

**Supplementary Material for:**

**Novel Surface Topography and Microhardness Analysis of Laser Clad Coating on TC4 Titanium Alloy Using Laser Induced Breakdown Spectroscopy and Machine Learning**

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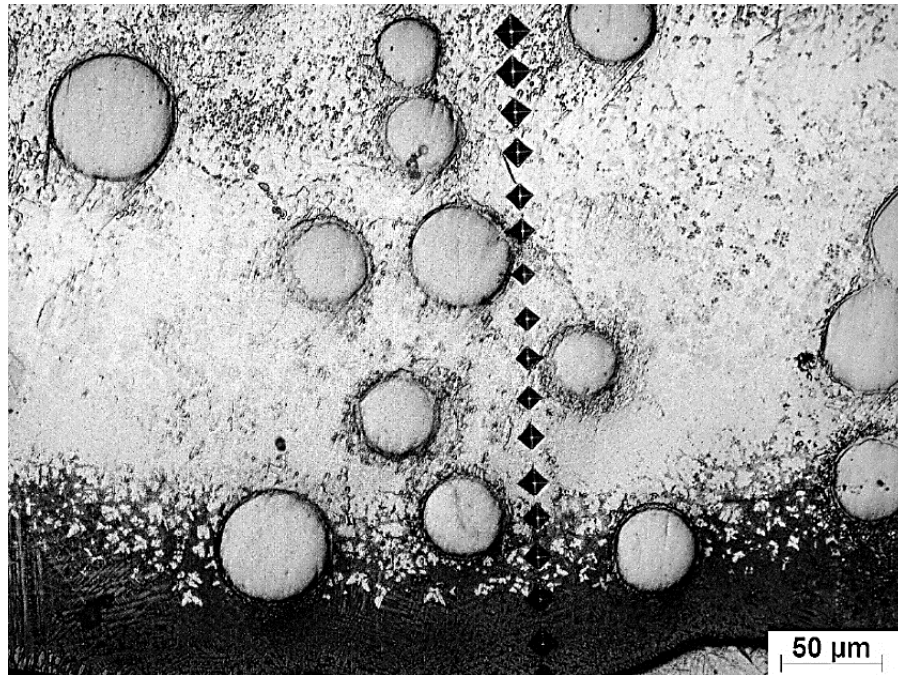
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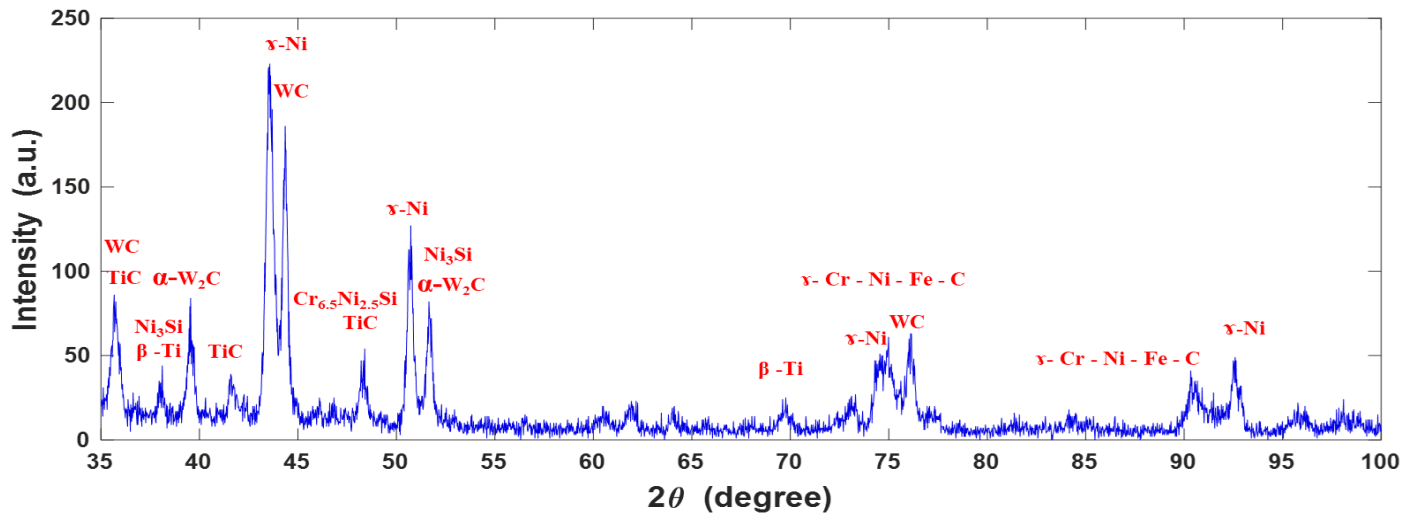
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**Measurement of coatings microhardness on metallographically prepared cross-sections by means of an HMV Vickers hardness tester**



