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A NEW THERMO-METALLURGICAL MODEL FOR WELDING AND QUENCHING RESIDUAL STRESSES COMPUTATIONS

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INTRODUCTION

Mechanical analysis of nuclear components may require consideration of residual stresses resulting from manufacturing processes. This is particularly the case for structures which have received no or only partial stress relieving treatment prior to entry into service. Although correct assessment of the quenching or welding thermal cycles undergone by the structures remains a delicate problem which can have considerable repercussions on the results obtained, it is essential that structural analysis involve phenomena induced by these cycles, which can include periods at very high temperatures. These phenomena involve both "usual" temperature effects on the thermo-mechanical characteristics of materials and also, for some steels, effects due to structural transformations occurring during cool-down from high temperatures.

The aim of this paper is to propose a model of cooling-induced structural transformations in the form of a *thermo-metallurgical constitutive equation.* The model, which has to remain compatible with usual space scale of computational mechanics, is described in the first part.

In the second part, the mechanical consequences of the structural transformations are discussed, together with their inclusion in an elasto-plastic structural analysis algorithm. The two main consequences considered are :

- inclusion of a plasticity law for a multiphase material (for present purposes, a law of mixture on the yield functions is adopted) ;
- occurrence of a transformation plasticity phenomenon, generating irreversible plastic type deformations during the transformations, even when the applied stresses are well below the current yield value.

The third part concerns a realistic butt welding computation of a stainless steel weld-end over a ferritic tube.

METALLURGICAL MODEL

Evidencing structural transformations

The dilatometric test consists in recording versus temperature the gradual deformation of small, unstressed test piece subjected to an assumedly homogeneous thermal history comprising heating to beyond 850°C and isothermal holding at this level followed by controlled cooling down to ambient temperature (see Figure 1). Such tests evidence the different structural transformations (or solid state phase changes) occurring in ferritic steel subjected to welding or quenching operations [1].

Heating induces the transformation : ferrite + pearlite (F+P) → austenite (γ). This transformation involves volumetric contraction and modification of some thermo-mechanical characteristics (thermal expansion coefficient (α) and yield stress (σ_y) notably). Cooling, depending on the rate, brings about the following transformations :

austenite (γ) → ferrite + pearlite (F+P) (1)

austenite (γ) → bainite (B) (2)

austenite (γ) → martensite (M) (3)

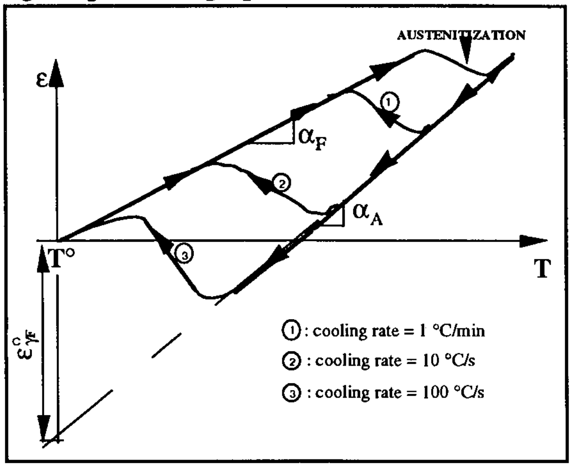

Fig 1 : Schematic dilatometric curves for a ferritic steel

These different transformations may be total, partial or consecutive. They are accompanied by volumetric expansion and give rise to metallurgical constituents having very similar thermal and elastic characteristics, but fairly different plastic properties (see Figure 2).

Characterizing the metallurgical structure

The incidence of these transformations on mechanical behaviour is obvious and cannot be accounted for in a conventional thermo-mechanical analysis where the variables are the temperature T, the stress tensor σ and the possible internal plasticity variables (ε^p , ...). In order to take the metallurgical phenomena into account, new internal variables have consequently to be introduced, characterizing the structural modifications in the material.

