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Modelling of the thermomechanical behaviour of coated structures using single and multi-level-set techniques coupled with the eXtended Finite Element Method

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ABSTRACT

The rapid evolution of manufacturing processes in many industrial sectors have largely highlighted the limitation of analytical and numerical modelling of heterogeneous structures integrating thin layers (joints, brazing, bonding coating). The present work proposes a multi-scale modelling of thin films applied to the problem of the thermomechanical behaviour of coated tools during machining operations. The approach relies on coupling X-FEM with the level-set functions within locally enriched elements and containing the coatings. The ability of the proposed numerical scheme is validated by solving 2D transient thermomechanical problems. The first obtained results show the effectiveness of the approach in terms of convergence and computational time, without any mesh refinement as required by the classic FEM approach. These results were systematically compared to the classical finite elements solution and experimental results. A parametric study about the number of Gauss points was leaded to evaluate its impact. The originality of this work is given with the specific application of thin layers and their thermomechanical behaviour such as coating, brazing, gluing, etc.

1. Introduction

Coatings deserve several applications in many industrial fields spanning from mechanical and electronics to optics. Coatings are generally deposited on a substrate to protect it against friction and wear phenomena. They are used to insure sensitive functions like thermal barriers to protect and isolate the substrate or to enhance the friction in the contact between two solids [1–3]. For example, the use of coated cutting tools in machining is crucial, allowing in part to operate effectively in the harshest environments such as dry machining [4] and high speed machining of hard materials (titanium based alloys, nickel based alloys, stainless steels, etc.). Increasingly, manufacturers and scientists have an important interest for the thermomechanical behaviour of coatings to understand and prevent their degradation. In fact, the presence of single or multi-thin layers in industrial structure, affects significantly the overall behaviour [5].

In a coating /substrate system, the systematic use of predictive models for the calculation of stress and temperature fields helps for the choice of materials. Moreover, it permits to verify the solution against the posed problem. The verification and optimization step is often carried out empirically based on:

– Experimental trials that are not always representative of the real in situ solicitations. Moreover, the results cannot be extrapolated easily through the whole pieces.
– Analytical methods that may contain restrictive assumptions.
– Numerical methods.

The main difficulty relies on the extremely small heterogeneity introduced by the deposit of a thin coating on a substrate.

The objective in this work is to set up a simplified numerical approach which allows to perform transient thermomechanical analysis of structures containing thin layers with small thicknesses (1–20 μm) as coatings and joints. Due to these small thicknesses, which rise the CPU calculation time, the chosen methodology must be able to take into account the presence of the coating without conforming mesh to the coating/substrate interface, i.e., it must capture the solution discontinuity that occurs when one or more material interfaces cross the mesh element. Moreover, the approach could give the possibility to integrate subsequently damage phenomena (crack propagation, delamination, wear …). To easily handle the topological changes of the interface when a non-conformed finite mesh is used, the geometric representation technique of the interface must be simple. This allows the control of the

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optimization process in industrial applications (e.g., for coated cutting tools, the choice of the thickness, the number of coating layers, the material nature and thermomechanical properties, …).

Whatever the analytical approach, the main conclusion is that the simplified assumptions considered in these approaches influence significantly the accuracy of the results. In addition, the studies are often completed on very simple geometries with such methods and damage prediction was never considered. Anyway, for the case of coating, references [6–11] can be cited, but they are all out of the scope of the presented work. It is clear that the standard finite elements method FEM can fulfill the specifications of this work (described previously). But, the mesh refinement close to the material interface is necessary to ensure the continuity of the mechanical and thermal fields [4,12,13], and the small mesh sizes generates a high CPU time for transient analyses which will be focused on the applications section of this article. To achieve the previous depicted objective of our study, it is important to keep on mind that the modelling of heterogeneous materials by numerical methods based on a spatial grid is facing fundamental problems. The most important of them is the achievement of the mesh. FEM definitively needs a conform mesh. This leads to a domain discretization which element size is around the thin layer thickness (1–20 µm). The principal consequence is that FEM is far away the objective of a small CPU calculation time. While considering now local effects, the expected model must take into account the layer(s) thickness(es), and so the localization of one or more material interfaces inside the non-compliant mesh. In the literature, methods such as the Meshfree Methods [14] and zero thickness elements (cohesive or double nodes elements [15]) raises some locks but remains insufficient. However, multi-scale methods must be pointed out for such aims like those of this study. Indeed, this type of modelling can deal with:

– The disappearance of the jump of properties between the coating and the substrate.
– The awareness of the coatings behaviour without any specific mesh refinement.
– The reduction of the CPU time calculation.

