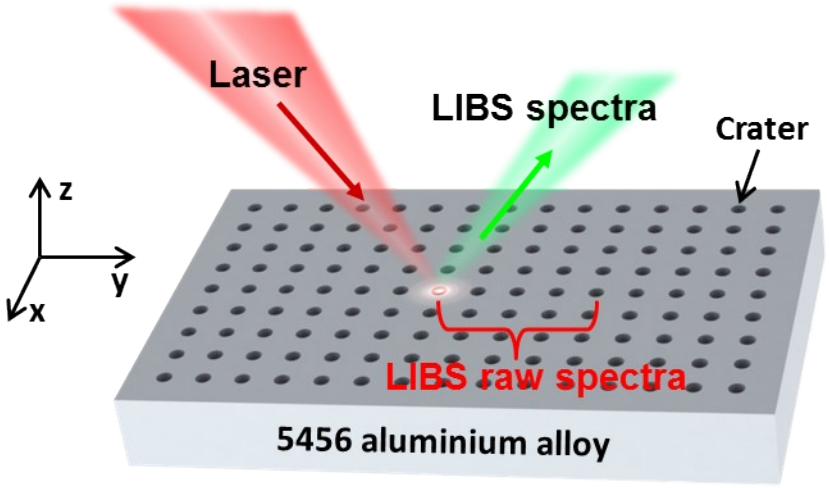

Figure S1. Schematic of the laser linear scanning on a sample surface for LIBS measurements.

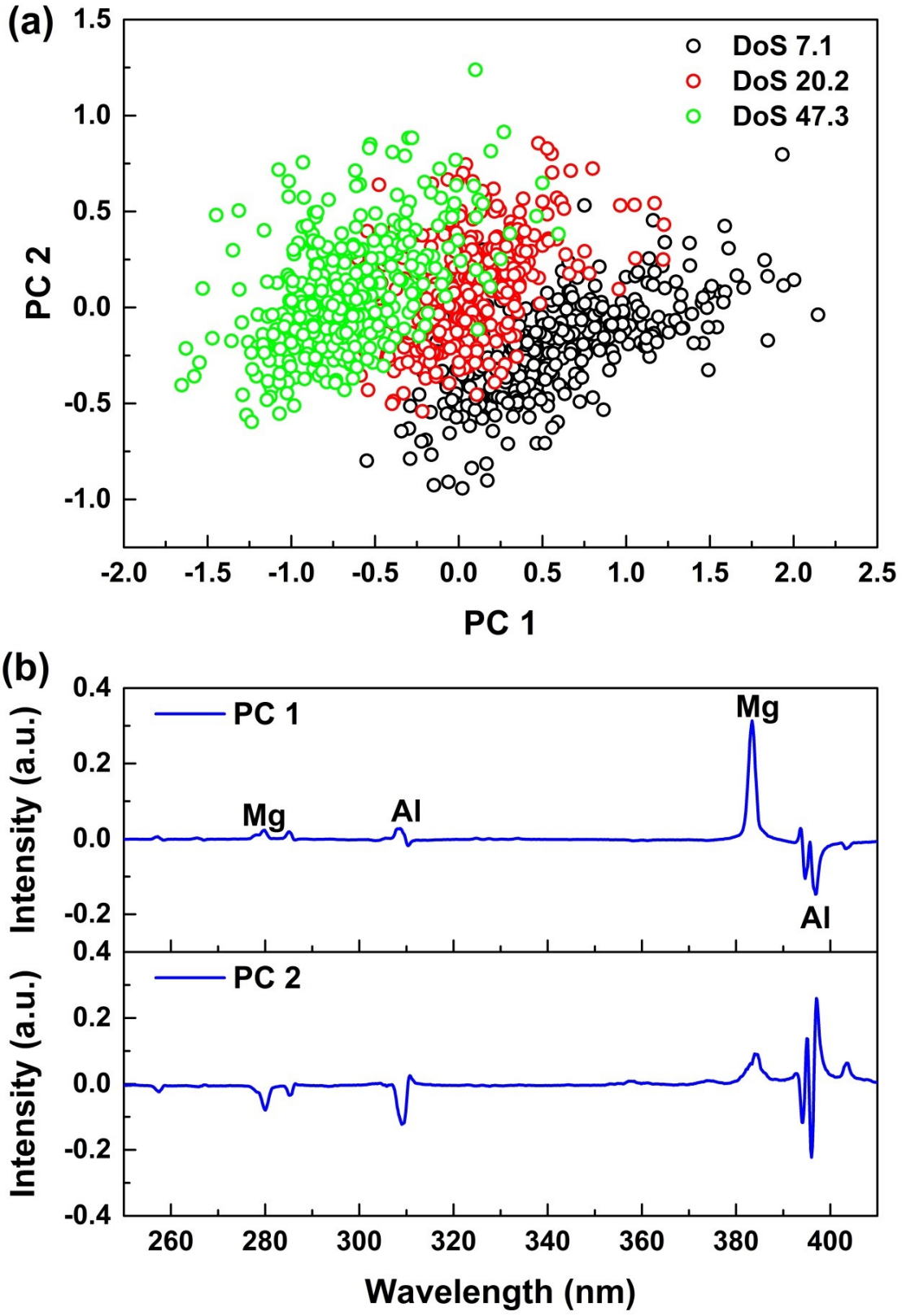

Figure S2. The (a) scores and (b) loadings of PC 1 and PC 2 in PCA.

Using a fixed laser beam, the sample was moved at a speed of 1 mm/s by a three-dimensional motorized stage. For each laser pulse, a crater was created on the sample surface for each LIBS spectrum taken. For all LIBS spectra used in this research, each was averaged from 5 laser pulse measurements to improve the signal stability and used as raw LIBS spectra for subsequent multivariate analyses using principal component and discriminant function analysis (PC-DFA).

Each raw spectrum has 1024 variables (wavelengths in the spectrum). PCA reduces the number of variables into principal components (PCs) which sequentially carry the most important information of the dataset. PC #1 and PC #2 carry the most and next important data information with 57.0% and 13%, respectively, of the total variance. The scores and loadings of PC 1 and PC 2 in PCA are shown in Figure S2 (a) and S2 (b), respectively. PC scores are the sequentially listed values of PCs after PCA transformation of LIBS spectra. PC loadings can be under-stood as the weights for each original variable (wavelength in spectral analysis) when calculating the PCs in PCA. As shown in Figure S2 (a), the LIBS spectra correlated with different DoS values are mainly classified by PC 1. Moreover, LIBS spectra correlated with lower DoS values have larger PC 1 scores. In addition, PC 1 loading (as shown in Figure S2 (b)) shows that the Mg I 383.5 nm emission line significantly contributes to positive PC 1 score. Hence, LIBS spectra contain higher Mg concentrations contribute more to positive PC 1 score, correlated with lower DoS values. This result is consistent with the material properties that materials with lower DoS values containing higher Mg concentration on the sample

surface after chemical etching due to less loss of β-phase (Mg_2Al_3 with Mg concentration of ~38 wt%)) precipitates which were preferentially dissolved during chemical etching.