MATHEMATICAL MODEL OF THE FUNCTION BETWEEN PARTICLES DISTRIBUTION OF SiC IN ALUMINUM MATRIX AND THE COMPOSITE MATERIAL RESISTANCE

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ABSTRACT

This work deals with a composite material with SiC particles mixed in an aluminum matrix. Qualitative analyses indicate that microstructural characteristics were very influenced by SiC particulate distribution. Several studies have recognized the deviations from the periodicity of reinforcement distribution can markedly influence the composite elastic and plastic deformation characteristics. The composite overall response is influenced by the physical and geometrical properties of the reinforcing phases. The finite element method, the Eshelby

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method and dislocation mechanisms are usually employed in the formulation of the composite constitutive response. The aim of this work is to study the relationship between the particle distribution and the metal matrix composite resistance and to propose a mathematical model for the composite elastic behavior. The proposed formulation was applied to establish the thermal stress field in an aluminum-SiC composite due to its fabrication process – the mixing is done at 600°C and the material is supposed to be used at room temperature. The analytical results, presented as stress probabilities, were compared with the numerical ones, presented as stress distributions from the numerical model, obtained with a commercial finite element code. Both results compare well with same trends and very close average values of the thermal stresses. It is also shown that, if the Maxwell-Boltzmann distribution law is used, it is possible to obtain the relationship between the distribution particles and the material resistance using the Eshelby's thermal stress.

Keywords:

Material

Metal – matrix composites (MMCs)

Particle – reinforced composites

Property

Modelling

I – INTRODUTION

The reinforcement of materials composite depends on SiC particles distribution in aluminum matrix either elastic or plastic behavior, although in different conditions of influence. It is important to highlight that while the amount of clusters increases, the composite resistance decreases. The greatest resistance occurs when the composite has uniform distribution. A mathematical model that evaluates the relationship between particles distribution and composite resistance is very important to the mechanical properties prediction of particulate composites.

The aim of this work is to study this relationship and to propose a mathematical model to elastic behavior, considering SiC particles in aluminum matrix. This is possible if the Maxwell – Boltzmann distribution law is used to relate the SiC distribution with the composite resistance by Eshelby's stress. The results of this model can be validated by finite elements method.

II – PROBABILITY OF A DISTRIBUTION

This work is an adjustment of Beiser[1] and Reif[2] considerations in statistical mechanics, which investigates the most probable behavior of particles distribution. In this work the state of a particles system is completely specified at a given instant if the position and potential energy (rather than the kinetic energy) of each constituent particles are known. This modelling suggests that the aluminum matrix should be divided into K cell whose areas are a_1, a_2, a_3,...,a_k. The SiC particles are thrown into the matrix in a completely random manner with no favored part to observe how many particles fall in each cell. After repeating the experience many times, a certain distribution of particles among the various cells occurs more often than any other in a perceptible way. This is the most probable distribution and the number of particles in each cell is proportional to the size of the cell. So this work studies this most probable distribution and offers the corresponding stress distribution.

III – MAXWELL – BOLTZMANN STATISTICAL

Beiser[1] has shown that Maxwell–Boltzmann distribution law is:

$$n_i = g_i \, e^{-\alpha} \, e^{-\beta u_i} \tag{1}$$

The most probable number of particles in any cell is n_i and the total number of particles is N. The *a priori* probability g_i that a particle falls into the *ith* cell is the ratio between the area a_i of the cell and the total area A of the entire matrix. The total priori probability is 1. The α and β which are independent of n_i's are called Lagrange multipliers. The "Function of Partition" is Known as $e^{-\beta u_i}$ and shows the distribution of particles between the various potential energy levels.

Maxwell – Boltzmann distribution law was used by Beiser[1] to divide the Kinetic energy between the molecules. The Kinetic energy will be changed to elastic potential energy[3] in this work. The question is: How the elastic potentials energies will be distributed between the various energies levels produced by N particles?

This elastic potential energy is function of stress produced by coefficient of thermal expansion (CTE) mismatch.

The mean matrix stress will be used to determine the approximate solution of this distribution law by Eshelby method shown by several authors[4,5,6,7] .

The α and β are obtained using the method showed by Beiser[1] and the mean matrix stress is showed by Clyne et al[4] and used in this work to determine the modified Maxwell-Boltzmann distribution law that indicates the partition of stress between the particles due to distribution of these particles into the aluminum matrix. In order to do so, it is convenient to consider a continuous distribution of energies, rather than the discrete set $u_1, u_2, \ldots, u_k$, so that Eq. (1) becomes

$$n(u)du = ge^{-\alpha} e^{-\beta u} du \qquad (2)$$

The number of particles whose energies lie between u and $u + du$ is interpreted as $n(u)du$ where u is the elastic potential energy.

In terms of stress the Eq. (2) becomes

$$n(\sigma)d\sigma = g e^{-\alpha} e^{-\beta\frac{\sigma^2}{2E}} d\sigma \tag{3}$$

where E is the Young's modulus.

