Computational Materials Science 62 (2012) 276–281

Contents lists available at SciVerse ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

How to minimise thermal fatigue in surface multi-treatments and coatings?

Pierre D’Ans [*], Marc Degrez

Université Libre de Bruxelles (ULB), Ecole Polytechnique de Bruxelles, 4MAT Department, 50, Avenue F.D. Roosevelt, CP194/3, 1050 Bruxelles, Belgium

ARTICLE INFO

Article history:
Received 1 February 2012
Received in revised form 23 April 2012
Accepted 1 May 2012
Available online 4 June 2012

Keywords:
Surface treatments
Physical vapour deposition
Thermal spray
Thermal fatigue
Performance indices

ABSTRACT

A tool is developed to rank surface treated materials with respect to thermal fatigue. It comprises a modelling of the temperature profile in the component and an adaptation of the Coffin–Manson model for surface treatments fatigue. It is used as a performance index and discussed onto several surface treatments and multi-treatments relevant for the protection of steel in aluminium foundry moulds, exposed to thermal fatigue, with some insight in the effect of surface treatments processes on the final result. The model reproduces the well-known capability of duplex PVD nitride onto nitriding to withstand thermal fatigue. Using thermal barrier coatings may also be relevant, but the internal stress must be sufficiently compressive to be resistant to the studied thermal cycles.

1. Introduction

Thermal stresses affect materials in many fields: aircrafts engines, foundry devices affected by moulding cycles, turbine blades for the energy industry, nuclear fusion reactors, etc. When applied cyclically or repeatedly over time, they often lead to thermal fatigue. For applications involving surface treated metals, such stresses arise from a combination of several factors:

1. The difference of the thermal expansion coefficients of the surface layer and the substrate.
2. The thermal gradients during thermal transients.
3. The residual stresses due to the surface treatment process itself, still present at uniform ambient temperature.

Contributions 1 and 3 mainly affect the layers. Contribution 2 affects both the substrate and the treatment layers.

Frequently, literature provides with extensive and successful mathematical descriptions of thermal flows in multi-materials [1] and crack propagations at failure for specific coatings categories [2]. Some works focus on modelling the thermal fatigue of the substrate [3,4]. Several simple bulk thermal fatigue cases (contribution 2) were modelled in Manson’s work [5], whereas modelling at least one contribution is presented elsewhere [6–10].

However, literature provides with very limited tools to compare coatings with totally different characteristics in terms of thermal fatigue lifetime for contributions 1–3. Such a semi-quantitative tool would be useful for designers to help to minimise the experimental investigations in thermal fatigue problems. The goal of this paper is to propose a way to fill this gap, by:

- Encompassing contributions 1–3 for single or multiple surface treatments.
- Using as much as possible parameters that can be found in the literature, instead of additional empirical parameters.

Surface treatments used for the aluminium die-casting operations are considered as a study case, since these treatments originate from different technologies and since the knowledge in this field is still quite empirical. Thermal fatigue acts there as a major failure mode for steel and its corrosion/sliding wear protective layers. Various treatments were compared: treatments aimed at reducing fatigue (nitriding [11–16], shot peening [17]), corrosion by molten aluminium (thin TiN coating [18–21], boriding [22–24]), and thermal gradients in the substrate (thin PVD thermally insulating oxide [25], thick zirconia [26] using plasma spray).

This paper first describes the model and the specific study case. Then, various surface treatments are ranked in terms of lifetimes in thermal cycling (with mechanical failure). A comparison is made with some important experimental results from the surface treatments literature.

2. Theory and calculation

The (x,y,z) Cartesian axis system sketched in Fig. 1 is assumed in the case of a double layer treatment. The studied treatments are represented in Fig. 2. The studied object is a 4 cm thick flat

---

[*] Corresponding author. Tel.: +32 (0)2 650 30 28; fax: +32 (0)2 650 27 86.
E-mail addresses: pdans@ulb.ac.be (P. D’Ans), mdegrez@ulb.ac.be (M. Degrez).