For the metallurgist, the obvious variables to introduce would be, for example, the crystal lattice parameters and alloy element content (carbon notably). But this very fine simulation scale would appear disproportionate to the material point notion used in mechanics and represented by the "homogeneous" dilatometric test piece. In such a test, several transformations can be induced successively producing, at ambient temperature, a test piece constituting a mixture of different phases. In this context, the metallurgical structure must consequently be considered to be characterized by the proportions of the phases present at a given point. *The additional variable to be introduced will thus be a vector* *quantity* $\mathbf{Z}$(M,t) = { Z_1, Z_2, Z_3, Z_4 } where Z_1, Z_2, Z_3, Z_4 *are the ferrite, pearlite, bainite and martensite proportions in M at time t* (the proportion of austenite being equal to the complement to 1 of the sum of the Z_i, i=1,4).

Postulating a law of mixture to define the thermal strain of a multiphase material, strain evolution during a dilatometric test can be described by the equation :

$$\varepsilon \equiv \varepsilon^{th} = \sum_{i=1}^{i=4} Z_i.\alpha_i.(T - T^0) + (1 - \sum_{i=1}^{i=4} Z_i).\ [\ \alpha_\gamma.(T - T^0) + \overset{0}{\varepsilon}_{\gamma F}\ ] \qquad (1)$$

where : T^0 is the reference temperature for which strain in the F, P, B, M phases is taken as null ;

α_i are the thermal expansion coefficients of the F, P, B, M phases and α_γ that of austenite ;

$\overset{0}{\varepsilon}_{\gamma F}$ is the γ phase strain with respect to phases F, P, B, M at temperature T^0.

Remark : For each dilatometric test, equation (1) can be used to reconstruct the $\mathbf{Z}$(t) evolution associated with a given thermal history T(t).

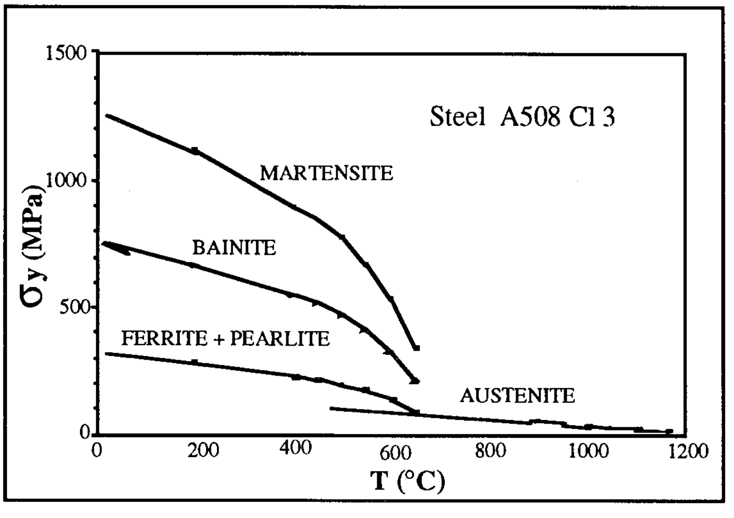

Fig 2 : Yield stress as a function of temperature for several phases of A508 Cl 3 steel

Modelling structural transformations

In the framework of thermodynamics of materials with internal variables [2-3-4], we postulate the existence of a function f and a finite number of additional internal variables η_k and functions ψ_k , such that :

$$\begin{cases} \dot{\mathbf{Z}} = f\,(q, \dot{q}, \mathbf{Z}, \eta_k) \\ \dot{\eta}_k = \psi_k\,(q, \dot{q}, \mathbf{Z}, \eta_k) \end{cases} \qquad (2)$$

where the q are pilot state variables of the thermodynamic process (*i.e.* those where evolution can be experimentally imposed or measured).

Pilot and internal variables choice will depend on the physical phenomena involved and the necessity for satisfactory fitting between experimental and computerized data.

For present purposes, the additional internal variables selected are *the austenitic grain size* d (characteristic of the austenitization conditions) and *the martensitic starting temperature* Ms which features in the empirical Koïstinen-Marbürger state equation describing the athermal kinetics of this transformation [5] :

$$Z_4 \ (T, Z_1, Z_2, Z_3, Ms) = [1 - \sum_{i=1}^{i=3} Z_i].\{1 - \exp(\beta\,[Ms - T]^+)\} \tag{3}$$

where : β is a material constant ($°C^{-1}$) ;

Ms is a function of the material and the remaining quantity of austenite at temperature T (to model the austenite stabilization phenomenon) ;

$[\,X\,]^+$ designates the positive part of X.

