Modelling of Heat Transfers, Phase Changes and Mechanical Behaviour during Welding

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ABSTRACT. *This paper describes the main models used in finite element software for welding simulations. Welding involves thermal transfers from the weld zone to the rest of the structure and thus leads to loadings due to thermal gradients and tools. Moreover, the temperature reaches locally relatively high values, so that the evolution of the microstructure in the material has to be taken into account. The main physical mechanisms involved during welding imply fully coupled thermal transfers and phase changes models, and thermo-mechanical models involving transformation induced plasticity. These models are described, and the concluding remarks outline particular points that are to be more investigated in the future.*

RÉSUMÉ. *Cet article décrit les principaux modèles utilisés dans les codes de calcul par éléments finis pour la simulation du soudage. Le soudage met en jeu des transferts thermiques de la zone soudée vers le reste de la structure et conduit ainsi à des sollicitations dues aux gradients thermiques et aux outillages. De plus, la température peut atteindre localement des valeurs relativement élevées, de sorte qu'il faut prendre en compte l'évolution de la microstructure dans le matériau. Les principaux phénomènes physiques en jeu lors du soudage nécessitent des modèles couplant fortement les transferts thermiques et les changements de phase, et des modèles thermomécaniques incluant la plasticité de transformation. Ces modèles sont décrits, et les remarques finales soulignent quelques points particuliers qu'il sera nécessaire de mieux étudier dans le futur.*

KEYWORDS: *welding, modelling, phase changes, temperature, plasticity.*

MOTS-CLÉS : *soudage, modélisation, changement de phases, température, plasticité.*

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1. Introduction

Microstructure changes, residual stresses and distortions are locally induced by welding processes. Their prediction by numerical simulations can considerably help for improving the mechanical behaviour of welded structures. For example, high residual stresses combined with hard phases can lead to brittle weld joints. Moreover, the prediction of distortions is very useful for example for the optimisation of the welding sequence.

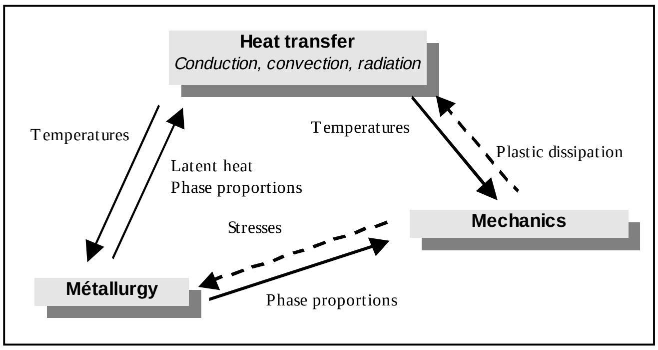

Figure 1. *Physical phenomena involved during welding, and their couplings*

Numerical simulations of welding are now possible with various finite element codes. In these codes, thermal transfers, metallurgical changes and mechanical behaviours are modelled and coupled according to various approaches. Figure 1 gives the physical phenomena involved during welding. The solid lines indicate the coupling phenomena, which are always taken into account during welding simulations. The dashed lines represent physical mechanisms, which are less important in our case, and thus, which are often neglected.

According to figure 1, it can be seen that heat transfers and metallurgical structures are fully coupled. It turns out that the first step in welding simulations consists of predicting the temperature field and the local phase proportions in the structure. This first step is described in the next paragraph. Then the temperatures and phase proportions are used as an input for the prediction of internal stresses and distortions. This second step is discussed in the third paragraph.

In this paper, the main models are always first detailed. Then other models are briefly described and referenced. Applications of these models can for example be found in a recent review paper on the present capabilities and future trends of the numerical simulation of welding in Europe (Boitout and Bergheau., 2003).

2. Thermal transfers and phase changes

It is well known that metallurgical structure of metals and heat transfer are fully coupled. Phase changes depend on temperature evolution, whereas temperature is influenced by contrasts of material characteristics between phases and latent heat effects. A lot of work has been performed on this subject, and classical models are now widely implemented into finite element computer codes (Leblond and Devaux, 1984, Fernandes *et al.*, 1985, Inoue and Wang, 1985, Habraken, 1988, Denis *et al.*, 1992, Reti *et al.*, 1999).