The Beiser[1] development is used to find $e^{-\alpha}$ and β.

Hence

$$n(\sigma)\, d\sigma = 4\pi N \left(\frac{\beta}{2E\pi}\right)^{3/2} \sigma^2 e^{-\beta\frac{\sigma^2}{2E}} d\sigma \tag{4}$$

The total energy U of the particles assembly is used to find β, so

$$U = \frac{3}{2}\frac{N}{\beta} \tag{5}$$

The total energy U can also be written as

$$U = uN \tag{6}$$

The elastic potential energy u is function of the mean matrix stress[3,4] which determines the approximate solution of the distribution law.

$$\frac{3}{2}\frac{N}{\beta} = \frac{f C_M [\,(\mathrm{S}-\mathrm{I})\,\varepsilon^*_{\mathrm{kl}}\,]^2}{2} N \tag{7}$$

where $\varepsilon^*_{\mathrm{kl}}$ is called the eigenstrain[4,5], S is the Eshelby tensor, I is the identity matrix and f is the volume fraction of particles or inclusions.

Hence

$$\beta = \frac{3}{f\, C_M\, [(\mathrm{S}-\mathrm{I})\,\varepsilon^*_{\mathrm{kl}}]^2} \tag{8}$$

So the Eq. (4) becomes the modified Maxwell–Boltzmann distribution law

$$n(\sigma) = 4\pi N \left(\frac{3}{2C_M K\pi}\right)^{3/2} \sigma^2 e^{-\frac{3\sigma^2}{K2C_M}} \tag{9}$$

With

$$K = f\, C_M\, [\,(\mathrm{S}-\mathrm{I})\,\varepsilon^*_{\mathrm{kl}}]^2 \tag{10}$$

Or

$$K = f C_M \{(S - I)\{(C_M - C_I)[S - f(S-1)] - C_M\}^{-1} C_I\ (\alpha_I - \alpha_M)\Delta T\}^2 \tag{11}$$

where C_M and C_I are called the elastic tensor components of the matrix and particles, respectively, α_M and α_I are CTE tensors of the matrix and particles, respectively, and ΔT is the temperature change.

$C_{Mii} = E_M (1 - \nu_M) / (1 - 2\nu_M)(1 + \nu_M)$;

$C_{Mij} = E_M\ \nu_M / (1 - 2\nu_M)(1 + \nu_M)$;

$C_{M44} = E_M / 2(1 + \nu_M)$;

$C_{Iii} = E_I (1 - \nu_I) / (1 - 2\nu_I)(1 + \nu_I)$; (12)

$C_{Iij} = E_I\ \nu_I / (1 - 2\nu_I)(1 + \nu_I)$;

$C_{I44} = E_I / 2(1 + \nu_I)$

The above-mentioned equation is the stress distribution function into the composite material with random spatial distribution of SiC particles in aluminum matrix.

It is convenient to consider the L constant which can be used to facilitate the derivative of equation (9):

$$L = 4\pi N \left(\frac{3}{2C_M K\pi} \right)^{3/2} \tag{13}$$

This L must be replaced on the equation (9):

$$n(\sigma) = L\sigma^2\, e^{-\frac{3\sigma^2}{2KC_M}} \tag{14}$$

II.7 – The Most Probable Stress

The maximum value will be obtained from the derivative of equation (14). This is the most probable stress (σ_p):

$$\sigma_p^2 = \frac{2fC_M^2\{(S-I)\{(C_M-C_I)[S-f(S-I)]-C_M\}^{-1}C_I\,(\alpha_I-\alpha_M)\Delta T\}^2}{3} \qquad (15)$$

II.8 – The Mean Stress

The mean stress is obtained through the formula :

$$\bar{\sigma} = \frac{\int_0^\infty \sigma\, n(\sigma)\, d\sigma}{N} \qquad (16)$$

With

$$n(\sigma) = \frac{4N}{\sqrt{\pi}}\frac{1}{\sigma_p}\left(\frac{\sigma^2}{\sigma_p^2}\right)e^{-(\frac{\sigma^2}{\sigma_p^2})} \qquad (17)$$

The solution of this equation is :

$$\bar{\sigma} = 1.13\sigma_p \text{ (Mean stress)} \qquad (18)$$

II.9 – The Quadratic Mean Stress

The quadratic mean stress is:

$$\bar{\sigma}^2 = \frac{\int_0^\infty \sigma_{ij}^2\, n(\sigma)\, d\sigma}{N} \qquad (19)$$

The solution of this equation is

$$\bar{\bar{\sigma}} = 1.225\sigma_p \qquad (20)$$

II.10 – Materials and Simulation Method

In composite materials the phases have different coefficients of thermal expansion (CTE) and this CTE mismatch is large. The composite manufacturing at elevated temperature results in the development of an appreciable internal stress and strain mismatch during the cooling process. In Al/SiC system the fabrication temperature is usually around 600 ^{0}C.