Since the pilot variables are the temperature T and the strain ε or stress σ tensor, the general form of the proposed model will be :

$$\begin{cases} \dot{Z} = f\,(T, \dot{T}, \sigma, \dot{\sigma}, Z, d, Ms) \\ \dot{d} = \delta\,(T, \dot{T}, \sigma, \dot{\sigma}, Z, d, Ms) \\ \dot{Ms} = \mu\,(T, \dot{T}, \sigma, \dot{\sigma}, Z, d, Ms) \end{cases} \tag{4}$$

Reduction of variables - model simplification

The stress state is known to influence metallurgical behaviour [6]. However, this influence has only been experimentally quantified in very specific situations [7] (constant uniaxial stress condition, isothermal transformations) which are scarcely representative of the actual welding or quenching conditions to which components are submitted. In the first version of the proposed model, this influence is disregarded.

Furthermore, the austenitic grain size is due only to the thermal history during austenitic stage : it is unchanged by cooling. The d variable consequently features only as a parameter in the model of metallurgical behaviour during cooling, which is the subject of the present investigations. We thus obtain :

$$\begin{cases} \dot{Z} = f\,(T, \dot{T}, Z, Ms\,;\,d) \\ \dot{Ms} = \mu\,(T, \dot{T}, Z, Ms\,;\,d) \\ d = d^c \end{cases} \tag{5}$$

where d^c is the grain size resulting from austenitization.

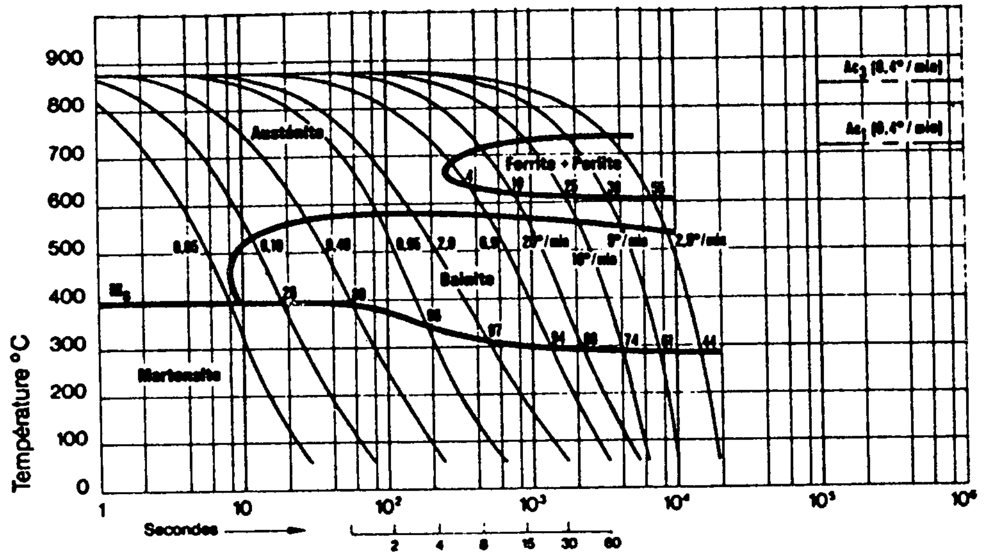

Fig. 3 : C.C.T. Diagram for a A508 Cl 3 steel

Identification postulates and final form of the proposed model

A C.C.T (Continuous Cooling Transformations) diagram synthesizes results obtained for different dilatometric tests (*i.e.* different cooling rates) for identical austenitization conditions (*i.e.* a d^c value). This involves, for each experimental thermal case history, the nature of the transformations induced, the temperatures from start and finish and the final proportions of each phase formed (see Figure 3).