2.1. *Thermal transfers in multiphase materials*

Thermal transfers in a solid Ω are classically governed by the following heat equation:

$$\begin{cases} \rho \dfrac{dH}{dt} - \mathrm{div}\left(\lambda \,\mathbf{grad} T\right) - Q = 0 \quad \text{in} \quad \mathbf{\Omega} \\ \lambda \,\mathbf{grad} T \mathbf{.} n = q \quad \text{on} \quad \partial \mathbf{\Omega}_q \\ T = T_p \quad \text{on} \quad \partial \mathbf{\Omega}_T \end{cases} \qquad [1]$$

In this equation, ρ, H and λ are respectively the mass density, the enthalpy per unit mass and the thermal conductivity of the material, and Q is a heat source per unit volume. On the boundary $\partial\Omega$ of the solid, either a heat flux density q or a temperature T_p is prescribed, the former being eventually temperature dependent.

The heat power density used for welding is often represented by a heat source per unit volume Q or by a heat flux density q, both of them being expressed as a function of the local coordinates x, y and z. For example, a half ellipsoidal shaped function q(x,y) has been proposed for TIG welding (Goldak *et al.*, 1984), and a gaussian shaped function Q(x,y,z) is often used for high energy welding sources like laser or electron beam.

Temperature evolutions lead to phase changes, which have to be taken into account. If the proportion of phase number k is denoted by p_k, then the phase changes are considered by modifying the material properties as follows (subscript k denotes the material property associated with phase k):

$$\rho = \sum_{\text{phases}} p_k \rho_k \ , \quad H = \sum_{\text{phases}} p_k H_k \ , \quad \lambda = \sum_{\text{phases}} p_k \lambda_k \ \text{ and } \ \sum_{\text{phases}} p_k = 1 \qquad [2]$$

Equation [1] involves the time derivative of the enthalpy per unit mass. In the case of two phases, this quantity is obtained from equation [2] as follows :

$$\frac{dH}{dt} = \left[\left(1 - p_2\right) \frac{dH_1}{dT} + p_2 \frac{dH_2}{dT} \right] \frac{dT}{dt} + \frac{dp_2}{dt} \left(H_2 - H_1\right) \qquad [3]$$

It can be seen in this equation that the phase change $p_1 \rightarrow p_2$ involves a heat capacity and a latent heat effect given respectively by $(1\text{-}p_2)dH_1/dT+p_2dH_2/dT$ and $(H_2\text{-}H_1)dp_2/dt$.

2.2. *Phase changes*

For an hypoeutectoid steel, the main transformations to consider during welding are the austenitic transformation during heating, and the ferritic, pearlitic, bainitic and martensitic transformations during cooling. Many approaches can be used to describe these transformations. A general formulation of multiple phase changes has been proposed (Fortunier *et al*., 2000). This formulation is based on:

– Avrami type kinetics when the phase change is governed by diffusion (Avrami, 1939, 1940, 1941),

– The Koistinen-Marburger law for martensitic type transformations (Koistinen and Marburger, 1959).

– The Avrami type kinetics is classically used to model a phase change governed by diffusion. According to this kinetic, the proportion of product phase p is given as a function of time along an isothermal path by:

$$p = P\left(1 - e^{-(ft)^n}\right) \qquad [4]$$

In this expression, P is the phase proportion obtained at the end of the transformation, f a frequency and n an exponent, which are generally obtained from IT diagrams by using the so-called *Avrami plot* method. However, welding processes involve non-isothermal paths, and a particular differential form of equation [4] has to be used in order to retrieve this equation along isothermal paths. The rate of phase change is thus written as follows (parameters P, n and f can be temperature dependent):

$$\dot{p} = nf\,\left(P - p\right)\left[\boldsymbol{ln}\left(\frac{P}{P - p}\right)\right]^{\frac{n-1}{n}} \qquad [5]$$

According to the Koistinen-Marburger law, the proportion of martensite p formed at temperature T is given by the following equation:

$$p(T) = \begin{cases} 0 \text{ when } T > M_s \\ 1 - e^{b(T - M_s)} \text{ when } T \leq M_s \end{cases} \tag{[6]}$$

where b is a kinetic factor homogeneous to the inverse of a temperature and M_s the starting temperature of the martensitic transformation. These coefficients are material dependent. For example, in the case of steels, the M_s coefficient is a function of the carbon content in the transformed austenite. Martensitic type transformations can also be expressed in a differential form. This is simply done by differentiating equation [6]. We obtain:

$$\dot{p} = \begin{cases} -b(1-p)\dot{T} \quad \text{when } T \leq M_s \text{ and } \dot{T} \leq 0 \\ 0 \quad \text{otherwise} \end{cases} \tag{[7]}$$

