Modeling of distortion induced by the nitriding process

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Résumé :
Cette étude présente un outil de prédimensionnement capable de simuler les déformations résiduelles de pièces complexes engendrées au cours du traitement de nitruration. Ce procédé thermochimique est destiné à améliorer la tenue en service des pièces mécaniques. Le modèle est constitué d’une première étape d’identification de la déformation volumique apparente engendrée par le traitement, dans le cas d’une géométrie simple. Un problème de diffusion équivalent produisant cette déformation est ensuite mis en place afin de s’extraire de la géométrie des pièces. Enfin, ce dernier est intégré à un code de calcul par éléments finis pour simuler des pièces de géométries complexes. Les résultats sont confrontés à des mesures expérimentales de déplacements sur une maquette de cas industriel.

Abstract :
This work deals with a pre-dimensioning tool able to simulate distortions of complex parts generated during nitriding process. Nitriding is a thermochemical process which is used to improve the fatigue life of structural parts. The first step of the model consists in identifying apparent volumic strains generated by the treatment for a simple geometry. Then, an equivalent diffusion problem producing this strain has been implemented in order to be independent from the parts geometry. Finally, the latter is integrated into a finite elements code to simulate parts with complex geometries. The results are compared to experimental measurements on an industrial case.

Mots clefs : Nitriding process ; Modeling ; Distortion

1 Introduction
Thermochemical treatments such as nitriding are usually used to improve the fatigue life of structural parts. Benefits of residual stress generated by this kind of treatment is well known \cite{1, 2, 3}. Many studies have been performed to describe the microstructure of nitrided layers. Several are available to model residual stress development \cite{4, 5}, but few deal with the distortion of mechanical parts. However, in the aeronautic industry, the mass of structural parts tends to be constantly reduced. This specificity implies the design of thinner parts which are more favorable to distortions. These distortions, usually neglected, have to be mastered in order to ensure the compliance of treated parts.

The nitriding process involves complex multi-physic phenomena at the source of distortion. In this work, the case study is the gaseous nitriding of 32CrMoV13 low alloy steel treated during 120 hours. In this kind of steel, nitrogen atoms diffuse from the surface and interact with iron and alloying elements. Nitrides are formed from initial carbides or alloying elements in iron solid solution. Carbon atoms released during the dissolution of initial carbides can diffuse in the depth and form new carbides such as cementite or be evacuated from the steel, which involves decarburizing on the surface \cite{6}. This microstructure evolution involves volume changes of nitrided layers, resulting in macroscopic residual stress and distortions \cite{4}.
This work focuses on the mechanical aspect of the treatment. It allows to provide a pre-dimensioning tool, whose computational time is reduced while simulating complex geometrical parts. Volumic eigenstrain (accompanying precipitations) is considered as the source of residual stress and distortions. In the model, the volumic strain is identified from the curvature of a thin plate nitrided on one face [7] using the radius curvature method.

Once the volumic strain is identified, it is imposed numerically to the studied structure thanks to an equivalent diffusion problem. Volumic strain is considered as a dilatation accompanying the diffusion of an equivalent quantity. The main assumption consists in considering that volumic strain generated by nitrogen and carbon diffusion coupled with precipitation can be obtained by the diffusion and the dilatation of a unique equivalent quantity. The benefit of this approach lies in its simplicity, its reduced computational time and its instant integration in usual finite elements methods.

2 Mechanical approach of the treatment

The aim of this study being the prediction of distortions, the behavior law is supposed to be linear elastic. Therefore, visco-plastic phenomena are neglected. The mechanical problem is to find \((u, \sigma)(x)\) sufficiently regular at every point \(x\) of a domain \(\Omega\) occupied by the studied solid (\(\partial\Omega\) is its boundary) [8] such as:

\[
\begin{align*}
\text{Kinematic compatibility} : & \quad \varepsilon = \frac{1}{2}(\nabla u^T + \nabla u) \\
\text{Equation of equilibrium} : & \quad \text{div}(\sigma) = 0 \\
\text{Constitutive law} : & \quad \sigma = K \varepsilon_e
\end{align*}
\]

with \(u\) the displacement field, \(\sigma\) the Cauchy stress tensor and \(K\) the Hooke tensor. \(\varepsilon\) is the total strain tensor, \(\varepsilon_e\) the elastic strain, \(\varepsilon_f\) the macroscopic volumic apparent eigenstrain generated by nitriding. It is considered purely hydrostatic due to quasi-random distribution of nitrides in ferrite. Assuming the infinitesimal strain theory is verified, the total strain can be separated in a summation of an elastic and apparent volumic strain [8]. Fig. 1 schematically shows the generation of residual stress and distortion, caused by volumic strain mismatch.