To identify the model, the following assumptions are made :

(i) for a given steel, the C.C.T. diagrams and the Koïstinen-Marbürger state equation completely characterize its metallurgical behaviour during cooling ;

(ii) in addition, for a given thermal case history, the ferritic, pearlitic and bainitic transformation kinetics can be approached by piecewise linear functions of the temperature (this postulate enables simple reconstruction of the **Z**(t) evolutions associated with each thermo-metallurgical history of the C.C.T. diagrams) ;

(iii) finally, a C.C.T. diagram enables the identification of an empirical equation linking Ms and $\sum_{i=1}^{i=3} Z_i$:

$$Ms(Z\,;d) = Ms_0(d) + A(d).[\sum_{i=1}^{i=3} Z_i - Z^s(d)]^+ \qquad (6)$$

In the light of these assumptions, the final form of the model is consequently :

$$\left\{\begin{array}{ll} \dot{\mathbf{z}} = \varphi(T, \dot{T}, \mathbf{z}\,; d) \ \text{ with } \mathbf{z} = \{Z_1, Z_2, Z_3\} & \text{(a)} \\ Z_4\ (T, \mathbf{z}, Ms) = [1 - \sum_{i=1}^{i=3} Z_i].\{1 - \exp(\beta\,[Ms - T]^+)\} & \text{(b)} \\ Ms = Ms_0(d) + A(d).[\sum_{i=1}^{i=3} Z_i - Z^s(d)]^+ & \text{(c)} \\ d = d^c & \text{(d)} \end{array}\right. \qquad (7)$$

Solving the evolution problem

For continuous cooling (without isothermal step), there is no satisfactory theoretical model enabling a specific shape to be given to function φ defined in equation (7a). In addition, the great number of variables included makes it very difficult (and highly uncertain) to adjust on a predetermined φ shape based on experimental data. Models using this kind of assumption do not consider $\dot{T}$ as a true variable and include its influence only via a parameter (generally $\dot{T}(T=700°C)$ [8]).

To calculate φ $(T, \dot{T}, \mathbf{z} ; d)$, we make use of the fact that the thermo-metallurgical histories featured in a C.C.T. diagram are each specific solution to the evolution differential equation (7a). They can consequently be used to compute the φ value for each of the thermo-metallurgical states $(T, \dot{T}, \mathbf{z} ; d)$ featured in this diagram. Numerical processing of the diagrams will enable construction of a set of "septuplets" $\Sigma = \{ T, \dot{T}, \mathbf{z}, d, \varphi (T, \dot{T}, \mathbf{z} ; d) \}$. Computation of transformation progression at a given time t will then be based on interpolation in set Σ [9]. Since the interpolation quality will depend on the density of set Σ, postulate (ii) will be used to define a virtual set, comprising about 10,000 "septuplets" based on a "skeleton" of only about 500 "septuplets".

The model was implemented in the EDF/DER finite element code (*Code Aster*), where it is currently used for metallurgical simulations as post-processing of linear or non-linear thermal computations (coupling, *i.e.* inclusion of solid state transformation latent heat, being formally possible). The first validation test consisted in numerical simulation of the dilatometric tests used to draw up the C.C.T. diagram for A508 Cl 3 steel austenitized 1 hour at 900°C. On 42 tests, discrepancies between computed and experimental results averaged about 2°C for transformation start and finish temperatures and about 2% for the final proportions of the phases formed.

It should also be noted that since the form of the differential equation governing structural transformation evolution is unspecified, the model can be further enhanced by inclusion of any new experimental results.

MECHANICAL CONSEQUENCES

Quenching or welding type operations affect mechanical evolution by the structural transformations they induce. Stress influence on transformation kinetics is disregarded as is that of strain energy rate in the heat equation.

Determination of mechanical evolution in the case of a process involving structural transformations thus requires two successive uncoupled computations :

- the first will be a thermo-metallurgical one enabling determination of thermal T(t) and metallurgical **Z**(t) evolutions ;
- the second will be an elasto-plastic one taking effects due to thermal and structural evolutions into account.

Three main thermo-metallurgical effects play a role in mechanical analysis equations :

- thermal strain ;
- modifications of the material mechanical characteristics ;
- transformation plasticity.

Thermal strain modifications are characterized by a dilatometric test (see Figure 1). Postulating a law of mixture to define thermal strain of a multiphase material, we obtain (see equation (1)) :

$$\varepsilon \equiv \varepsilon^{th} = \sum_{i=1}^{i=4} Z_i.\alpha_i.(T - T^0) + (1 - \sum_{i=1}^{i=4} Z_i).\ [\ \alpha_\gamma.(T - T^0) + \varepsilon^0_{\gamma F}\ ]$$

Elastic characteristics (Young's modulus, Poisson's ratio) are little affected by metallurgical composition, so only their temperature dependence is included.

