Mechanical Behavior of Interfaces in Nickel-Based Superalloys: Finite Element Method Analysis.

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ABSTRACT:

In this paper we use the Finite Elements Method (FEM) to model the mechanical behavior of γ/γ' two-phase single-crystal superalloys. All calculations have been performed in elasticity for a three-dimensional finite element model analysis: we take into account real morphology (cubic with rounded edges) and the cubic crystallographic structure of the disordered γ phase and ordered γ' phase. We compare results of our 3D Finite Element model with the experimental literature and 2D models for equivalent VON MISES stresses, stored elastic energy and deformations. We are particularly interested in γ - γ' interfaces, which play a significant role in the behavior of industrial superalloys: misfit parameter and elastic energy. These interfaces play a significant role in the behavior of nickel-based superalloys.

Based on our results we criticize isotropic modelings, 2D models and values of misfit calculated in the existing literature. Our models are in agreement with the experiments because they take into account the real geometry and crystallography.

INTRODUCTION

Nickel-based superalloys allow improvement of the mechanical properties and extension of the field application of two-phase materials. They are used a great deal in the aircraft industry to manufacture single-crystal turbine blades because of their excellent mechanical properties at high temperatures. They consist of two cubic structures phases: γ disordered and γ' ordered. The specificity of these superalloys lies in the very particular morphology of their microstructure, a morphology that results from the existence of the distortions of coherence and the strongly anisotropic elastic behavior of the two phases. The γ' phase may appear in spherical or cuboids precipitates [1,2].

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Optimization of mechanical properties is achieved by a judicious choice of γ' volume fraction, size and misfit δ /3,4,5/. The macroscopic elastic limit increases with temperature until it reaches a maximum, beyond this peak it decreases (at a given temperature this limit depends on the orientation) /6/. γ and γ' phases have slightly different cell parameters although they are perfectly coherent. This difference in dimensions generates a stress field in material and in particular residual stresses at interfaces.

Up to now little work has been carried out in order to understand the role of the interfaces in the behavior of superalloys. Blavette *et al.* /7/ have analyzed by atomic probe the interfaces of a single-crystal, nickel-based superalloy crept at 1050 °C and have then tried to understand the influence of the applied stress on the γ/γ' interfaces' chemical composition: they note subtle variations between the two types of interfaces according to their orientation compared to the direction of the load. In this article we study the mechanical behavior of the interfaces.

Various methods have been used to estimate the misfit: Lahrman *et al.* /8/, Tian /9/, Fredholm /5/, Royer *et al.* /10/, Grose *et al.* /11/ and Nathal *et al.* /12/. It differs according to the analyzed direction because of the anisotropy due to crystallography and geometry of the precipitates. The fact that the γ' phase has a coefficient of thermal expansion lower than that of the matrix is one of the reasons for the algebraic decrease in the misfit. Currently, Völkl *et al.* /13/ are using three different methods to measure the nonconstrained misfit in the CMSX-4 alloy. These authors carried out *inter alia* calculations by the Finite Element Method (FEM) and Convergent Beam Electron Diffraction (CBED). The various quoted authors have often arrived at divergences between their various measurements of the misfit for the same superalloy. These variations may be explained by the strong dependence of the misfit on the shape of the precipitates. In addition the applied boundary conditions influence the results in a very significant way.

Finally, few results exist from calculations by the three-dimensional FEM, hence the significance of our study.

1. MATERIALS

1.1. Modeling:

In our modeling the material is supposed to be periodic, which is rather close to reality, and the boundary conditions obey this assumption of periodicity. The two phases constituting the studied material are supposed to have a perfect connection.

We use the numerical values based on data of the images observed under electronic microscopes in previous work. In Figure 1, drawn from the thesis of Benyoucef /14/, we note that the various precipitates called in the literature “cuboids” are in fact parallelepipeds with rounded corners.

Hazotte *et al.* /15,16/ showed that minimal elastic energy is obtained for the morphology formed from eight cubes. But initially the microstructure of material modeled in this study by F.E. calculations was represented by a cube (precipitate) surrounded by channels (matrix).

Fig. 1: Microstructure of MC2 superalloy. The matrix γ is in dark contrast and the precipitates γ' are in clear.

