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Crack initiation and propagation in FeAl matrix

D, Renowicz ^a, S.J. Skrzypek ^{b, *}

^a Department of Mechanics of Materials, Faculty of Materials Engineering and Metallurgy, Silesian University of Technology, ul. Krasińskiego 8, 40-019 Katowice, Poland ^b Department of Physical and Powder Metallurgy, Faculty of Metals Engineering and Industrial Computer Science, University of Science and Technology-AGH, Al. Mickiewicza 30, 30-059, Kraków, Poland

* Corresponding author: E-mail address: skrzypek@uci.agh.edu.pl

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ABSTRACT

Purpose: of this paper is evaluation of macroscopic and microscopic residual stresses and their influence on nucleation and development of cracking in Fe-Al-C cast alloy

Design/methodology/approach: In the case of particular chemical composition of Fe-Al-C alloy phenomena of its self-disintegration appears. Fracture mechanic methods with additional consideration of residual stresses were applied. The last one was measured by X-ray diffraction method.

Findings: Measurnaments and calculations proved that crack nucleation and development is controlled by diffusion of hydrogen and oxygen to chemical reaction with Al_4C_3 precipitations. This process is enhanced by existing residual stresses. When total stress approaches to critical stress level the cracks gradually develops.

Research limitations/implications: Microstructure of high-aluminium alloy (35.5 wt.% Al) consisted of brittle matrix with Al₄C₃ precipitations. Microstructure of this matrix appeared in a form of intermetallic compound as a superlattice FeAl.

Practical implications: These kind of intermetallics is practically applied in high temperature working machine components. In many cases they are under high level of residual stresses. Any progress in describing of cracking in this type of microstructure has real practical importance. Modeling of crack nucleation and farther its growth using finite elements method confirmed with real measurements make an interesting approach in characterization of cracking of the alloys.

Originality/value: Morfology of Al_4C_3 precipitation in FeAl superstructure alloy and its self-disintegration process can be ruled by chemical composition and solidification conditions. The elaborated physical model of cracking can be used to estimate durability of this Fe-Al-C alloy.

Keywords: Crack resistance; Fracture mechanic; X-ray phase analysis; Computational material science

1. Introduction

Durability of machine parts depends on many factors and one of them are interactions having distortion nature.. They appear in a form of crystal defects and lattice curvature connected with elastic strains/stresses which are created by mechanical, chemical, metallurgical and heat flow factors. Among them there are welding or assembly stresses [1-6], phase transformations [7] and thermal residual stresses. [8-10] and hydrogen interaction as well [11]. There are also distortions caused by chemical forces like due to chemical reactions between Al_4C_3 and oxygen and water vapor in high aluminium Fe-Al-C cast alloy. This is known phenomena which finally produces cracking and self-disintegration [12, 13]. Calculation and measurnement of microstresses around grains and carbide precipitation and in intermetallic matrix are presented in this work. The level of macroscopic residual stresses were caused by solidification process and during degradation Al_4C_3 carbides in a form of plate.

2. Experimental

Macro and microscopic residual stresses were measured with X-ray diffraction methods. The diffractometer D8 Advance with cobalt tube radiation was used. The modified $g-\sin^2\psi$ metod with grazing incidence angle X-ray diffraction geometry were applied [14-16]. This metodolgy anabled tomography like measurnaments in non-destructive way. This geometry of diffractin is characterized with small and constant incidence angle and with constant effective depth of penetration which is regulated with incidence angle of X-ray beam [16].

Using this non-destructive technique it was possible to repeat measurnaments of the same area on the sample versus time of chemical reaction and cracking development. A phase analysis, lattice parameter and lattice elastic strains can be measured with this diffraction [17].

Bragg equation and some crystallographic relations were used in measurement methodology of residual stresses:

$$a_{\varphi\psi} = d_{hkl}\sqrt{h^2 + k^2 + l^2} = \frac{\lambda}{2\sin\Theta}$$
(1)

where: $a_{\phi\psi}$ - lattice parameter measured in direction defined with ϕ and ψ angels, d_{hkl} - interplanar distance between crystallographic planes {hkl}, λ - wavelength, Θ - Bragg angle, ψ - angle between normal to the sample and normal to diffracting planes {hkl}, ϕ angle between x axis of the sample and direction of measured stress component.

An elastic strain measured in particular direction can be expressed with equation

$$\varepsilon_{\varphi\psi} = \frac{d_{\varphi\psi} - d_0}{d_0} \tag{2}$$

where: d_0 - interplanar distance between crystallographic planes {hkl} in unstressed sample (powder).

An elastic strain $\varepsilon_{\phi\psi}$ can be transformed into sample coordinates with relation:

$$\varepsilon_{\varphi\psi} = \varepsilon_1 a_1^2 + \varepsilon_2 a_2^2 + \varepsilon_3 a_3^2 \tag{3}$$

 $\epsilon_1, \epsilon_2, \epsilon_3$ - main strains, a_1, a_2, a_3 - direction cosine of the angles between strain measurement direction and principal direction 1, 2, 3.

Using above equation and Hook's law for plane stress field, principle equation of $\sin^2 \psi$ diffraction method can be derived: [16,17]:

$$\varepsilon_{\varphi\psi} = \frac{1+\nu}{E} \sigma_{\varphi} \sin^2 \psi - \frac{\nu}{E} (\sigma_1 + \sigma_2)$$
(4)

where: $\sigma_{\phi} = \sigma_1 \cos^2 \phi + \sigma_2 \sin^2 \phi$, σ_1 i σ_2 – principle plane stresses, E, v - elastic mechanical constances.