Plastic characteristics (yield stress especially) are strongly affected. Here again, the material has to be considered as a multiphase structure with different characteristics for each phase. The macroscopic material "plastic characteristics" are obtained by a law of mixture. More precisely, the yield function f is expressed by (isotropic hardening case) :

$$f\,(\sigma,p) = \sigma_{eq} - R(T,Z).p - \sigma_y(T,Z) \qquad (8)$$

where : $R(T,Z) = \sum_{i=1}^{i=4} Z_i.R_i(T) + [1 - \sum_{i=1}^{i=4} Z_i].R_\gamma(T)$

is the linear isotropic hardening coefficient, R_i being that of phase i ;

$\sigma_y(T,Z) = \sum_{i=1}^{i=4} Z_i.\sigma_{yi}(T) + [1 - \sum_{i=1}^{i=4} Z_i].\sigma_{y\gamma}(T)$

is the yield strength, σ_{yi} being that of phase i ;

σ_{eq} is the von Mises equivalent stress and p denotes cumulated plastic strain.

Transformation plasticity

During dilatometric tests under uniaxial stress states, it is observed that transformations occurring under stress can induce irreversible strains, even if the applied stress does not exceed the yield stress of the material at the temperature considered (see Figure 4). This phenomenon is commonly known as "transformation plasticity". Two microscopic phenomena are proposed in explanation of this macroscopic phenomenon :

- incompatibility of microscopic strain fields owing to specific volume differences between the phases (Greenwood and Johnson) [10] ;
- orientation of the martensite plates during their formation under the effects of the applied stress (Magee) [11].

In the case of a single transformation, these tests exhibit linearity between the applied macroscopic stress and the value of the final irreversible strain, whence the experimental model proposed by Desalos [12]:

$$\dot{\varepsilon}_i^{pt}(\sigma,Z_i) = k_i.\,G_i.(Z_i).\sigma \tag{9}$$

where k_i is a constant (MPa^{-1})and G_i is a function of the transformed phase proportion Z_i such that $G_i(0)=0$ and $G_i(1)=1$.

A 3D generalization of this experimental model was proposed by Leblond [13] for a single transformation :

$$\dot{\varepsilon}_i^{pt}(\sigma,Z_i) = \frac{3}{2}\,k_i.F_i\,(Z_i).\dot{Z}_i.\sigma^d \quad \text{with} \quad F_i = G_i' \tag{10}$$

This generalization is based on the following heuristic considerations :

- as in plasticity, the equation has to be "incremental" ;
- transformation plasticity only progresses during transformations ;
- it must be proportional to the applied stress ;
- as in usual plasticity, it occurs without volume changes, implying dependence with respect to the stress deviator rather than to the whole stress tensor ;
- finally, integration of this equation in a constant stress uniaxial case should give back the experimental equation (9).

The transformation plasticity phenomenon can be observed for ferritic, pearlitic, bainitic and martensitic type structural transformations. Since these transformations may occur simultaneously we obtain :

$$\dot{\varepsilon}^{pt}\,(\sigma,Z) = \sum_{i=1}^{i=4} \dot{\varepsilon}_i^{pt}(\sigma,Z_i) = \frac{3}{2}\,\sigma^d.\sum_{i=1}^{i=4} k_i.F_i\,(Z_i).\dot{Z}_i \tag{11}$$

