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Multiscale thermo-mechanical analysis of multi-layered coatings in solar thermal applications

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ABSTRACT

Solar selective coatings can be multi-layered materials that optimize the solar absorption while reducing thermal radiation losses, granting the material long-term stability. These layers are deposited on structural materials (e.g., stainless steel, Inconel) in order to enhance the optical and thermal properties of the heat transfer system. However, interesting questions regarding their mechanical stability arise when operating at high temperatures. In this work, a full thermo-mechanical multiscale methodology is presented, covering the nano-, micro-, and macroscopic scales. In such methodology, fundamental material properties are determined by means of molecular dynamics simulations that are consequently implemented at the microstructural level by means of finite element analyses. On the other hand, the macroscale problem is solved while taking into account the effect of the microstructure via thermo-mechanical homogenization on a representative volume element (RVE). The methodology presented herein has been successfully implemented in a reference problem in concentrating solar power plants, namely the characterization of a carbon-based nanocomposite and the obtained results are in agreement with the expected theoretical values, demonstrating that it is now possible to apply successfully the concepts behind Integrated Computational Materials Engineering to design new coatings for complex realistic thermo-mechanical applications.

1. Introduction

One of the most difficult challenges in Solar Thermal Electricity (STE) power plants is the increase in the operating temperature beyond current limits in order to boost the efficiency of the cycle in concentrated solar power (CSP) plants.

There are two major CSP plant configurations, namely central receiver systems (CRS) and parabolic trough (Fig. 1a and b, respectively). A key component in both configurations is the receiver tube, through which solar heat radiation is transferred to the so-called heat transfer fluid (HTF), increasing its temperature before feeding the power block [1]. In the former configuration, tubes are arranged within an exposed cavity; while in the latter, the absorber tube is located at the focal point of the collector, usually inside the vacuum chamber conformed by another external glass tube. The thermal performance of this component strongly depends on the optical and thermo-mechanical properties of the tube materials.

The final goal of the receiver tube is therefore to heat the HTF that will eventually run (directly or by means of steam via an intermediate heat exchanger) the turbine. Thus, the purpose of the tube is to absorb as much solar radiation as possible, conduct it, and finally heat the HTF by forced convection [2].

Solar selective coatings (SSCs) [3,4] are multi-layered materials that optimize the solar absorption while reducing the thermal radiation losses, granting the long-term structural stability. A variety of thin film architectures can be exploited as SSCs for obtaining spectral selectivity. One of the most efficient configurations is based on a multi-layer stack, whose composing layers are usually arranged as depicted in Fig. 2, and described in the following [5]:

a) an antireflective (AR) layer (e.g., Al_2O_3, SiO_2), transparent to solar radiation to increase solar absorption and chemically stable in air at high temperature so as to reduce corrosion;
b) an absorber layer (e.g., transition-metal nanocomposites, cermets), which must offer optimal optical properties regarding absorption and conductivity as well as thermo-mechanical stability;

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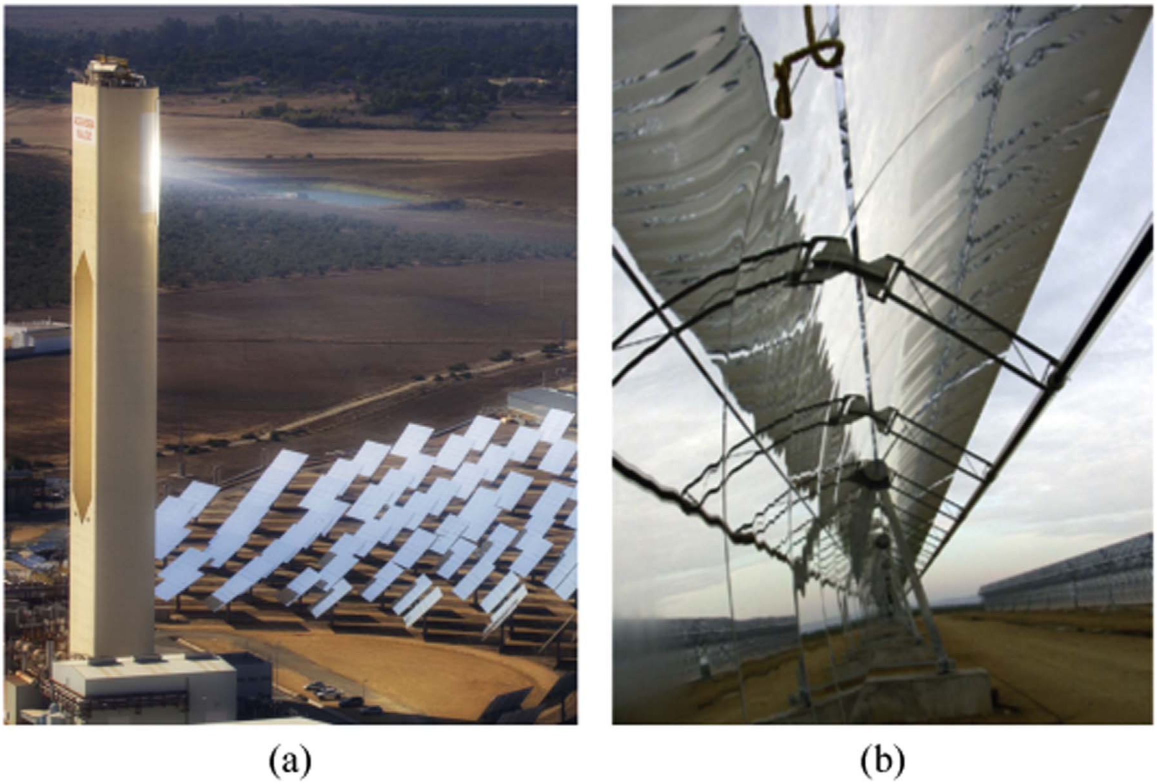
(a) (b)