So, the most probable stress is determinated considering elastic behavior and the following datas:

1) Young's modulus of matrix : E = 73GPa
2) CTE of aluminum: $\alpha_M = 23.6 \times 10^{-6}\ C^{-1}$
3) CTE of SiC particles: $\alpha_I = 4 \times 10^{-6}\ C^{-1}$
4) Temperature change: cooling down from its manufacturing temperature to room temperature or $\Delta T = -580\ ^0C$

II.10 – Results

II.10.1 – The Most Probable Stress Determination

1) Thermal strain tensor is given by $\varepsilon^{**}{}_{kl} = (\alpha_I - \alpha_M)\Delta T$:

$$e^{**}_{kl} = \begin{bmatrix} 0.011368 \\ 0.011368 \\ 0.011368 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

2) The elastic constant tensor of aluminum matrix is given by:

$$C_M = \begin{bmatrix} 10.8160 & 5.3273 & 5.3273 & 0 & 0 & 0 \\ 5.3273 & 10.8160 & 5.3273 & 0 & 0 & 0 \\ 5.3273 & 5.3273 & 10.8160 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2.7443 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2.7443 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2.7443 \end{bmatrix} x10^{10}$$

3) The elastic constant tensor of the inclusion:

$$C_I = \begin{bmatrix} 48.3700 & 9.9100 & 9.9100 & 0 & 0 & 0 \\ 9.9100 & 48.3700 & 9.9100 & 0 & 0 & 0 \\ 9.9100 & 9.9100 & 48.3700 & 0 & 0 & 0 \\ 0 & 0 & 0 & 19.2300 & 0 & 0 \\ 0 & 0 & 0 & 0 & 19.2300 & 0 \\ 0 & 0 & 0 & 0 & 0 & 19.2300 \end{bmatrix} x10^{10}$$

4) Eshelby's tensor related to spherical inclusion:

$$S = \begin{bmatrix} 0.53234 & 0.06468 & 0.06468 & 0 & 0 & 0 \\ 0.06468 & 0.53234 & 0.06468 & 0 & 0 & 0 \\ 0.06468 & 0.06468 & 0.53234 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.23383 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.23383 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.23383 \end{bmatrix}$$

5) The following volume fractions were considered for calculations: 17.9%, 24.4%, 31% and 35.2%. The most probable stress (σ_p), the mean stress ($\overline{\sigma}$) and the quadratic mean stress ($\overline{\overline{\sigma}}$) to spherical particles are given in table I, considering the volume fractions.

III – DISCUSSION

Twenty-four simulations were done using the finite elements method with different particle distributions and volume fractions and all obtained results were consistent with the mathematical model. From these, four selected results regarding thermal stress distributions will be shown in this paper for the already mentioned volume fractions.

The figures (1), (3), (5) and (7) clearly shows that the graphics of thermal stress distributions to volume fractions of 17.9, 24.4, 31 and 35.2% are coincident with stress range obtained by FEM simulations like shows the figure (2), (4), (6) and (8) for the elastic problem case. These figures indicates the coherence on the obtained results.

It is normal to suppose that the introduction of high volume fraction of SiC particles to Al matrix could notably increase the amount of clusters and decreases the composite resistance[9]. Recent studies showed that high volume fraction of reinforcement could reduce the CTE of matrix, leading to the low CTE values of the composite[10] and the non–uniformity of the SiC particles and aspect ratio have a strong effect on the local and global damage behavior and stress-strain relationship[11].

The stress magnitude and SiC distribution are determined by the thermomechanical process history of the materials. The mechanical behavior of particulate metal–matrix composite is also dependent of the matrix alloy and the reinforcement[12].

Considering the stress distribution graphics obtained by mathematical model, the area between two stress values is the amount of particles per stress unit.

IV – CONCLUSIONS

The present mathematical model analyses the elastic response of two–phase composite as function of the spatial distribution of reinforcement. The following conclusions may be drawn from the results of this study:

1) The non–uniformity of the SiC particles distribution has a strong effect on the stress-strain relationship of the composites materials. This effect also depends of the reinforcement volume fraction. There is a broad consensus on this issue.

2) As it stands, the approach presented here indicates a method to take into account the clustering effect on thermal stress. This method showed the same efficiency that the FEM to estimate that thermal stress.

3) This work produced a mathematical model in order to obtain the elastic response although the factors that govern matrix plasticity will be studied in the future to determine the plastic behavior of composites materials.