The choice of a periodic approach in three-dimensional modeling allows us to reduce the calculation in a cubic unit cell representative of the whole material, maybe in an eighth of a single precipitate surrounded in a coherent way on its three faces by channels forming the matrix (for a 3D mesh). γ/γ' interfaces are supposed to be aligned parallel to the $\{001\}$ planes of the cube. For reasons of volume of calculations this choice of periodic approach is obligatory, and, in fact, all models of massive material assume implicitly the periodicity of the structure. Boundary conditions imposed on the studied structure are symmetry conditions.

Very dubious results encountered in the literature /17/ and the images obtained by with scanning and transmission microscopes /14,17/ have spurred us to describe better the geometry of the two-phase structure, to eliminate the case of sharp edges and to take into account round-offs of the edges and to introduce them to net the eighth of a cube. Let us notice that in the actual material the radius of curvature of these edges varies from one precipitate to another, as one can see on microscopic images.

We are interested in calculation within the framework of isotropic and anisotropic elasticity. The single grains of superalloys have a cubic crystallography, their elastic behavior is anisotropic and they are thus characterized by three independent constants: the elastic constants obtained are those of a composite body made up of the two phases with distinct elastic properties.

In the case of materials with a linear elastic behavior, the macroscopic law of behavior connecting the

tensor of stresses σ to that of strains ε by the tensor of moduli C is written:

$$\sigma = C \varepsilon \quad (1)$$

For reasons of cubic symmetry only three elastic constants, C_{11} , C_{12} and C_{44} , are to be defined in the crystallographic reference mark. The following tables taken from the literature give the values of these constants.

Table 1

Elastic moduli of γ and γ' phases at 25°C and 980°C /18/.

Constants	Matrix (γ)		Precipitate (γ')	
T (°C)	25	980	25	980
E (GPa)	123.4	92.0	115.1	85.0
ν	0.387	0.405	0.387	0.401
α ($10^{-5}/^{\circ}\text{K}$)	1.58		1.32	

Table 2

Elastic constants of γ and γ' phases at 25°C and 1050°C /19,20/.

Constants	Matrix (γ)		Precipitate (γ')	
T (°C)	25	1050	25	1050
C_{11} (GPa)	218.5	109.3	166.9	124.8
C_{12} (GPa)	117.4	58.7	89.7	67.1
C_{44} (GPa)	143.4	71.7	109.5	81.9

where E is Young's modulus, ν Poisson's ratio and α the linear thermal expansion coefficient.

The misfit will be simulated as a difference between the coefficients of thermal expansion of the two phases γ and γ' , which represents a thermal loading of the structure. We show elsewhere [submitted paper] that at 820°C the boundaries are without constraint.

Finally we shall proceed to the superposition of the precedent load and of a field of tensions (traction/compression) in order to evaluate the local stresses of the γ/γ' microstructure of the nickel-based superalloy.

1.2. Finite Element mesh

We use the computer code CAST3M, obtained by courtesy of the “Commissariat à l’Energie Atomique”.

The FEM allows solution of the preceding intricate problem by using a simple approximation of the unknown fields. While going from a coarse mesh to a finer one, we vary the number of elements in the rounded corners. Figure 2 gives the evolution of the density of elastic energy vs the number of elements in the rounded corners of the precipitate, the material being considered isotropic (Figure 2-a) or anisotropic (Figure 2-b); this last figure also gives the result for the structure with sharp edges of the precipitate. We note that from 15000 elements results are stable and the anisotropic material minimizes elastic energy.

Fig. 2: Evolution of the density of elastic energy vs the number of elements of meshes: a) Isotropic case; b) Anisotropic case.

We have considered the total error (Figure 3) in calculating the true stresses with the two types of meshes (with sharp edges (3-a) and rounded ones (3-b)). In the cubic case with sharp edges, error evolution is higher than with round-offs. On the other hand, the error obtained for meshes with precipitates with rounded corners decreases slightly to a total number of elements of 21,500 (which corresponds to the mesh 22*22*22); after that it no longer varies and the anisotropic structure gives better results than the isotropic one.

Fig. 3: Estimate of the total error in the calculation of the real stresses, refinement and validation of the mesh (isotropic and anisotropic cases). a) cubic structure, b) structure with rounded corners of precipitate.