According to equations [5] and [7], any single phase transformation can be described in a differentiated form, so that phase changes along any thermal path T**(t)** can be evaluated by integrating these equations. Moreover, equations [7] can simply be expressed in the form of equation [5] by stating that n=1, P=1, and that f depends on the thermal path as follows :

$$f = \begin{cases} -b\dot{T} \quad \text{when } T \leq M_s \text{ and } \dot{T} \leq 0 \\ 0 \quad \text{otherwise} \end{cases} \tag{[8]}$$

In general, different phases may be present simultaneously, and transform into another in a given volume element. In this case, if p_i denotes the current proportion of phase number i, we can define a “driving force” of the i⟶j transformation by $E_{ij}=P_{ij}(p_i+p_j)-p_j$, where P_{ij} is the maximal proportion of phase j that one can obtain from phase i. It should be noted that if the driving force E_{ij} is positive, then the driving force E_{ji} (corresponding to the j⟶i transformation) is negative. These driving forces thus indicate the “direction” of the transformation between phases i and j.

We can now solve the problem of many phase transformations by just replacing p_i by $p_i/(p_i+p_j)$ in equation [5]. Then the variation of the proportion of phase j results from all the possible transformations i⟶j and j⟶i, which are assumed to occur independently. Thus we have the following relation:

$$\dot{p}_j = \sum_{j \neq i} A_{ij} \tag{[9]}$$

where A_{ij} can be considered as the "activity" of the reaction between phases i and j (i.e. transformation i→j or j→i). This activity is finally obtained from equation [5]:

$$A_{ij}=\begin{cases} n_{ij}f_{ij}E_{ij}\left[\boldsymbol{ln}\left(1+\dfrac{p_j}{E_{ij}}\right)\right]^{\frac{n_{ij}-1}{n_{ij}}} & \text{if } E_{ij}>0 \quad (i\rightarrow j\text{ transformation}) \\[2ex] -n_{ji}f_{ji}E_{ji}\left[\boldsymbol{ln}\left(1+\dfrac{p_i}{E_{ji}}\right)\right]^{\frac{n_{ji}-1}{n_{ji}}} & \text{if } E_{ji}>0 \quad (j\rightarrow i\text{ transformation}) \\[2ex] 0\text{ otherwise} \quad (\text{no transformation}) & \end{cases} \tag*{[10]}$$

Parameters P, n and f in this equation are reaction dependent, and the activities A_{ij} form a skew-symmetric matrix (A_{ij} represents the proportion of phase i which is transformed into phase j by unit of time, so that $A_{ij}+A_{ji}=0$). Thus the sum of the rates of change of the phase proportions vanishes, as desired.

Different numerical schemes can be used to perform time integration of these equations. For example, for Avrami type kinetics, the thermal path can be divided into several isothermal time steps $\mathbf{[t, t+\Delta t]}$, along which an integrated form of the kinetics is applied (Pumphey and Jones, 1948, Denis *et al*, 1992), but a classical second order Runge-Kutta method can also be used (Leblond and Devaux, 1984, Fortunier *et al.*, 2000).

2.3. *Working example*

When phase changes are studied on a given material, thermal paths are imposed, and dilatometry measurements are often used to detect phase transformations. During these experiments, it is generally assumed that the temperature in the specimen is homogeneous, so that the heat flux density q in equation [1] vanishes. The thermal path of these experiments is thus schematised by the internal heat source term in equation [1]. This term represents the heat quantity which is put into (for heating) of extracted from (for cooling) the specimen by unit of time, and equation [1] reads:

$$Q-\rho\dot{H}=0 \quad \text{in} \quad \boldsymbol{\Omega} \tag*{[11]}$$

According to this equation, a thermal path T(t) is obtained by monitoring Q(t). It turns out from equations [11] and [2] that the temperature change rate in the specimen and the internal heat source are related by:

$$\frac{Q}{\rho} = \dot{T} \sum_i p_i \frac{dH_i}{dT} + \sum_i \dot{p}_i H_i \qquad [12]$$

In this equation, the rates of change of the phase proportions are obtained from equations [9] and [10]. If N denotes the total number of phases that may be present in the specimen, then we can define a vector with N+2 components consisting at any instant of:

– the temperature T,

– the heat source or sink Q,

– the phase proportions $p_1, \ldots, p_N$.