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Table I – Results obtained by the most probable stress equation, mean and quadratic mean equation, using the mathematical model

VOLUME FRACTION f (%)	THE MOST PROBABLE STRESS σ_p (MPa)	MEAN STRESS $\overline{\sigma} = 1{,}13\sigma_p$ (MPa)	QUADRATIC MEAN STRESS $\overline{\overline{\sigma}} = 1{,}225\sigma_p$ (MPa)
17.9	352	398	432
24.4	404	456	495
31	447	505	547
35.2	471	532	577

Figure 1 – Distribution function of stress to volume fraction of 17.9% of SiC in aluminum matrix

Figure 2 – Finite element results (Pa) for the volume fraction of 17.9% of SiC in aluminum matrix

Figure 3 – Distribution function of stress to volume fraction of 24.4% of SiC in aluminum matrix

Figure 4 – Finite element results (Pa) for the volume fraction of 24.4% of SiC in aluminum matrix

Figure 5 – Distribution function of stress to volume fraction of 31% of SiC in aluminum matrix

Figure 6 – Finite element results (Pa) for the volume fraction of 31% of SiC in aluminum matrix

Figure 7 – Distribution function of stress to volume fraction of 35.2% of SiC in aluminum matrix

Figure 8 – Finite element results (Pa) for the volume fraction of 35.2% of SiC in aluminum matrix

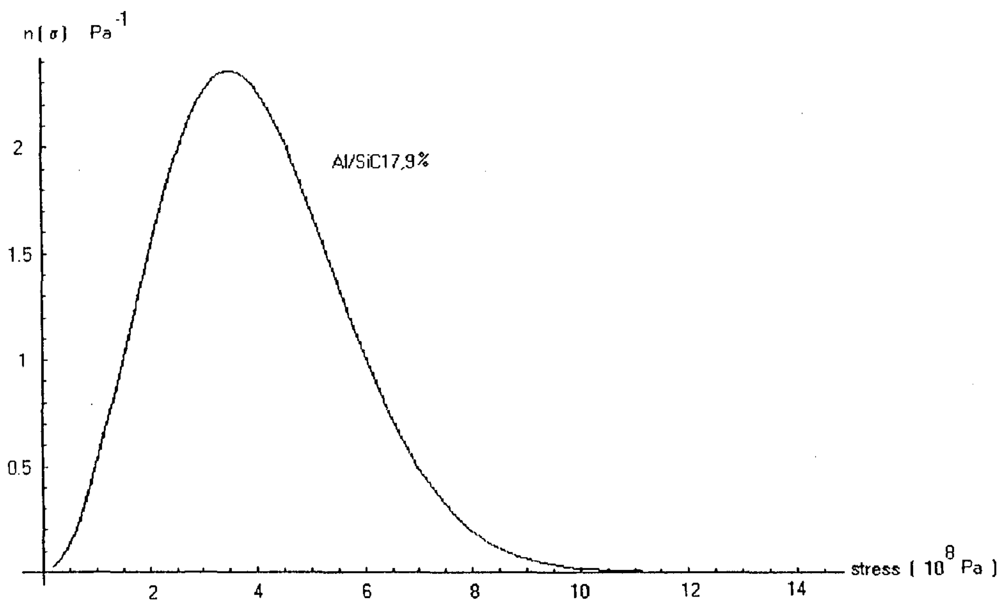

Figure 1

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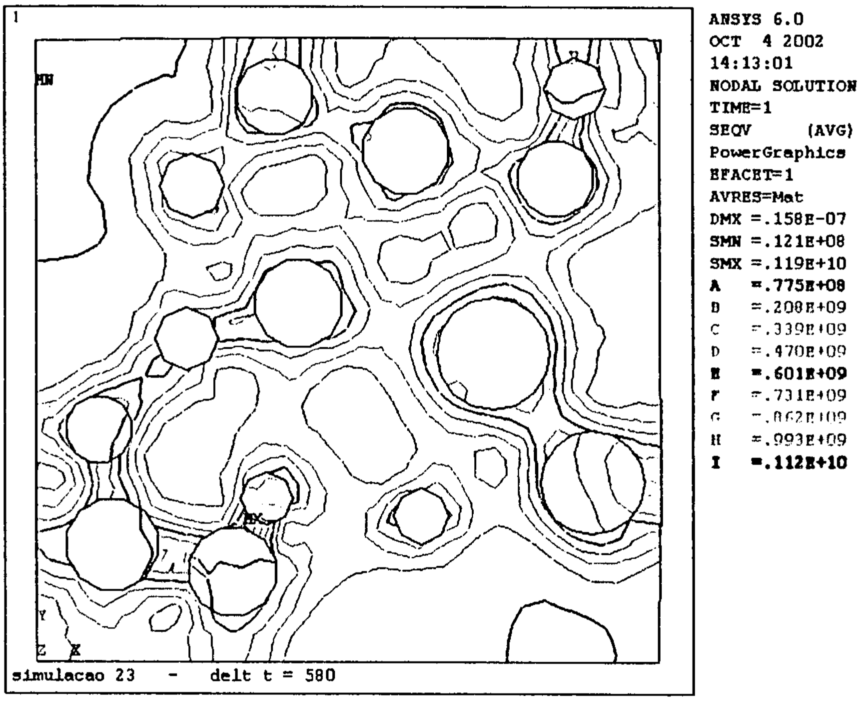

Figure 2

Zoroastro de Miranda Boari – Waldemar Alfredo Monteiro – Carlos Alexándre de Jesus Miranda