**Fig. S-1.** The appearance of hardness traces throughout the metal matrix coating of a sample processed at  $20 \text{ g}\cdot\text{min}^{-1}$ .

## Identification of matrix phases observed in the clad layer using X-ray diffraction spectrum



**Fig. S-2.** X-ray diffraction spectrum of the clad layer with 60 WC + 40 NiCrBSiC blended powder at a powder feeding rate of 20 g.min<sup>-1</sup>.

### Belsley collinearity diagnostics

Belsley collinearity diagnostics were applied to LIBS data represented by a matrix of  $249 \times 246$  elements to measure the strength and sources of multicollinearity among the 246 variables. In brief, it computes the 246 singular values of the matrix and the variance decomposition matrix that comprises  $246 \times 246$  variance decomposition proportions in which each row is associated with one singular value. Then, the singular values were arranged in descending order and converted into indices of variance decomposition (Figure S-3(a)). Since the separate near dependences of the data matrix appear only for the highest indices, the location of high proportions exceeding a predetermined tolerance for the highest indices was utilized to identify the dependent variables. A tolerance value of 0.5 was chosen according to [1]. Considering the variance decomposition proportions of the last twelve rows corresponding to the highest 12 indices given in Figure S-3(b), it is clear that the last row associated with the highest index has a number of 17 proportions above the tolerance suggesting that these variables are dependent and exhibit multicollinearity. It can be also observed that the row of variance decomposition matrix related to the second-highest index has another two high proportions that exceed the tolerance. While their preceding row cannot identify any variable dependency, not two or more variables are observed above the tolerance that is required for dependency. Then, such dependent emissions lines had to be associated with less significant canonical correlation coefficients (less than  $5 \times 10^{-5}$ ). The variance decomposition proportions of the last twelve rows corresponding to the highest 12 indices after removing the emission lines which have absolute correlation coefficients less than  $5 \times 10^{-5}$  given in Figure S-3(c) depicts no source of multicollinearity among the variables.

