Bandgap tuning of niobium-based oxides in thin film combinatorial libraries

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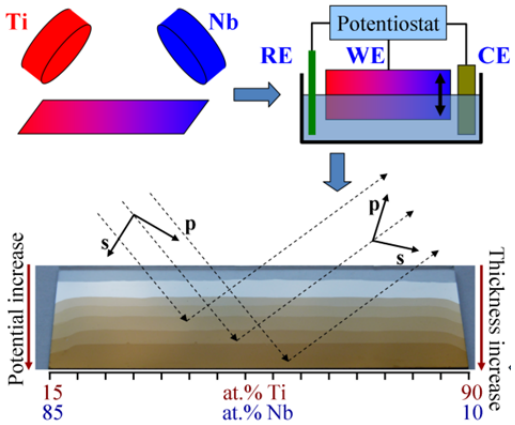
Oxides of Nb, Ta and Ti show promising capabilities for nanocomposite formation enhancing photocatalytic activities in electrochemical energy production and/or storage applications. Variable angle spectroscopic ellipsometry (VASE) is used for optical properties mapping of anodic oxides grown on Nb-Ta and Nb-Ti thin film combinatorial libraries. The microstructure of the Nb-based parent metal alloys was tuned in order to avoid compositionally induced microstructure dissimilarities between alloys. Upon step-wise anodization up to 10 V vs SHE VASE was used to calculate the oxide. The mixed oxides showed absorption close to visible photon energies and presented indications that an in-depth compositional gradient may be present. Individual bandgaps of Nb-based mixed oxides were mapped as a function of composition and a non-linear behavior was identified [1, 2]. The deviation from the linear model predicted by the mixed matter theory when applied for calculating the metal alloys electronegativities was explained by an in-depth compositional gradient of the mixed oxides. Surface enrichment of minority species in oxidized form triggered a depletion of that species at the metal/oxide interface shifting the metal alloys electronegativities in a non-linear manner. Compositional tuning of the parent metals revealed the possibility of mixed oxides bandgap tuning.



[1] W. Limberger, C.C. Mardare, C. Cobet, J. Zuo, A.W. Hassel, A.I. Mardare, RSC Adv. 6 (2016) 79934

[2] P. Bleckenwegner, C.C. Mardare, C. Cobet, J.P. Kollender, A.W. Hassel, A.I. Mardare, ACS Comb. Sci., 19 (2017) 121