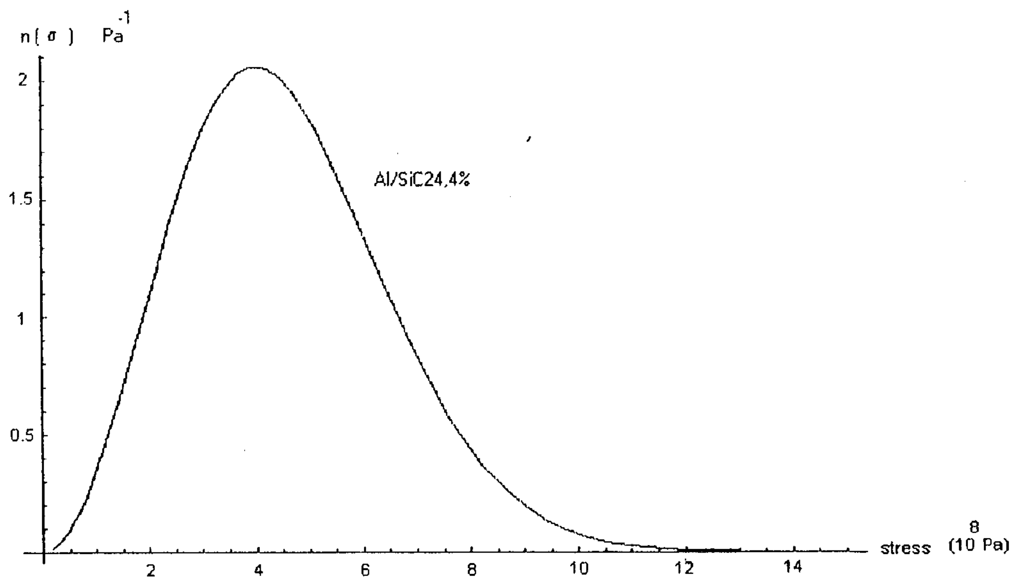

Figure 3

Zoroastro de Miranda Boari – Waldemar Alfredo Monteiro – Carlos Alexandre de Jesus Miranda

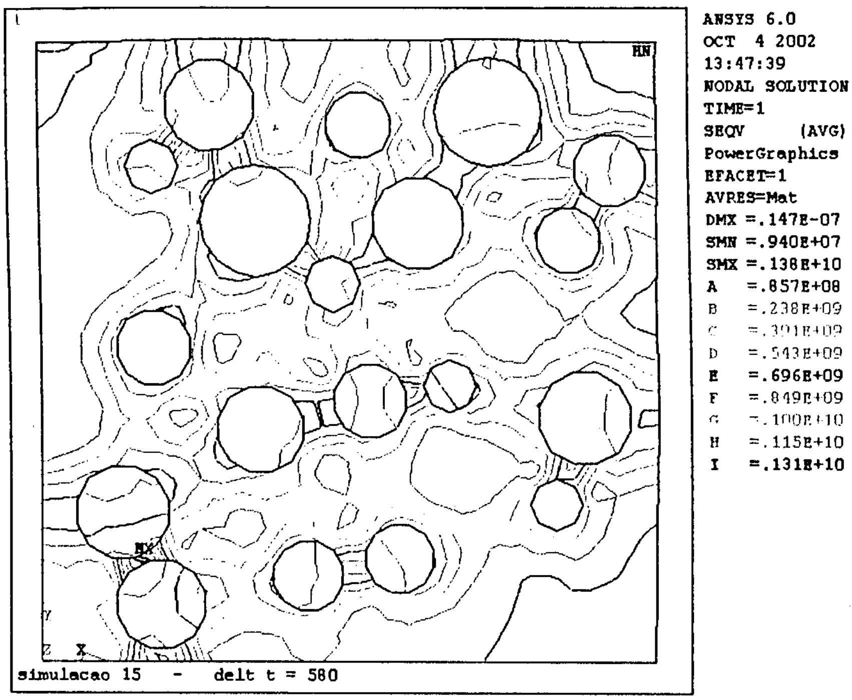

Figure 4

Zoroastro de Miranda Boari – Waldemar Alfredo Monteiro – Carlos Alexandre de Jesus Miranda