Starting from this last mesh we wanted to know how the total error will evolve by fixing this time the number of elements in the round-offs and by varying only those outside; Figure 3 shows that this error remains constant.

The mesh is thus stable and converging from a number of elements of 21,500 distributed in a precise way between the interior of the round-offs and the other zones.

2. RESULTS

2.1. Analysis of morphology

From Figure 1 we have measured for a range of 62 grains the lengths a and b defined in Figure 4 (a being taken by convention smaller than b). In Figure 4-a we give the distribution of the grains vs the characteristic length $(a*b)^{\frac{1}{2}}$. We note that the average characteristic length is $241nm$. We also give (Figure 4-b) the

Fig. 4: a) Illustration of the average length characteristic of precipitate; b) distribution of the grains vs the ratio; c) diagram illustrating the localization of the standard grain.

distribution of grains vs ratio $\frac{a}{b}$. This ratio varies from 0.3 to 1 and the average ratio is 0.71. The standard grain corresponding to $(a * b)^{\frac{1}{2}} = 241nm$ and $\frac{a}{b} = 0.71$ thus has the dimensions $a = 203nm$ and $b = 286nm$; we notice that it corresponds to a cuboid with an edge of approximately 240nm but to no observed grain. We take the ratio $\frac{a}{b}$ for the 62 grains vs the characteristic length $(a * b)^{\frac{1}{2}}$. We note that 61% of these 62 grains

are in the rectangle traced in Figure 4-c. The standard grain corresponds to the blue square being practically the center of this rectangle.

To specify the shape of the grains we used the same region of image 1 and estimated 248 radii of curvatures. We note that the most frequent radius of curvature R is close to 40nm . The values thus determined cover a range of values from 22nm to 65nm . These values are definitely lower (approximately one tenth) than those determined by Espie, which range roughly from 180nm to 620nm , but these last dimensions exceed half of the side of a precipitate.

Considering the cuboidal precipitate dimensions A , B and R , defined in Figure 5, and the surface proportion $P_s = 76\%$ that we estimated by analysis of the image in Figure 1 we will use for modeling, taking into account what precedes, $R = 40\text{nm}$, $2A = 240\text{nm}$. One finds then $B = 136\text{nm}$ and a volume proportion $P_v = 0.642$, that is, 64.2% of precipitates in volume.

Fig. 5: Diagram used for the calculation of the volume of the eighth of a precipitate in the matrix.

2.2. Calculation of misfit

One calculates the strains in several nodes of the mesh along the direction $[100]$ with the aim of determining the misfit, a significant parameter for evaluation of the stresses due to this misfit. We see on these nodes in Figure 6.

If no stress is applied, for a temperature of 1050°C we obtain the misfit corresponding, in fact, to the amplitude of the tetragonal distortion, and the computed value is $-0.7 \cdot 10^{-3}$. This value is coherent with that found by Royer /21/.

Let us notice that from the experimental point of view the determination of the misfit is very delicate /12/. The measurement of the misfit has been the subject of many reflections and was for a long time prone to controversies; the “FEM” proves necessary and effective in solving this type of problem, allowing us to determine infinitely small values provided that one has a morphological representation very near to the real structure and a good smoothness of the meshes, which is true in our case. We give additional precise details on the misfit in the section on “interfaces”.

Fig. 6: Distribution of normal strain along x direction: ϵ_x^y and ϵ_y^x .

2.3. VON MISES equivalent stresses

The precise knowledge of the distribution of internal stresses allows us to understand the effect of coherence between the two γ and γ' phases on the mechanical behavior of the single-crystal superalloys.

We point out that for the cubic ones with centered faces the criterion of VON MISES – the criterion of energy of distortion – is physically justified. The VM equivalent stresses are calculated by our finite elements model in both phases with isotropic and anisotropic elasticity.

To bring us closer to the real case, we superimposed on the internal stresses due to the misfit a stress σ_a of 100MPa applied to the higher and lower faces of the structure; σ_a obviously corresponds to the mechanical load on the industrial superalloys when they are working. We note that a strong evolution of the microstructure of these superalloys occurs under the effect of temperature and applied stresses.