For these reasons, this article focus on the detail of some selected multiscale approaches to assess their effectiveness and relevance in relation to the coatings problems. The Arlequin method [16] allows overlapping mechanical states in the same zone of modelling. In fact, the studied domain can be divided according to several distinct regions, requiring different levels of analysis. The calculations can be then carried out simultaneously at the different scales. When trying to adopt this approach to the coatings application, it is difficult to relate the subdivision field and the mesh in the local domain "coating" increases the CPU time calculation. As well as the choice of the space approximation of the Lagrange multiplier is not always easy. Homogenization methods must be also mentioned. For example, in the composite materials domain, the square finite elements EF^2 [17] has been used to describe the behaviour of the strong heterogeneity of such materials. The idea is to describe the microstructure evolution using a simple approach that doesn't require any explicit resolution of the problem at each Gauss point. This generates an excessive computation time and high memory consumption. Therefore the use parallel computing should be required. Despite of the fact that Variational method [18] allows to consider microscopic effects within a relatively coarse FE approximation by a kind of regularization process, enrichment functions defining the microscopic part remain localized to one or more finite elements and lead therefore to a relative poor enrichment. Furthermore, the various micro sub-problems do not have any effect on each other. This could lead to some difficulties when applying for the coating case with local behaviour (damage, cracks …).

In contrast, Du et al. [5] compared two multi-scale methods to analyse the thermal field distribution in coated cutting tools. Both methods are based on the boundary element approach. One of these methods is dedicated to coatings with very low thicknesses, unlike the other method can be devoted to a wide variety of coatings thicknesses. In comparison, multi-scales approaches based on the concept of enrichment are worthy of the research field of this work. They are based on the partition of unity method (PUM) [19], which enrichment functions are multiplied by the partition of unity functions to construct the local enrichment. The enrichment concept was developed in the Generalized Finite Element Method (GFEM) [20], and improved later within the eXtended Finite Element Method (XFEM) [21]. A more general review on these enriched methods was given in [22]. Many authors used these methods to handle strongly discontinuous problems such as crack propagation [23] and weakly discontinuous problems such as material interfaces [21,24].

Ifis et al. [25,26] have developed the hybrid method “MAX-FEM” to analyse structures containing thin layers especially brazed joints. The principle of this method is to enrich the approximation of the global problem "macro" solution by local information of the "micro" problem. By exploiting the similarity between the analytical Matched Asymptotic Expansions approach (MAE [27]) and the XFEM method, the authors were able to define a procedure describing the heterogeneous behaviour of a structure containing a thin layer, without any mesh refinement and while keeping good accuracy of the overall solution. This method is detailed in the works of Ifis et al. in [25,26]. However, despite these great advantages, this method was proved to be limited when it comes to deal with geometries containing curved thin layers, or layers with non-uniform thicknesses. Moreover, at its actual development step, the coupling only integrates thermo-elastic behaviours. Anyway, since its extrapolation to the coatings problem could be easily completed, first results are presented in [28,29]. In fact, even if the MAX-FEM remains the starting point of the work presented here, other ways of investigations needed to be found to handle with its limits. For this purpose, and in order to reduce the number of degrees of freedom due to the additional term in the XFEM formulation, an interface-enriched generalized FEM (IGFEM) [30] has been proposed. In the same principle, the XFEM/Level-Set function coupling [21] operates the level set function principle to localize the material interface. In fact, surfaces that are not represented explicitly by mesh boundaries can be implicitly represented by the iso-zero values of a level set function. This allows to choose a mesh which is not conforming to the coating layers boundaries and to use large elements size. In this way, the XFEM method can be used to solve large-scale problems without large CPU penalty. For this reason, it was chosen in this work to deal with the coatings problems.

The paper is organized as follows. Section 2 presents the principle of the XFEM with the different improvements and strategies which were applied to achieve the objective of this work: easy material interfaces representation and CPU calculation time reduction. Section 3 describes the problem of interest, i.e., the transient thermomechanical equations. Then detailed two-dimensional studies on simple and complex coated structures with single and multi-thin layers are presented and comparisons with the FEM, MAX-FEM method and the work of Du et al. [5] are performed and discussed.

2. The principle of the XFEM/Level-set coupling

In this work, the XFEM method has been developed to perform a transient thermo-elastic analysis of coated structures with one or several coating layers. In order to take into account the presence of coatings without the need of a specific space grid, that allows to minimize the huge CPU calculation time caused by low coatings thicknesses.

A domain $\boldsymbol{\Omega} = \boldsymbol{\Omega}_1 \cup \boldsymbol{\Omega}_2$, containing a singularity Γ, is subjected to an imposed constant temperature T_{imp} and displacement $\boldsymbol{u}_{imp}$ which are specified on a Dirichlet boundary, denoted by Γ_{Tu} and to a heat flux density φ_{imp} and a pressure $\boldsymbol{p}_{imp}$ specified on a Neumann boundary