MICROMECHANICAL NUMERICAL MODEL FOR THE EVALUATION OF THE ELASTIC PROPERTIES AMORPHOUS TITANIUM DIOXIDE THIN FILM

N. Cefis[1], M. G. Beghi[2]

[1]*Department of Civil and Environmental Engineering (DICA), Politecnico di Milano, Milan, Italy, e-mail: nicola.cefis@polimi.it*

[2]*Department of Energy, Politecnico di Milano, Milan, Italy, e-mail: marco.beghi@polimi.it*

In this communication we present a numerical methodology for the mechanical assessment of thin films in amorphous titanium dioxide deposited by PLD (Pulsed Laser Deposition) technique on crystalline substrates. The morphology of these films includes columnar structures in amorphous titanium dioxide interspersed with empty regions. These films are widely used for several civil and industrial applications in which the photocatalytic properties of titanium dioxide are exploited when they are exposed to UV rays (evaporative systems, surfaces of buildings in urban environment, dye-sensitized solar cell [1]).

The novel numerical procedure aims at estimating the elastic moduli of nanostructured films through two subsequent steps. In the first step, starting from the SEM images of the frontal morphology, a model of the Reference Volume Element (RVE) is provided. In the second step, assuming a priori the elastic parameters for the amorphous titanium dioxide [2], a homogenization procedure with periodic boundary conditions is utilized to estimate the macroscopic response [3]. Such a procedure was implemented in Abaqus environment. The elastic parameters thus obtained turn out to be in satisfactory agreement with those provided by optical techniques based on Brillouin scattering [4].

References

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