Before nitriding

\[\varepsilon = 0\]
\[\sigma = 0\]

After nitriding

\[\varepsilon = \varepsilon_f\]
\[\sigma = 0\]

Verifying strain compatibility

\[\varepsilon = \varepsilon_f + \varepsilon_e\]

\[\sigma = K \varepsilon_e\]

Figure 1 – Schematic approach of the generation of residual stress and distortion.

3 Apparent volumic strain identification

Goret used the curvature radius method to evaluate residual stresses [7]. A thin plate is nitrided on one face in order to generate a bending moment which curves the plate. Its curvature radius
$R$ is assumed to be constant. Successive material removals are performed using chemical etching and the evolution of the curvature radius $R$ is measured using a 3D coordinate measuring machine (Fig. 3).

The curvature $\chi$ in respect to the removed thickness $e$ and the apparent volumic strain can be calculated in the case of a plate geometry ($H$ its thickness, $z$ the depth in the nitrided layer):

$$\chi(e, \varepsilon_f) = \frac{1}{R(e, \varepsilon_f)} = \frac{6(H + e) \int_e^H \varepsilon_f(z) \, dz + 2 \int_e^H z \, \varepsilon_f(z) \, dz}{(H - e)^3}$$

In order to calculate the curvature, the in-depth apparent volumic strain profile is assumed to be piecewise polynomial (Fig. 2) such as:

$$\varepsilon_f(z) = \begin{cases} az^2 + bz + c & \forall \ z \in [0; z_M] \\ dz^3 + e z^2 + fz + g & \forall \ z \in [z_M; z_F] \end{cases} = \varepsilon_f(z, \varepsilon_0, \varepsilon_M, z_M, z_F)$$

where $(a, b, c, d, e, f, g)$ are constants which depend on $(\varepsilon_0, \varepsilon_M, z_M, z_F)$. The choice made about the apparent volumic stress profile is based on phenomenological considerations. Indeed, the condition $\varepsilon_0 \leq \varepsilon_M$ comes from the observation of decarburizing close to the surface [5] which involves an elementary volumic strain gradient. Maximal point $(z_m, \varepsilon_M)$ is directly linked to the maximal compression stress level observed around $300 \mu m$ in depth [7]. At last, end of diffusion layer is similar to a diffusion front which has a tangent to zero in $z_F$.

![Figure 2](image1.png) \hspace{1cm} ![Figure 3](image2.png)

**Figure 2** – Theoretical in-depth apparent volumic strain profile, assumed to be piecewise polynomial.

**Figure 3** – Curvature of a thin plate nitrided on one face in respect to removed thickness [7].

The identification of apparent volumic strain is to find the parameters $\{\varepsilon_0, \varepsilon_M, z_M, z_F\}$ minimizing the cost function $I$ defined in the least squares sense by:

$$I = \sum_{k=1}^{N} [\chi^{\text{exp}}(e_k) - \chi(e_k, \varepsilon_0, \varepsilon_M, z_M, z_F)]^2$$

with $\chi^{\text{exp}}(e_k)$ the experimental curvature at $e_k$ depth of $k^{th}$ material removal and $N$ the number of measurement points taken into account in the minimization problem. The simplex optimization algorithm is used to determine the four optimal parameters.
The experimental results (Fig. 3) show a remaining residual curvature even after the total removal of the nitrided layer (depth over 1.1 mm). It means that plastic and visco-plastic effects appear in the non-treated material during treatment. The considered model does not account for these phenomena, and expects a zero curvature once the nitrided layer is removed. It can explain the significant discrepancy between the experiment and the model prediction.

Furthermore, the simulation is about prediction of distortions on mechanical parts which have not been chemically etched. This is why optimization of apparent volumic strain is only performed on the first measured point, which corresponds to a minimal material removal ($N = 1$).

Finally, $\varepsilon_f(z)$ is an "apparent" volumic strain which is not only related to microstructure volume changes, but also accounts (in a global manner) for plastic and visco-plastic effects.