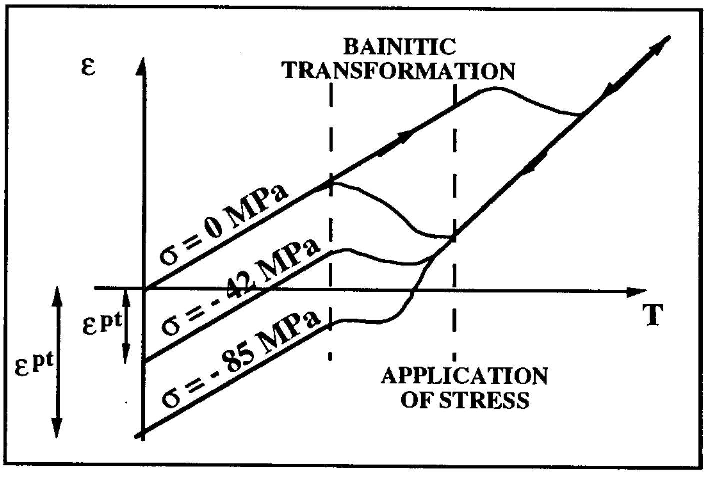

Fig 4 : Dilatometric curves under constant uniaxial compressive stresses for a A508 Cl 3 steel [10].

Constitutive equations

In brief, inclusion of structural transformation effects in elasto-plastic computations [14] leads to the following constitutive equations :

$$\left\{\begin{array}{l} \varepsilon = \varepsilon^e + \varepsilon^{th} + \varepsilon^p + \varepsilon^{pt} \\ \sigma = \mathbf{A}(T).\varepsilon^e \\ \dot{\varepsilon}^p = \dot{\lambda}\,\dfrac{\partial f}{\partial \sigma}(\sigma,p\,;T,\mathbf{Z}) \\ \dot{p} = \dot{\lambda}\,\dfrac{\partial f}{\partial p}(\sigma,p\,;T,\mathbf{Z}) \\ \dot{\varepsilon}^{pt} = \dfrac{3}{2}\,\sigma^d.\displaystyle\sum_{i=1}^{i=4} k_i\,.F_i\,(Z_i).\dot{Z}_i \\ \varepsilon^{th}\,(T,\mathbf{Z}) = \displaystyle\sum_{i=1}^{i=4} Z_i.\alpha_i.(T - T^0) + (1 - \sum_{i=1}^{i=4} Z_i).\,[\,\alpha_\gamma.(T - T^0) + \varepsilon^0_{\gamma F}\,] \\ \dot{\lambda} = 0 \text{ if } f\,(\sigma,p\,;T,\mathbf{Z}) < 0 \\ \dot{\lambda} \geq 0 \text{ if } f\,(\sigma,p\,;T,\mathbf{Z}) = 0 \end{array}\right. \qquad (12)$$

where : ε^e, ε^{th}, ε^p, ε^{pt}	are respectively the elastic, thermal, plastic and transformation plasticity strains ;
$\mathbf{A} = (A_{ijkl})$	the elastic compliance tensor ;
λ	the plastic strain rate parameter ;
f	the yield function given by (8) ;
p	the cumulated plastic strain ;
T(t) and **Z**(t)	the temperature and the metallurgical structure variable.

Resolution algorithm

In the elasto-plastic computations, the temperature and metallurgical structure evolutions are known (determined by a thermo-metallurgical computation performed beforehand).

In the EDF/DER finite element computation code (*Code Aster*), an implicit method is used for the time discretization of the elasto-plastic model [16], including the transformation plasticity phenomenon [17]. Discretization of the incremental problem leads to a non-linear problem, solved by a Newton method [15].

Convergence in such a method much depends on the choice of a consistent tangent stiffness matrix, the expression of which is affected by the transformation plasticity phenomenon [17].

The Newton method iterative process is also highly sensitive to the initial solution option. In the *Code Aster*, the initial solution is obtained by solving the explicit rate problem, which is also considerably modified by the transformation plasticity. In the case of von Mises plasticity with linear isotropic hardening, the stress field derivative at time t, $\dot{\sigma}(t)$, is an enhanced function of $\varepsilon(\dot{u})$. The transformation plasticity thus produces a left hand side member in the rate problem which cannot be disregarded if we hope to converge after a reasonable number of iterations.

If we take the simple (and analytical) example of a cylindrical specimen under tensile stressing subjected to a homogeneous temperature field T(t) and structural composition field **Z**(t) and in which the transformation plasticity strain exceeds the plastic strain, the number of iterations required to converge to the analytical solution drops from about a hundred to less than ten, providing the initial solution is correctly estimated.

In the *Code Aster* computation options, the transformation plasticity phenomenon can be omitted, in which case only the other structural transformation effects will be considered. On the other hand, when transformation plasticity is taken into account, it can occur even when the structure plastifies.