The results are illustrated in Figure 7. The loadings of the channels parallel and perpendicular to σ_a are close. It is noted that the precipitate is less charged (in a homogeneous way) than the matrix channels and we point out that the yield stress of the precipitate is higher than that of the matrix, except at low temperatures where they are relatively weak (about 300MPa/14°).

We note that the isotropic structure is approximately 6 times more charged than the anisotropic one, both in the channels and the precipitate. Of course, it is the anisotropic calculation that corresponds to reality because the crystallographic structure is anisotropic. One can notice that in the anisotropic (the less loaded) case, which corresponds to actual material, the yield stress of the precipitates (560MPa around 900°C/14°) is not reached by the calculated VM stress, whereas the matrix yield stress (70MPa at 900°C) exceeds the calculated VM stress.

Fig. 7: Distribution of Von Mises equivalent stresses (MPa): a) in isotropic modeling; b) in anisotropic modeling. Superposition of a thermal field of 1050°C and a compression of 100 MPa in both cases.

2.4. Interfaces

As before, we have carried out an isotropic and an anisotropic calculation. Figure 8 gives the elastic energy in the two-phase material and in interfaces: it is noted that the anisotropic structure minimizes energy compared to the isotropic one.

This figure highlights (green-yellow colored strip) the characteristic of the interface: from the point of view of elastic energy, it is a true zone of transition between the precipitate and the matrix. However, as one can see on the curves of Figure 8, the elastic energy varies along the interface and differently according to whether the interface is perpendicular or parallel to the applied stress. Here also the anisotropic calculation is very different from the isotropic one, in particular in the round-offs: it is noted that the elastic energy is minimized in the anisotropic case, which corresponds to reality, whereas it reaches a maximum in the isotropic case.

For the line described in Figure 8 by the nodes C_1 , C_2 , C_5 and C_{10} we give the normal and tangential strains at the interface (Figure 9), that is from C_1 to C_2 ϵ_{xx} tangential deformation and ϵ_{zz} normal deformation and, of course, from C_5 to C_{10} the reverse, ϵ_{xx} normal deformation and ϵ_{zz} tangential deformation. These results are in agreement with the literature that shows that the normal misfit is greater than the tangential one.

From C_2 to C_5 ϵ_{xx} and ϵ_{zz} are not relevant; we could easily calculate the normal and tangential strains in this zone, but in the round-offs, i.e. from C_2 to C_5 , the misfit, both normal as tangential, is difficult to define.

It is noted again that the anisotropic structure is more advantageous than the isotropic one: the network is deformed less at the interface; the corresponding misfit, both the tangential and the normal, is weaker.

Fig. 8: Total elastic energy (J/m^3) for two-phase material and interface: a) and b): isotropic modeling, c) and d): anisotropic modeling.

Fig. 9: Distribution of interfacial strains along X and Z directions (nm): a) isotropic model, b) anisotropic model.

DISCUSSION AND CONCLUSION

We note that a modeling by finite elements is correct only if one is concerned with convergence of calculations, which we are.

In the anisotropic case, total elastic energy calculated with the model with sharp edges is higher than that of the model with round-offs, which proves that, simply from the point of view of elastic energy, the precipitates have an interest to grow with round-offs, as seen indeed under the electronic microscope.

We showed, in addition, that the increase in the radius of curvature generates a reduction in the VM equivalent stresses estimated in the cuboidal precipitate: when the radius becomes very large, the precipitate geometry deviates from reality, the mesh becomes less and less sharp and the stress concentration is reduced.

The calculations we performed underline, by comparison with the existing literature, the difference between the 2D and 3D elastic approaches. Thus results of our calculations differ from those obtained in 2D and quoted in the literature. With regard to the VM stresses, the values that we obtain are definitely higher than those obtained by 2D modeling (approximately 60%) and this is in agreement with the experimental literature [22]. We think that this is due to the fact that 2D modeling is incorrect because it assumes a state of plane stresses or plane strains, which cannot correspond to reality taking into account the geometry of the material. We notice, however, that a study in 2D for thin blades with $\langle 001 \rangle$ normals is relevant because the loading corresponds to a state of plane stresses. For lack of data in the literature we could not compare the elastic energy for 2D and 3D modelings.