4 Equivalent diffusion problem

Once apparent volumic strain is calculated, it is considered like the solution of one dimensional equivalent diffusion problem. A convection boundary condition is chosen. The diffusion problem is to find $(C, q)$ sufficiently regular in $\Omega = [0; H]$ such as:

\[
\begin{align*}
\text{Diffusion equation:} & \\
\frac{\partial C(z,t)}{\partial t} - a \frac{\partial^2 C(z,t)}{\partial t^2} &= 0 \quad \forall (z,t) \in (\Omega \times [0; t_1]) \\
\text{Constitutive law:} & \\
q(z,t) &= -\lambda \frac{\partial C(z,t)}{\partial z} \quad \forall (z,t) \in (\Omega \times [0; t_1]) \\
\text{Boundary conditions:} & \\
q(z_{\partial \Omega},t) &= -h(C_{ext}(t) - C(z_{\partial \Omega},t)) \quad \forall (z,t) \in (\partial \Omega \times [0; t_1]) \\
\text{Solution at $t_1$ time:} & \\
\varepsilon_{diff}^f(z) &= \alpha C(z,t_1)
\end{align*}
\]

(5)

where $C(z,t)$ is a diffusing equivalent quantity and $q$ its flux. Identification is an inverse problem which consists in finding an unstationary external equivalent quantity $C_{ext}(t)$ which gives $\varepsilon_{diff}^f(z) = \alpha C(z,t_1)$, for given parameters $(a, \lambda, h, \alpha)$ and at a given time $t_1$ corresponding to the end of the simulation.

5 Identification of an external equivalent quantity

The one dimensional diffusion problem is resolved using Crank-Nicolson numerical scheme. In order to reduce the solution search space, $C_{ext}(t)$ belongs to the family of piecewise T-periodic sinusoidal functions such as $T = \frac{N_s}{2t_1}$. $N_s$ is the number of sinusoidal segments on the time interval $[0; t_1]$. For each segment, the only unknown is the sinus amplitude $C_{max}^i$ where $i \in [1; N_s]$. The optimization problem is to find the parameters $(t_1, N_s, C_{max}^i)$ which minimize the cost function:

\[
J = \int_0^H \left[ \varepsilon_f(z) - \varepsilon_{diff}^f(z) \right]^2 dz
\]

(6)

Simplex algorithm is used in the same manner as for the identification of apparent volumic strain. Fig. 4 shows the optimal external unstationary equivalent quantity. It is evaluated to best fit the apparent volumic strain (at $t = t_1$, Fig. 5) which is experimentally identified in the third section.
Figure 4 – External equivalent quantity which is the boundary condition numerically applied to the surface layer of the treated material.

Figure 5 – Comparison of in-depth apparent volumic strain resulting from numerical diffusion at $t = t_1$ and from experimental identification.

6 Results

Once the external equivalent quantity $C_{ext}(t)$ identified, it is numerically applied on each "nitrided" surface of a finite element model. In order to validate the model, an industrial complex geometry case (Fig. 6) is simulated using an industrial finite element code (Fig. 7), then compared (Fig. 8) to experimental measurements acquired by a 3D coordinate measuring machine.

Figure 6 – Industrial case for validation. All surfaces are nitrided. Landmarks 1 to 7 correspond to the measurement results shown in Fig. 8 (Design details are suppressed).

Figure 7 – Theoretical distortion. Blue section is the undeformed geometry before treatment; in color, the geometry after treatment ($\times$ 100). Axial and radial displacements are shown in Fig. 8.

Seven measurements of distortions — part geometry before and after nitriding — have been carried out in different zones (see landmark Fig. 6). Fig. 8 compares these experiments with the simulation results. Measures 1 and 2 correspond to axial displacements. The maximal absolute discrepancy is around 34 $\mu$m, and the relative one around 13 %. The next measurements correspond to radial displacements, with a maximal absolute discrepancy around 32 $\mu$m. The relative discrepancy becomes not relevant because of the low level of displacements compared to the measurement uncertainty.
7 Conclusions

This work presented a simplified model for the prediction of structural parts distortions generated by nitriding. Our results showed that these deformations can be accurately related to apparent volumic eigenstrains. These eigenstrains - involved during nitriding - were assumed to be the only source of distortions. They could be identified from a nitrided plate and then simulated thanks to an equivalent diffusion problem. Furthermore, the boundary condition identified in the latter diffusion problem was supposed to characterize the distortions generated by a given set of nitriding parameters applied to a fixed material. Thus, only one nitrided plate was needed to identify the boundary condition to be imposed to future simulations. It allows to predict distortions for any complex geometry for the same fixed material and nitriding parameters. The results of such simulations were compared to experimental measurements and gave a good estimation of the real distortions. Thus, our simulation method proved to be a good pre dimensioning tool to anticipate distortions. Moreover, the presented approach is not limited to nitriding — because there is no description of nitriding specific micro structural transformation — but could enable to model distortions of any phenomena generating volume changes such that the macroscopic free strain is hydrostatic.

Références