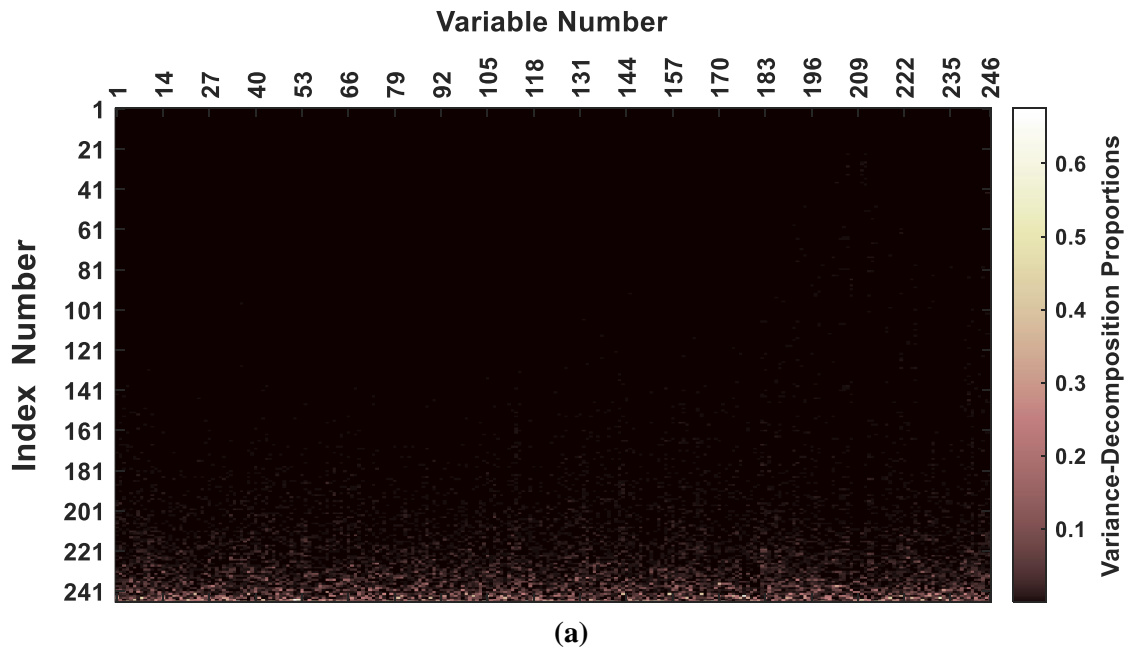
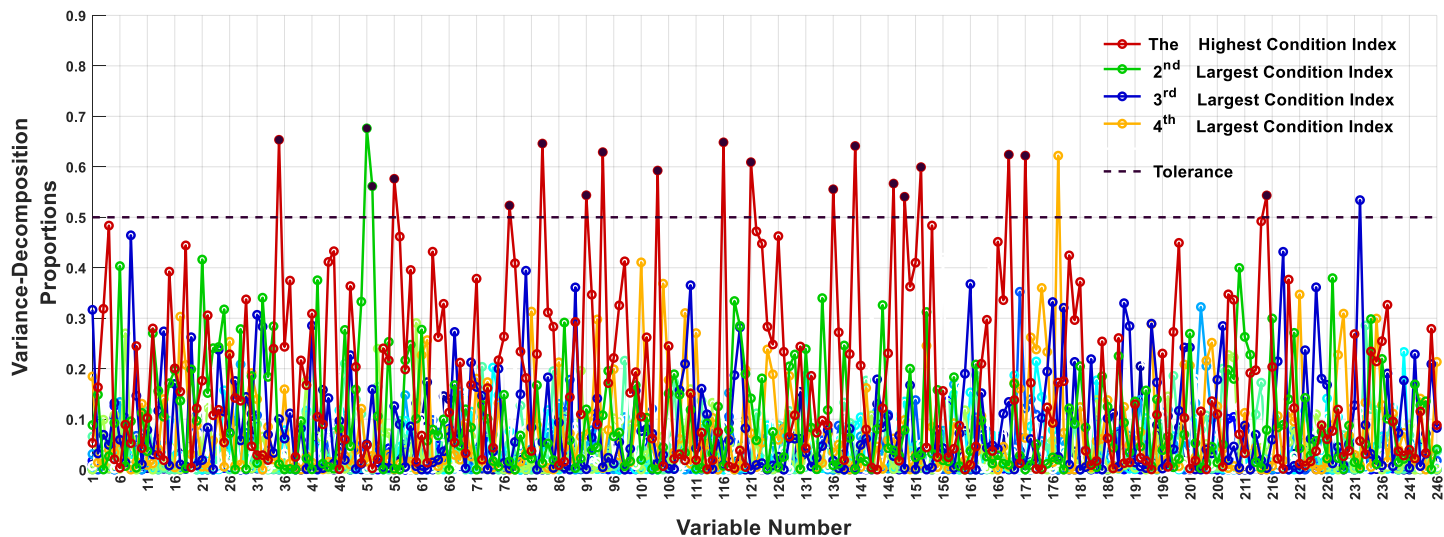