APPLICATION

The application presented here concerns the axisymetric computation of a butt-welding of a stainless steel weld-end (AISI 316, without structural transformation) over a ferritic steel tube (AISI A508 Cl 3, with structural transformations) fitted at its bottom. The welding metal is also a stainless steel (AISI 308). The overall geometry is shown figure 7. The mesh contains about 214 parabolic elements and 511 nodes. The thermo-metallurgical simulation of the welding was realized in one pass (2,800 seconds on a Cray YMP). It takes into account the liquid-solid state changes and the radiation thermal exchanges. The figure 5 depicts the metallurgical evolutions of a material point in ferritic steel H.A.Z. (Heat Affected Zone). After the thermo-metallurgical computation, three mechanical computations were realized. The first one (see figure 6) does not take into account the structural evolutions (2,500 s). The second one involves metallurgical transformation modifications of mechanical characteristics (also specific mass) of all the phases, but neglect the transformation plasticity (3,800 s). Whereas the third includes all effects and thus the transformation plasticity (4,200 s). The results show that the structural transformations change considerably and over a large region the stresses evolution along the outside boundary of the tube. The influence of transformation plasticity is more confined in the H.A.Z. immediate neighbourhood and is less important.

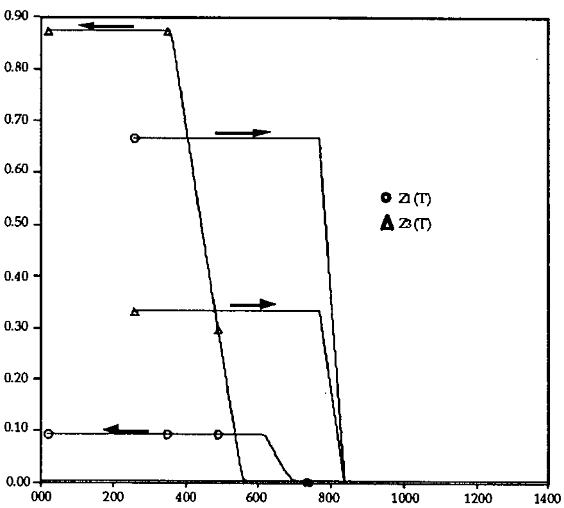

Fig 5 : Metallurgical evolutions versus temperature for node 68.