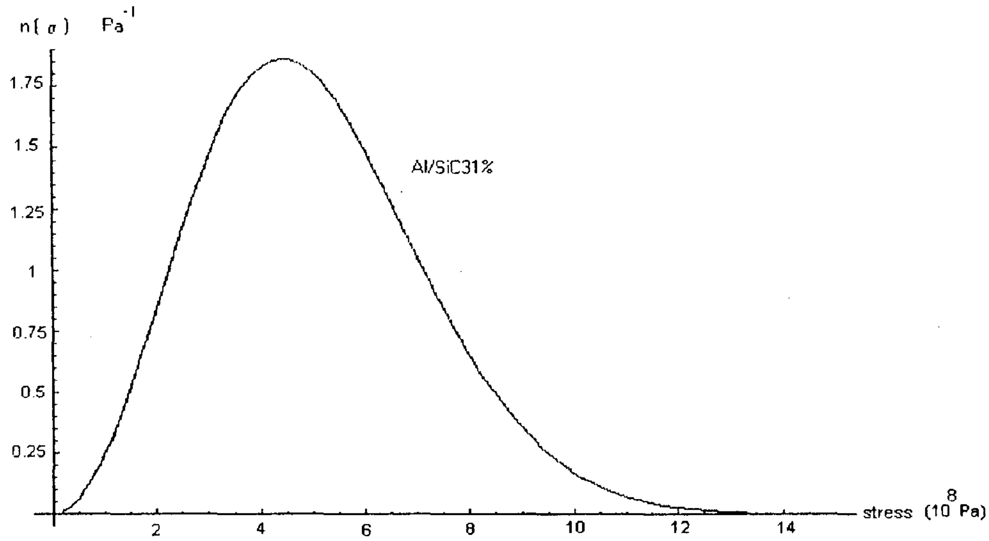

Figure 5

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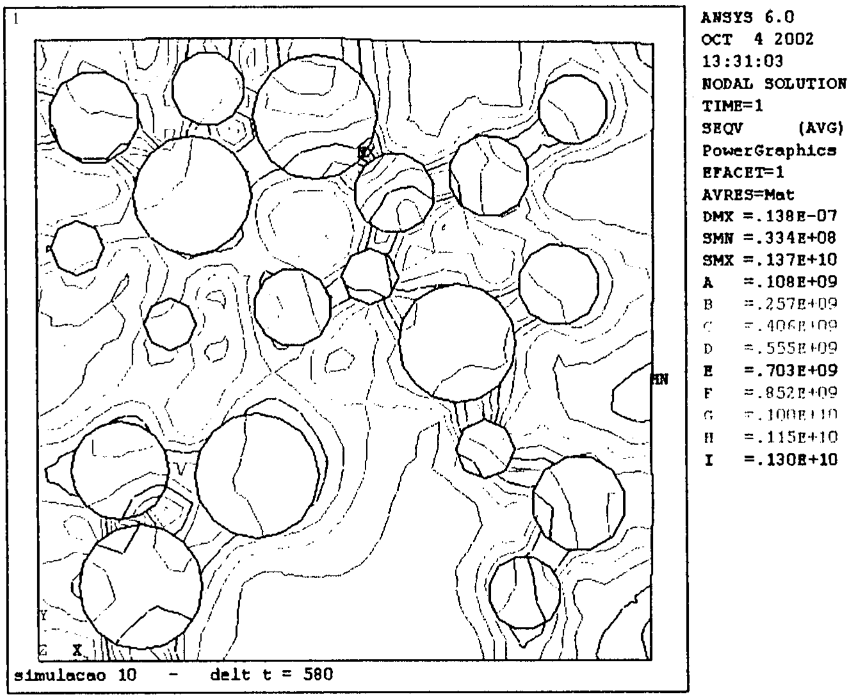

Figure 6

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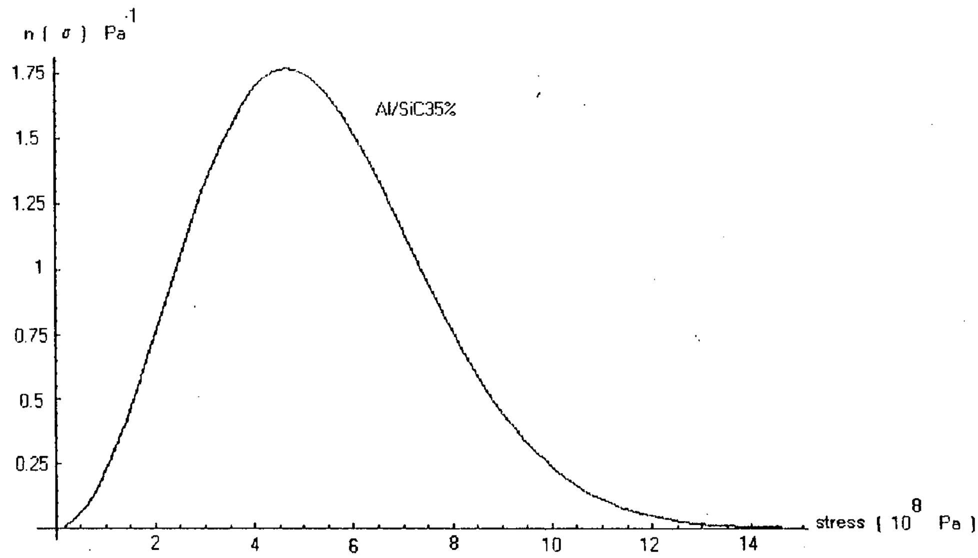