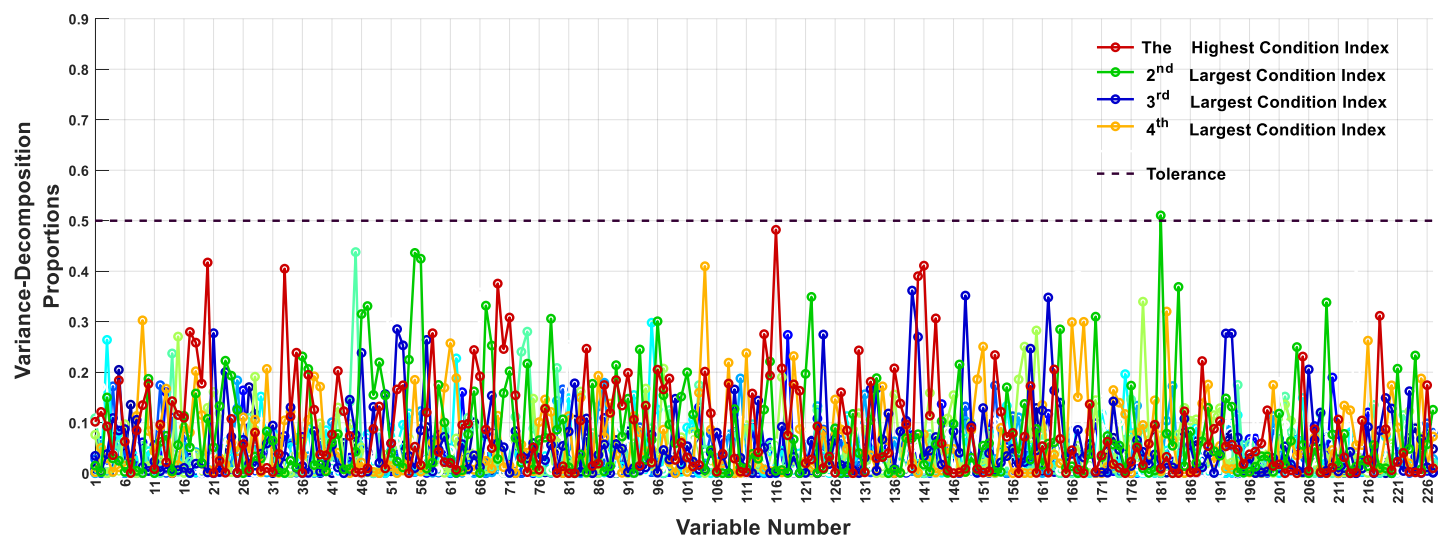


