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Correlation between experimental results and ab initio calculations in TiN-based decorative coatings

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Ti-X-N films (X = Ca, La, Mg, Sn or Y) were deposited on stainless steel substrates using a hybrid reactive arc evaporation - magnetron sputtering process. The X content into the films was adjusted by the pulsed DC current applied to the X sputtering target. The deposited films were characterised by XRD, EDS, UV-visible spectrometry and SEM. The nature of the X element is shown to strongly influence the structure of the deposited films. Using Ca, Mg and Y, a (Ti,X)N solid solution is evidenced using XRD. As a function of the y = X/Ti content, coatings exhibit nice coppery or violet colours suitable for decorative applications. On the other hand, Ti-La-N and Ti-Sn-N films are amorphous and bi-phased (TiN + Sn), respectively showing a rapid evolution from golden-like to grey metallic colours. To rationalize these observations, first-principles density functional theory (DFT) calculations were performed on Ti-X-N bulk, as a function of the y = X/Ti ratio. The results show that the blue/red shift of the Ti-X-N absorption band (with respect to y) can be directly correlated to the nature of the X element (number of electrons and orbitals involved) by means of local Ti à X or X à Ti electron transfers. Phase stability diagrams were also computed to correlate the crystallized or amorphous nature of the Ti-X-N films to the X element nature and size. This study aims at providing simple concepts and rules to be used as a starting point for the design of new coloured coatings.

Keywords
Decorative coatings
ab initio calculations