Figure 7

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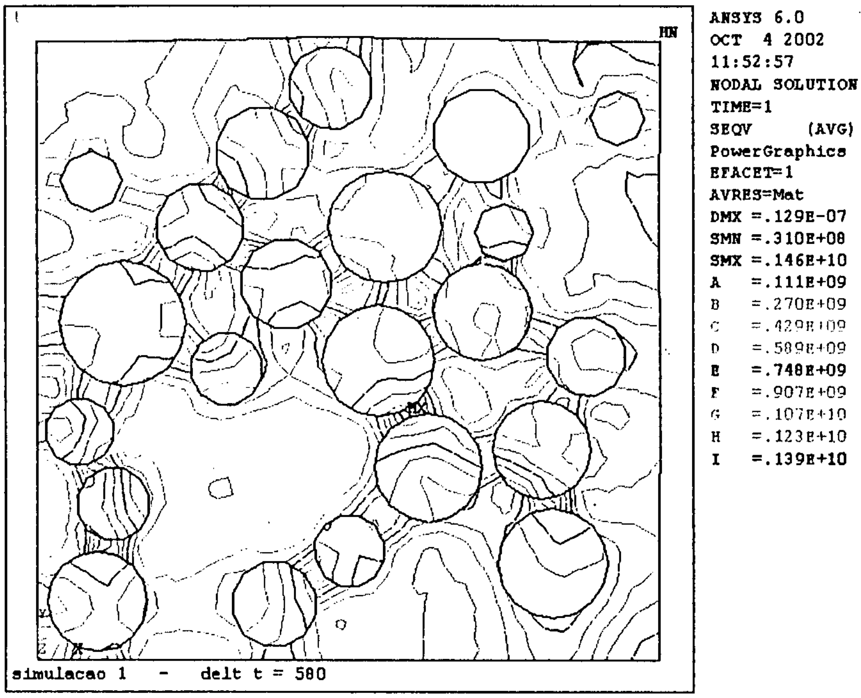

Figure 8

Zoroastro de Miranda Boari – Waldemar Alfredo Monteiro – Carlos Alexandre de Jesus Miranda

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Declaro que ZOROASTRO DE MIRANDA BOARI apresentou trabalho oral entitulado MATHEMATICAL MODEL OF THE FUNCTION BETWEEN PARTICLES DISTRIBUTION OF SiC IN ALUMINIUM MATRIX AND THE COMPOSITE MATERIAL RESISTANCE no II Encontro da SBPMat – Sociedade Brasileira de Pesquisa em Materiais, realizado de 26 a 29 de outubro de 2003, no Rio de Janeiro.

Rio de Janeiro, 26 de Outubro de 2003.

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3. Existirão 4 sessões orais do Simpósio E: duas para cada dia de encontro. O dia, horário e sala da sua apresentação serão divulgadas oportunamente no site do evento www.sbpmat.org.br/encontro, assim como na programação final.

4. Palestrantes convidados irão dispor de 30 minutos (26 + 4 para perguntas) de apresentação. Contribuições orais estarão limitadas a 15 minutos (12 + 3 para perguntas).

5. As salas onde terão lugar as apresentações orais estarão devidamente equipadas com equipamento audiovisual (retroprojetores e datashow). As apresentações devem ser preferencialmente em inglês. No caso do apresentador preferir a exposição em português, o material a ser projetado deve ser obrigatoriamente em inglês.

6. Convidamos a submeter este abstract como trabalho completo para ser publicado em um número especial da revista *Composites Structures* (http://www.elsevier.com/locate/compstruct) ou *Materials Research* (www.nit.ufscar.br/matres), a critério do autor. A extensão do artigo está limitada a 6 páginas no formato revista. Os artigos submetidos serão devidamente analisados por um corpo revisor, segundo critérios usuais de cada revista. Instruções para os autores podem ser encontradas na home page das referidas revistas.

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durante o próximo ciclo, comparando-se com os tamanhos críticos dos mesmos, levando-se em conta as incertezas envolvidas, às quais acrescenta-se a incerteza quanto ao crescimento do defeito.

. Verificar se o ferramental a ser usado nos testes é adequado

. Analisar os resultados dos testes e identificar a necessidade de eventuais testes adicionais

. Avaliar os resultados dos testes quanto ao CM e ao OA.

Deve ser preparado e aprovado um procedimento que defina os objetivos dos testes e identifique os procedimentos a serem adotados durante a inspeção dos tubos do GV (que parâmetros/dados devem ser obtidos para cada tipo de defeito), durante os testes (níveis de pressão a serem atingidos, limites de vazamento, etc.) e pós-testes (é recomendável que todos os tubos testados sejam reparados (plugueados, enluvados, etc.).

Obs.

1. É necessário, também, no planejamento dos testes, prever a necessidade de expandir o escopo dos testes (quantidade de tubos testados) pela eventual falha (no caso do teste de pressão) ou vazamento excessivo de um dado tubo pelo impacto que tal expansão pode causar no planejamento da parada.

2. faz parte do escopo dos testes o exame NDE e o reparo dos tubos testados.