Fig. S-3. Cont.



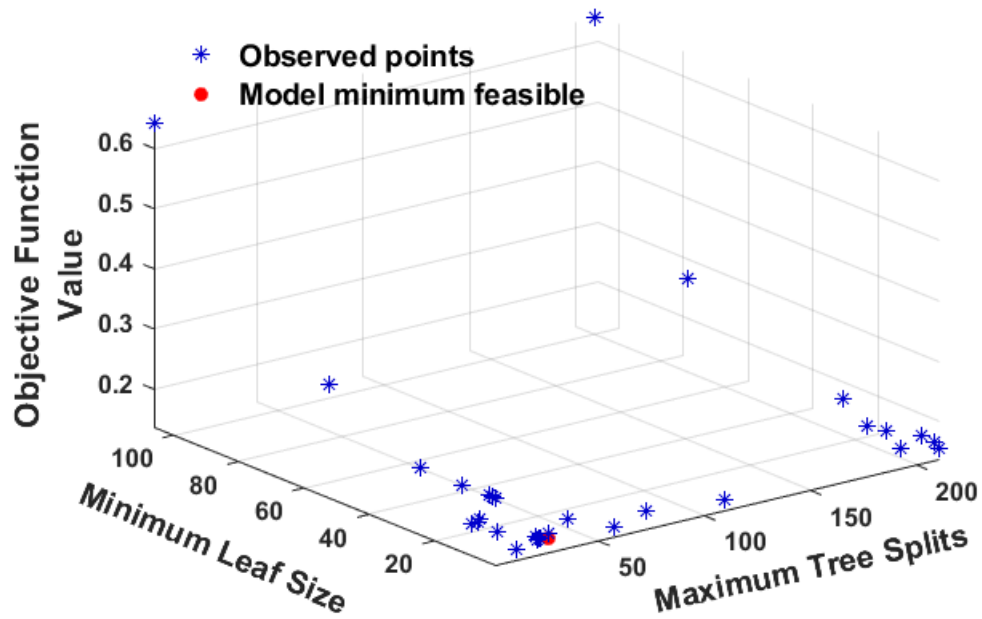
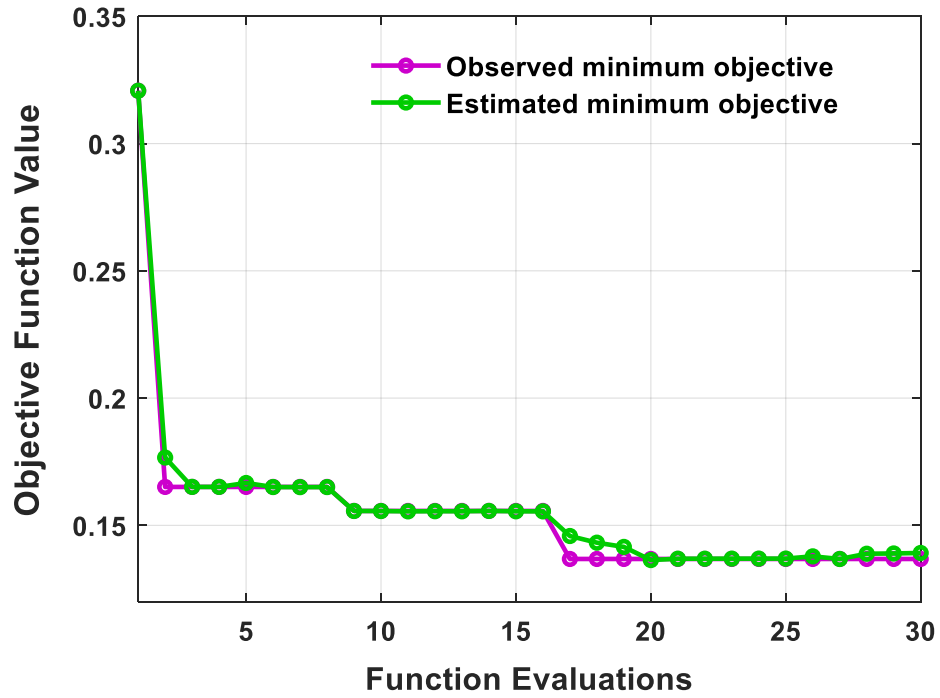
(b)



(c)

**Fig. S-3.** Belsley collinearity diagnostics for evaluating the source of collinearity among variables: (a) the variance decomposition matrix for the selected 246 variables, (b) and (c) the variance decomposition proportions of the last twelve rows corresponding to the highest 12 indices before and after removing the emission lines which have absolute correlation coefficients less than  $5 \times 10^{-5}$ , respectively.

The hyperparameters as returned by the optimization model for 50 classification trees



**Fig. S-4.** Bayesian optimization results for locating the maximum number of decision splits and minimum leaf size for achieving the unique minimum objective.