When a thermal path is applied to a specimen, then either T(t) or Q(t) is known, and the N+1 remaining components of the vector are determined by integrating equations [12] and [9], [10]. This allows for the simulation of any thermal path applied to a given material. In the case of IT diagrams, isothermal phase changes are detected at different temperatures, so that T(t) is known and constant. In the case of CCT diagrams, phase changes are followed along continuous cooling paths. These paths are obtained by prescribing a linear function T(t) or a constant value Q.

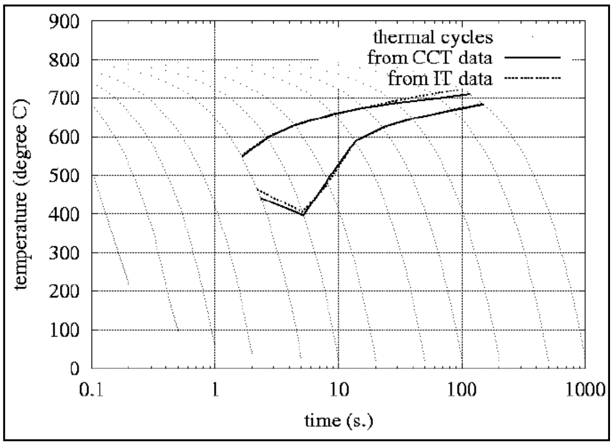

Figure 2. *0.8% carbon steel CCT diagrams recalculated by prescribing T(t)*

Figures 2 and 3 give calculated CCT diagrams corresponding to a 0.8% carbon steel (Fortunier *et al.*, 2000). Metallurgical data have been obtained from IT or from

CCT diagrams using an identification procedure described in Pont *et al.* (1994). It can be seen in this figure that:

– Metallurgical data obtained from IT (dashed lines) or from CCT (solid lines) diagrams give quite similar results;

– Prescribing T(t) or Q(t) can lead to relatively different recalculated CCT diagrams. This is mainly due to the latent heat effects during phase changes (see figure 3).

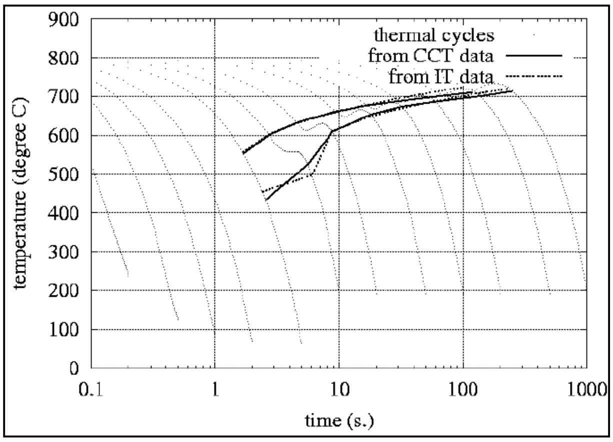

Figure 3. *0.8% carbon steel CCT diagrams recalculated by prescribing Q*

2.4. *Other models*

A model directly based on CCT diagrams has been incorporated in some finite element software (Waeckel, 1994). This model is also based on a differential form of the phase changes, but the function in equation [5] is replaced by non explicit values computed at each point using information read on the CCT diagram. As a consequence, this model really sticks to the CCT diagram and cannot be used out of its boundaries, for example when the cooling rates exceeds the cooling rates of the diagram. However, the main advantage of this approach is that there is no need to identify parameters.

The modelling of the tempering is also very important when residual stresses and distortions during a multi-pass welding operation are to be computed. Indeed, tempering effects result in the lowering of the yield stress of the material. In a multi-pass welding process, each pass generates a tempering effect on the heat affected zone induced by the previous weld beads. The consequences are very important on the residual stresses. A dedicated model has been proposed for tempering of martensite with three independent kinetics, each of them using a Johnson-Mehl-Avrami law (Aubry *et al.*, 1997):

– precipitation of carbides in martensite,

– transformation of retained austenite into ferrite and cementite,

– transformation of carbides into cementite.