A seção 5.0 (***Test Procedure***) de [1] tem uma lista detalhada dos procedimentos recomendados para cada uma destas fases (pré-teste, teste e pós-teste) sugerindo alternativas para algumas situações que podem ocorrer (como quando há um vazamento excessivo que impeça a continuidade do teste de pressão até o nível ΔP previsto)

IV.4 – Condição de Monitoramento e Avaliação Operacional - CM e OA

Apesar de definidas em relatório anteriores, veja-se por exemplo a referência [6], a seguir apresenta-se sucintamente a conceituação da Condição de Monitoramento (CM) e Avaliação Operacional (OA) que devem ser verificadas por ocasião da inspeção nos GVs de uma usina nuclear.

Para qualquer tipo de defeito, segundo [3], a pressão de colapso dos tubos associada a condição CM ou à condição OA deve ser avaliada com probabilidade de 0,90, com um grau de confiança de 50% (indicada por 90/50). Isto é interpretado da seguinte forma: quando se afirma que nos tubos, com um certo tipo defeito de um dado tamanho, o valor associado à condição CM, ou à condição OA, é a pressão de colapso PB, isto significa que se espera que, em 90% das vezes os tubos com aquele defeito (tamanho) não sofrerão colapso quando a pressão atuante atingir o valor PB. Para efeitos de verificação, o valor PB dever ser o valor ΔP dado pela eq. (1.1)

Na condição CM se verifica o nível de integridade com que os tubos do GV terminaram o ciclo operacional recém concluído, a partir da comparação dos tamanhos críticos dos defeitos com as dimensões medidas, sempre considerando-se as incertezas envolvidas (correlações, analista, técnica de NDE, material, etc.). Na condição OA se considera o quanto cada defeito crescerá, durante o próximo ciclo, comparando-se com os tamanhos críticos dos mesmos, levando-se em conta as incertezas envolvidas, às quais acrescenta-se a incerteza quanto ao crescimento do defeito.

E-O3 MATHEMATICAL MODEL OF THE FUNCTION BETWEEN PARTICLES DISTRIBUTION OF SiC IN ALUMINUM MATRIX AND THE COMPOSITE MATERIAL RESISTANCE

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This work deals with a composite material with SiC particles mixed in an aluminum matrix. Qualitative analyses indicate that microstructural characteristics were very influenced by SiC particulate distribution. Several studies have recognized the deviations from the periodicity of reinforcement distribution can markedly influence the composite elastic and plastic deformation characteristics. The composite overall response is influenced by the physical and geometrical properties of the reinforcing phases. The finite element method, the Eshelby method and dislocation mechanisms are usually employed in the formulation of the composite constitutive response. The aim of this work is to study the relationship between the particle distribution and the metal matrix composite resistance and to propose a mathematical model for the composite elastic behavior. The proposed formulation was applied to establish the thermal stress field in an aluminum-SiC composite due to its fabrication process – the mixing is done at 600°C and the material is supposed to be used at room temperature. The analytical results, presented as stress probabilities, were compared with the numerical ones, presented as stress distributions from the numerical model, obtained with a commercial finite element code. Both results compare well with same trends and very close average values of the thermal stresses. It is also shown that, if the Maxwell-Boltzmann distribution law is used, it is possible to obtain the relationship between the distribution particles and the material resistance through the Eshelby's thermal stress.

E-O4 STEAM CURING AND DELAYED ETTRINGITE FORMATION IN BRAZILIAN CEMENTS

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Delayed ettringite formation may be defined as the formation of ettringite in a cementitious material by a process that begins after hardening has substantially complete. The reaction occurs between the anhydrous cement compound C3A and sulphates in the paste. In recent years delayed ettringite formation has become a topic of major significance to the international community. Early ettringite formation, which occurs immediately (within hours) in a plastic fresh mixture, does not produce any damaging expansion and is associated with the regulation of setting time of Portland cement paste. Delayed ettringite formation may be defined as the formation of ettringite in a cementicious material by a process that begins after hardening is substantially complete and in which none of the sulphate comes from outside the cement paste. Delayed ettringite formation (DEF) can damage concrete that has experienced a temperature above about 70°C. This process is associated with expansion. Expansion results from formation of ettringite crystals of submicrometre size in the paste, the large crystals largely observed in cracks and voids being recrystallization products. The rate and ultimate extent of expansion are influenced by factors of three types: chemistry, which determines how much ettringite can be formed; paste microstructure, which determines the stress produced by its formation; and concrete and mortar microstructure, which determines the response of the material to those stresses. Image analysis by Scanning Electron Microscopy (SEM) promotes the observation of ettringite crystals in Portland cement pastes, mortars and concretes. The aim of this work was to observe the DEF in steam-cured concretes made with Brazilian Portland cements (Blastfurnace Slag Cement – CP III, and High Initial Compressive Strength Portland Cement – CPV-ARI). The steam temperature was 80°C. The image analysis showed that DEF was observed in both cements.