The comparison of isotropic and anisotropic modeling confirms the interest in the use of the suitably directed superalloys for manufacture of the turbine blades of turbojets. In the cubic ones one knows that the $\langle 001 \rangle$ axes are among the most resistant to a given mechanical loading. It is thus coherent that the anisotropic structure charged in tension (traction/compression) along $\langle 001 \rangle$ axis minimizes the stored energy and the VM stress compared to the isotropic structure, as shown by our calculations.

However, the elastic models are naturally insufficient, as shown by the literature in electronic microscopy; nevertheless the VM curves which we give confirm that in fact the matrix channels should at first deform plastically, as confirmed by experimental results in microscopy. One can speak of the beginning of a mechanism of plasticity with the elastic model. We intend to go further in this last point with a viscoplastic modeling.

Our calculations on the misfit are in agreement with the literature: the normal misfit is higher than the tangential misfit. Anisotropic calculation gives a misfit smaller than the isotropic one; this shows that, generally in models of the literature, the misfit is over estimated because it is calculated isotropically, which does not correspond to reality.

Finally, our model is in good agreement with reality: it takes into account the real geometry and crystallography and it agrees with the experimental results.

REFERENCES

1. P. Caron, T. Khan, 1983, *Mat. Sci. and Eng.* 61, 173.
2. A. Royer, P. Bastie, M. Veron, A. Jacques, 2000, *Journal de physique IV*, vol 10, n° 4.
3. M. V. Nathal, 1987, *Metall. Trans., A*, 18A, 1961.
4. M.V. Nathal, R. A. Mackay and R. V. Miner, 1989, *Metall. Trans., A*, 20A, 133.
5. A. Fredholm, 1987, These, Ecole des Mines de Paris.
6. N. Clement, 1986, *J. Microsc. Spectrosc. Electron.*, Vol 11, pp. 195-204.
7. D. Blavette, L. Letellier, A. Racine and A. Hazotte, 1996, *Microsc. Microanal. Microstruct.*, 7, pp. 185-193.
8. D. F. Lahrman, R. D. Field, R. Darolia, and H. L. Frazer, 1988, *Acta Metall.*, 36, 1309-1320.
9. W. H. Tian, Z. Horita, Y. Honda, H. Kunitaka, *et al.*, 1992, *Materials Transactions JIM*, vol. 33, 12, pp. 1084-1092.
10. A. Royer, P. Bastie, D. Bellet, and J. L. Strudel, *Phil. Magazine A*, 1995, vol. 72, n° 3, 669-689.
11. D. A. Grose, and G. S. Ansel, 1981, *Metallurgical Transactions A*, 12A, 1631.
12. M. V. Nathal, R. A. Mackay, R. G. Garlick, 1985, *Mat. Sci. and Eng.*, vol. 75, pp. 195-205.
13. R. Völkl, U. Glatzel and M. Feller-Kniepmeier, 1997, *Scripta Materialia*, vol 38, n° 6, pp. 893-900.
14. M. Benyoucef, These, 1994, UPS-Toulouse.
15. A. Hazotte, T. Grosdidier, S. Denis, 1996, *Scripta Materialia*, vol 34, n°4, pp. 601-608.
16. A. Hazotte, A. Racine, S. Denis, 1996, *Colloque C1, supplément au journal de physique III. Journal de physique IV*, vol 6, pp. 119-128.
17. L. Espie, These, 1996, ENSMP, Paris.
18. U. Glatzel, and M. Feller-Kniepmeier, 1989, *Scripta Metall.*, vol 23, n°11, pp. 1839-1844.
19. J. F. Ganghoffer, A. Hazotte, S. Denis, and A. Simon, 1991, *Scripta Metall. & Mater.*, vol 25, pp. 2491-2496.
20. A. Hazotte, D. Bellet, J. F. Ganghoffer, S. Denis, P. Bastie, and A. Simon, 1992, *Physic. Mag. Letters*, vol 66, 4, pp. 189-196.
21. A. Royer, Thèse, 1993, Université Josef Fournier - Grenoble I.
22. L. Müller, U. Glatzel and M. Feller-Kniepmeier, 1992, *Acta Metall. Mater.*, vol. 40, n°6, 1321-1327.