Equation [5] can also be used to model pseudo-transformations from an as-quenched structure to a tempered one (Leblond and Devaux, 1984).

Finally, the effects of stresses on transformation kinetics have also been examined (Denis *et al.*, 1987). Practically, the lack of material data is a strong limitation to the application of the models.

3. Mechanical behaviour

The mechanical analysis is based on the usual equations describing the static equilibrium of the welded structure. This analysis is often uncoupled from the analysis of the thermal transfers. Thus, the mechanical computation is achieved by using temperatures and phase proportions obtained previously at each point of the structure. The effects considered are:

– the thermal dilatations and the volume changes during phase transformations,

– the influence of the phase proportions on the local mechanical characteristics, and the transformation induced plasticity.

3.1. *Thermal dilatations and volume changes due to phase transformations*

The volume changes due to transformations are the main cause for the residual stresses and distortions. To include those changes in a computation, a simple solution consists in changing the standard thermal strain into the following thermal and metallurgical strain:

$$\varepsilon^{th}(T) = \sum_{\text{phases}} p_k . \varepsilon_k^{th}(T) \qquad [13]$$

where ε_k^{th} represent the thermal strain of each individual phase.

Figure 4 gives the evolution of the total thermal strain in a specimen submitted to a free dilatometry test. It can be seen in this figure that, in order to reproduce the volume changes due to transformations, the ε_k^{th} terms in equation [13] differs not only by their slopes (which correspond to the heat expansion coefficients of each phase k), but also by their values at the origin (Leblond *et al.*, 1986).

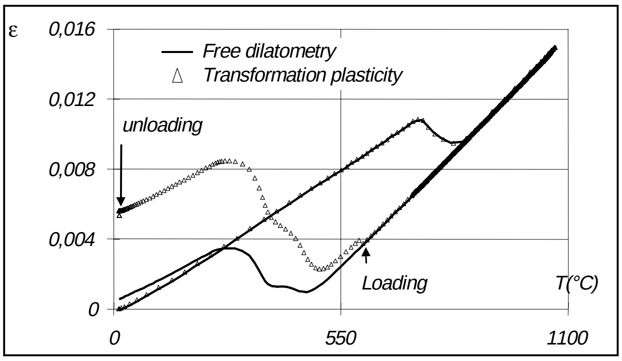

Figure 4. *Free dilatometry and transformation plasticity tests (Petit, 2000)*

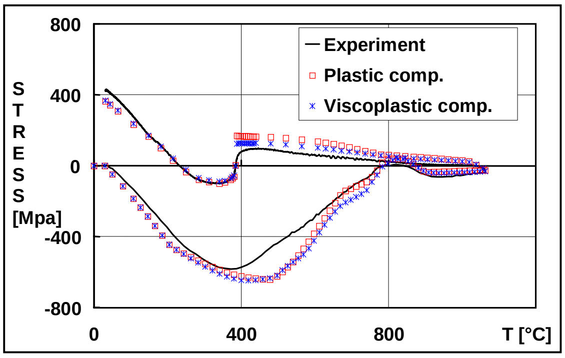

Figure 5. *Satoh test (Vincent, 2002)*

Figure 5 gives the longitudinal stress evolution in a bar shaped specimen with fixed ends heated above the temperature corresponding to the end of the austenitic transformation and then cooled down. This test is refereed to as the Satoh test. It is difficult to control experimentally, but the effects of volume changes occurring during a transformation on the residual stresses can easily be observed.

As expected, the stress at high temperature is close to zero. At the beginning of the cooling period, tensile stresses are developed, which reach the yield strength of the material. When the transformation proceeds, due to the volume change, a sudden stress reversal is observed, leading to a compressive stress. It is clear that, as in the meantime the specimen continue shrinking, the stress value and the sign at the end of cooling strongly depend on the temperature start of the transformation, its range and the new phase volume condition.

3.2. *Local mechanical characteristics and Transformation induced plasticity*

When the elasticity constants are assumed to be the same for all the phases, it has been proved that the plastic strain rate can be expressed in the following form (Leblond *et al*., 1989):

$$\dot{\boldsymbol{\varepsilon}}_p = A\dot{\boldsymbol{\sigma}} + B\dot{T} + C\dot{p} \qquad [14]$$

Mathematical expressions for the different implied coefficients A, B and C can be derived from micro-mechanical analyses and elementary finite element simulations. Coefficients A and B correspond to classical thermo-mechanical models, whereas coefficient C is associated with transformation plasticity.