A microstresses were measured by X-ray diffraction method consisted in diffraction peak analysis. A physical widening of diffraction lines β were estimated with assumption of Gauss function fitting procedure [18].

$$\beta = \sqrt{B^2 - b^2} \tag{5}$$

here: B- half-width of measured diffraction line, b- half-width of reference sample.

Experimentally evaluated physical widening is used to calculate microstrains and microstresses [14,18]:

$$\overline{\varepsilon} = \frac{\beta}{4 \cdot tg\Theta} \tag{6}$$

Substituting microstrains to Hook's law microstresses (the second order of residual stresses) can be evaluated. Their range is of order of FeAl grains around Al_4C_3 precipitation.

For this purpose the diffraction line profile of {211} were analysied. A dyfractograms were recorded in normal envioremental conditions i.e. room tempereture, moisture 70%÷80%. Using grazing angle X-ray diffraction geometry it was possible to measure surface layers with thickness of g_1 = 3,75 µm, g_2 =7,5 µm, g_3 =10,5 µm, g_4 =14,0 µm during 0÷484 h in nondrstructive mode. X-ray diffraction patterns were recorded evry 24 hours. An example of microstresses distribution is presented on Figure 1.



Fig. 1. Microstresses σ_{II} distribution in surface layer versus time of self-disintegration

Proces of microcracking was developing in surface layer (thickness about $14 \mu m$), further calculations were curied out for the state of plane stress.

A local maximum of normal stresses was asumed as a characteristic criterion of the material as the stresses causing

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cracking in surface layer. Following values were taken into account:

$$\sigma_{\varphi} = \sigma_{I}, \text{and } \sigma_{3} = 0; \tag{7}$$

where: σ_I – macroscopic residual stress in surface plane, σ_3 -principal stress.

The macroscopic residual stress σ_{ϕ} was measured by $\sin^2 \psi$ method (eq.5), and procedure needs strain measurnament $\varepsilon_{\phi\psi}$ for choosen crystallographic planes {100},{110},{200} and {211} under different ψ angles [19]. An example of results for thickness of surface layer of g=3,75 µm is presented on Figure 2.

Residual stresses distribution σ_{ϕ} in surface layer of the sample versus time of self-disintegration for different thickness is presented on Figure 3.

Measurnaments were curied out from begining (state after casting) to the powder state what appeared after 484 hours. The irradiated area was defined by geometrical conditions and cross-section of the incidence X-ray beam and for Bragg-Brentano geometry. The surface was S=4,8-11,5 mm² and was changing continuously versus θ angle. In the case of grazing angle X-ray diffraction radiated area was twice larger but for particular incidence angle constant.



Fig. 2. Basic relation for measured macroscopic residual stress of FeAl lattice for g-sin² ψ method for the thickness of surface layer 3,75 μ m

Microscopic residual stresses σ_{II} in FeAl grains around Al₄C₃ precipitation was calculated from Hook's law with assumption of plain stress field:

$$\overline{\varepsilon} = \frac{1}{E} \left(\overline{\sigma}_1 - \nu \cdot \overline{\sigma}_2 \right) \tag{8}$$

where: σ_1 , σ_2 - are averaged main micro-stresses. For uniform tensile it was assumed $\overline{\sigma_1} = \overline{\sigma_2} = \sigma_{II}$. Above assumption is taken from fact that there are two neighboring areas where tensile and compression appear to fulfill equilibrium conditions. Therefore absolute value of second order stresses can be expressed as:

$$\sigma_{II} = \frac{\overline{\varepsilon} \cdot E}{1 - \nu} \tag{9}$$

The averaged crystal lattice microstrain can be treated as a measure of elastic cumulated energy in grains which can contribute in cracking process [20].

According to superposition rule total stress distributions in surface layers can be calculated. Superpose both i.e. solidification stresses and stress components due to chemical reaction of Al_4C_3 of self-disintegration the total stresses can be analyzed and presented on Figure 4.



Fig. 3. Macroscopic residual stresses change versus time of self-disintegration of FeAl in surface layer for different thickness g, μm

3. Analysis of the results

The obtained results of calculations and measurements confirmed importance of residual macro and micro-stresses in grains of FeAl superlattice around Al_4C_3 precipitation. Micro-stresses like oscillation fields from averaged macroscopic stress level energetically contributes in chemical reaction with environment and in self-disintegration process. The micro-stresses decrease versus time after 60 hours. After 484 hours they approach to zero what was found before (Fig.1.).



Fig. 4. Total stress distribution versus time of self-disintegration of FeAl in surface layer for different thickness g, μm

Macroscopic stresses at the very beginning were compressive. They changed in another way for the reason of self-disintegration of Al_4C_3 carbide. When cracking has started macroscopic stresses decreased and in time of cracking i.e. after 60-90 hours they approached to tensile (Fig. 3). The maximum of the total stresses indicate also that most intensive cracking took place after about 60-110 hours. A relaxation processes i.e. decrease of stresses appeared in that time.

4.Conclusions

The maximum of normal tensile stresses in FeAl grains of matrix was main cause of cracking. Nucleation of cracks and their development can be observed in microstructure. Some cracks in Al_4C_3 carbides appeared as the result of disintegration and their chemical reactions with moisture.

Direction of crack development and time relations of cracking and stresses change indicates on critical total stresses.

The results confirmed on algebraic add of micro and macroscopic residual stresses in particular directions can be treated as the fulfilling conditions for hypothesis of maximum normal stresses in self-disintegration process.

The measured compressive macroscopic residual stresses resulting from solidification superimposed with microscopic stresses and finally in carbide-matrix interface zone tensile total stresses caused cracking.

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