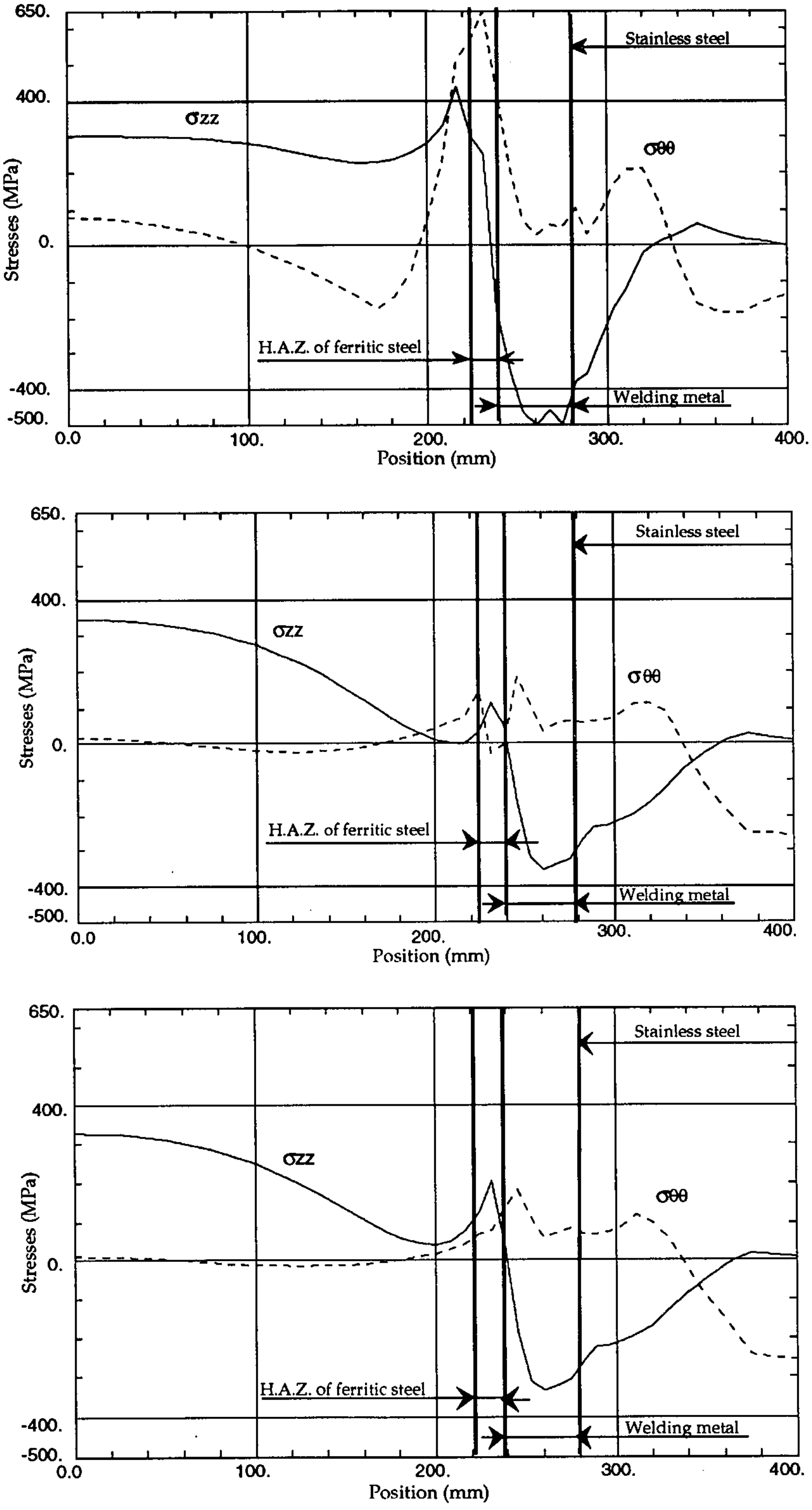

Fig 6 : Stresses versus position along outside face of the tube.

up : Thermo-mechanical computation.
middle : Thermo-metallurgical-mechanical computation without plasticity transformation.
down : Thermo-metallurgical-mechanical computation with plasticity transformation.

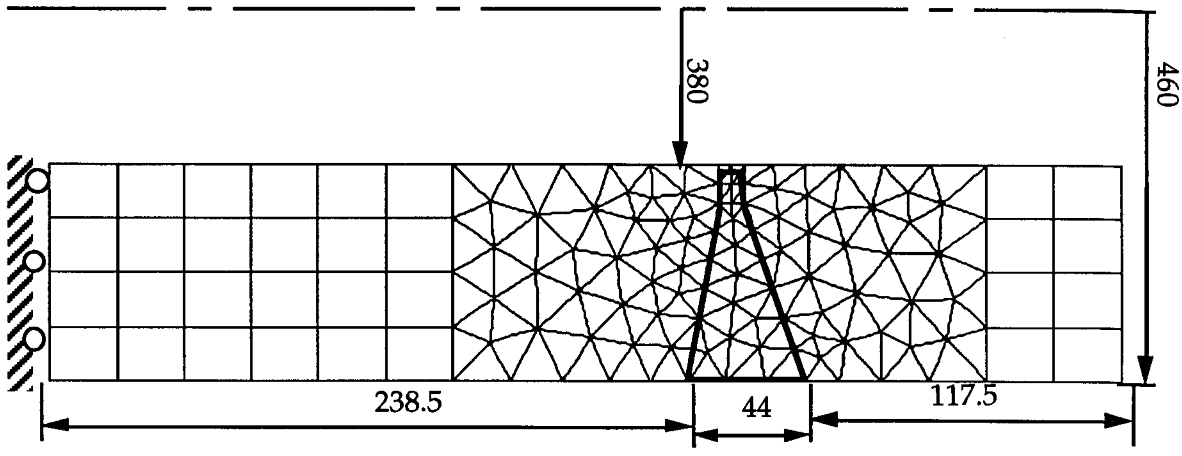

Fig 7 : Mesh of the structure.

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