Fig. 1. Solar selective coatings are present in two main concentrating solar power (CSP) plant configurations: a) central receiver systems and b) parabolic trough absorber tubes.

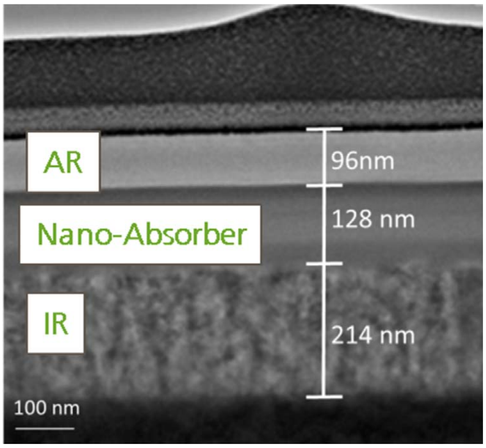

Fig. 2. Cross section scanning electron image of a complete selective stack structure developed for the present application. The stack consists (from substrate to the surface) of an infrared (IR) layer, an absorber nanocomposite coating (nanoabsorber), and an antireflective (AR) top film.

c) an infrared reflective (IR) layer (e.g., metal nitrides) beneath the absorber, with high reflectivity in the infrared region to reduce emissivity; and, finally,
d) a substrate (e.g., stainless steel or Ni-based alloys) layer, that hosts the HTF and provides mechanical resistance.

The composing materials of each of these layers are typically chosen (or designed) according to their particular optical properties (Fig. 3); therefore, major efforts by materials scientists in Abengoa Research have been devoted in the last years to the optical enhancement of SSCs [5]. However, important questions regarding their thermo-mechanical stability have to be considered.

In this work, a bottom-up multiscale methodology (Fig. 4), developed within the Abengoa's Virtual Materials Design (VMD) project [6], is reported in order to establish a virtual laboratory for testing new structured materials (e.g., SSCs) for renewable energy solutions. In this virtual laboratory, SSCs macroscopic properties required by the continuum models (usually modeled and solved by means of finite element analyses, FEA) are obtained from nanoscale molecular dynamics (MD) simulations in a succession of progressively higher scales with their corresponding interfaces. In this particular work, and in order to show the capabilities of this new tool, a new nanoabsorber layer composed by an amorphous carbon (a-C) matrix reinforced with titanium carbide (TiC) nanoparticles is analyzed. In this sense, original MD results are presented herein, especially for the case of a-C for which a large dispersion in the thermal and mechanical properties is found in the literature [7–9].

Multiscale analysis has been presented as a powerful tool in order to analyze complex heterogeneous media such as composite materials [10,11]. Moreover, it has been applied in two-level continuum thermo-mechanical problems [12,13] or, more recently, covering even three continuum scales [14,15]. With regard to applications, multiscale thermo-mechanical schemes have been successfully used in RVE-based problems (i.e., micro to macro transition) like, for instance, in metal matrix composites [16,17]. In this work, a novel thermo-mechanical homogenization scheme is presented, providing insights into the main features of the numerical simulation strategies, especially those regarding the implementation scheme.

Finally, the thermo-mechanical behavior of the different layers in a piece of the receiver tube is analyzed at the macroscale, providing useful information for the design of this type of components while validating the presented multiscale methodology and demonstrating that it is possible to conduct multiscale analyses, from *atoms to structures*, in a three-scale scheme. However, it must be remarked that, in the presence of other conditions such as finite strains, strain-