As soon as one considers the behavior of steels during transformation, transformation induced plasticity cannot be neglected. The transformation plasticity effect can be shown by combining a dilatometry test (figure 4) with an applied stress during the cooling transformation during. In this case, a relatively small stress (i.e. small compared to the yield stress of the weakest phase of the material at that time) applied during the transformation while cooling will generate a residual strain nearly proportional to the applied stress. This behavior can be associated with two mechanisms:

– The Greenwood-Johnson mechanism (Greenwood and Johnson, 1965), which states that the volume change during the transformation is enough to induce plasticity in the weakest phase (austenite). Those small strains are orientated in the direction of the applied stress.

– The Magee mechanism (Magee, 1966), which is related only to martensitic transformation and is the result of a specific orientation of the martensite needles during the transformation. This orientation is related to the local stress state.

In memory-shape alloys the Magee mechanism is the only mechanism responsible of their specific behaviour. In the case of welded structures, this mechanism is often neglected, the Greenwood-Johnson mechanism giving the main contribution to the transformation induced plastic deformation.

Transformation induced plasticity has been studied by many authors (Greenwood and Johnson, 1965, Magee, 1966, Abrassart, 1972, Giusti, 1981, Berveiller and Fischer., 1997, Fisher *et al*., 2000). Different models have been investigated to account for the Greenwood-Johnson mechanism. All the models can be written in the following form in a three-dimensional case:

$$\dot{\boldsymbol{\varepsilon}}_{pt} = \frac{3}{2} K\,\mathbf{S} f'(p)\dot{p} \qquad [15]$$

where **S** is the stress deviator, K a material parameter and f(p) a specific function of the local phase proportion p.

Numerical simulations of welding often use the following values for the K coefficient and the f(p) function (Leblond *et al.*, 1989):

$$K = \frac{2}{3\sigma_\gamma^y}\frac{\Delta V}{V} \quad \text{and} \quad f(p) = p - p\,\boldsymbol{log}\,p \qquad [16]$$

where $\Delta V/V$ represents the relative volume variation during the transformation and σ_γ^y, the austenite yield strength. Recently, these expressions have been slightly improved for small values of p (Taleb and Sidoroff, 2003).

The viscoplastic effects have been often neglected during welding simulations, since the welding processes only involve very short time durations. But, the mechanical properties of austenite at high temperature strongly depend on the strain rate, and these properties have an important effect on the final residual distortions (Bru *et al.*, 1996). Therefore, this effect must now be integrated in the models. Moreover, an experiment representative of a welding operation has pointed out that viscoplastic effects cannot be neglected (Cavallo, 1998, Vincent, 2002). Wang and Inoue (1985) present a model which makes no exception for the transformation plasticity. An elastic-viscoplastic model with combined hardening has also been developed (Colonna et al., 1992). The yield strength and the viscous parameters are obtained with mixture laws. A non-unified elastic-viscoplastic model has been developed (Videau *et al.*, 1994*)*, whereas a parallel model has also been programmed (Coret and Combescure, 2002). In the latter, the strain is assumed identical in all the phases and the macroscopic stress is obtained with a mixture law on the individual stresses in each phase. Finally, the model proposed by Leblond and coworkers (Leblond *et al.*, 1989) has recently been extended to visco-plasticity by considering the yield stress of the phases as a function of the viscoplastic strain rate (Vincent *et al.*, 2003).

4. Concluding remarks

The numerical simulations of welding are now widely used in industry during the design and/or production stages. Generally, such computations are done with general purpose finite element software or dedicated software.

The models presented in this paper have now been validated against microstructure and residual stresses. The main reason is that the low temperature material data, on which the residual stresses mainly depend, are relatively well known. Moreover, local models of the welded zone are generally sufficient to obtain acceptable results in this case.

However, distortion predictions is more difficult. Since distortions strongly depend on high temperature mechanical properties, the development of high temperature material database becomes necessary. Moreover, calculation of distortions involve the whole structure. Beside the improvement of computer capabilities, it seems that simplified methods have now to be extensively developed

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