0927-0256/$ - see front matter © 2012 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.commatsci.2012.05.010

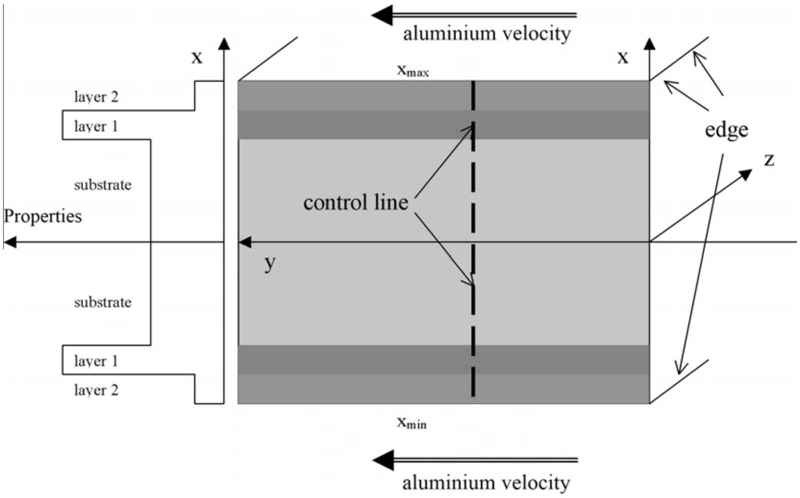

Fig. 1. Axis and properties definition (cross-section of the studied object).

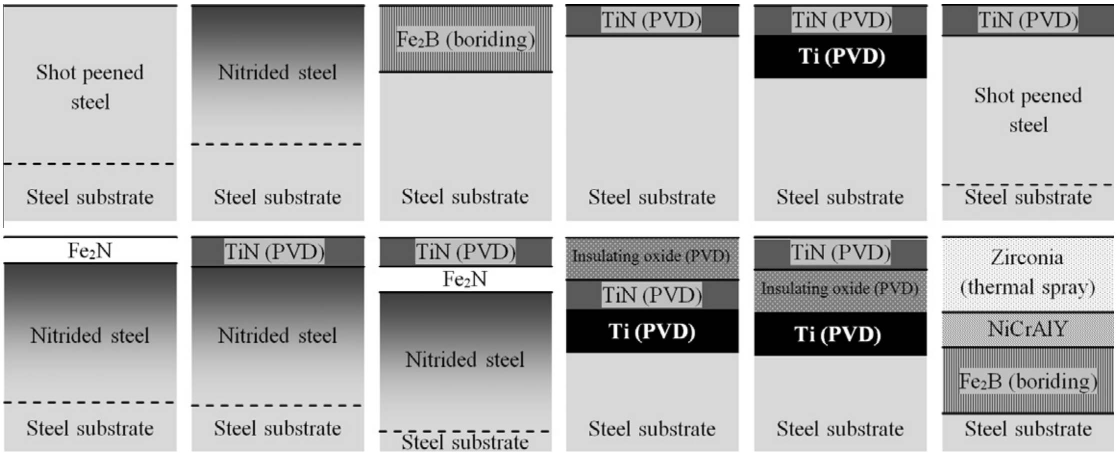

Fig. 2. Studied treatments.

semi-infinite plate, parallel to the y and z axis, symmetric with respect to the (y,z) plane. Such a simple geometry is used for a ranking purpose, but a more complex geometry can be used to model a complete mould during aluminium casting operations, for instance, to determine where failure occurs first.

The proposed methodology is based on the equations used in [27]. For a ranking purpose, it splits into the 9 following steps:

1. Definition of the studied surface treated material: substrate, surface treatment(s) and their respective thickness.
2. Definition of the cyclic time-dependent thermal boundary conditions.
3. For each material/treatment, data mining for: thermal expansion coefficient α, Young's modulus E, Poisson's modulus υ, ultimate strain ε_u, ultimate stress σ_u, specific heat C_p, density ρ, thermal conductivity k.

One further assumes that:

- The interfaces between the layers are flat and chemically stable.
- The materials properties are constant within a layer, as illustrated on the left-hand side of Fig. 1. In the cases of nitriding and shot peening, the actual layer is virtually sliced into thinner layers so that this assumption is acceptable within each of these. In the case of diffusion layers, several compound layers are sometimes obtained. They should be considered as distinct materials with distinct properties.

4. Define the process stresses σ_0 of each layer (biaxial along y and z). In the case of a thin enough coating, a uniform value is assumed along x. For deep treatments, a complex stress profile has to be assumed (think about shot peening, which generates compressive stress around the surface and tensile stress deeper; the same stands for the diffusion case of nitriding). It was then split into thin layers, each of which having a different value of σ_0.
5. Resolution of time-dependent heat transfer problem. The heat flow is assumed to be oriented along x, so that the 1-D Fourier equation has to be solved. Variable space and time integration steps are recommended, so that the space steps are shorter in the layers and their immediate surroundings. The time steps should also be shorter around the most important temperature changes.
6. For each time step, determination of the stress at each point of the treated layers and substrate: $\sigma(x,t)$ (t: time) in the one-dimension case. For each material, a stress–strain relationship is assumed. In this work, the materials were assumed either perfectly plastic or perfectly brittle, as sketched on Fig. 3. The stresses are biaxial along y and z