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복합재의 파괴와 hygrothermal 효과에 관한 연구

Fracture and Hygrothermal Effects in Composite Materials

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ABSTRACT

This is an explicit-implicit, finite element analysis for linear as well as nonlinear hygrothermal stress problems. Additional features, such as moisture diffusion equation, crack element and virtual crack extension(VCE) method for evaluating J-integral are implemented in this program.

The Linear Elastic Fracture Mechanics(LEFM) Theory is employed to estimate the crack driving force under the transient condition for and existing crack. Pores in materials are assumed to be saturated with moisture in the liquid form at the room temperature, which may vaporize as the temperature increases. The vaporization effects on the crack driving force are also studied. The ideal gas equation is employed to estimate the thermodynamic pressure due to vaporization at each time step after solving basic nodal values.

A set of field equations governing the time dependent response of porous media are derived from balance laws based on the mixture theory. Darcy's law is assumed for the fluid flow through the porous media. Perzyna's viscoplastic model incorporating the Von-Mises yield criterion are implemented. The Green-Naghdi stress rate is used for the invariant of stress tensor under superposed rigid body motion. Isotropic elements are used for the spatial discretization and an iterative scheme based on the full newton-Raphson method is used for solving the nonlinear governing equations.

국 문 요 약

본 연구는 선형, 비선형 hygrothermal 응력 문제를 위한 explicit-implicit 유한요소 해석 모델 개발에 관한 것이다. 부가적으로 moisture 확산 방정식, J-적분 평가를 위한 균열 요소 및 가상 균열 진전법이 도입된다.

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시간 변화에 따른 균열 추진력을 계산하기 위하여 선형 탄성 파괴 역학(LEFM)이론이 고려되며 재료의 기공은 실온에서 액체 상태의 습기로 포화되어 있으며 온도가 상승함에 따라 증기화된다는 가정하에서 균열 추진력과 증기 효과의 관계가 연구된다. 이상 기체방정식은 각 시간 단계에서 증기에 의한 열역학적 압력을 계산하기 위하여 이용된다.

다공질 재료의 시간 종속 응답을 지배하는 방정식들은 혼합이론에 기초하며 다공질 재료의 유체 흐름을 위한 Darcy의 법칙과 Von-Mises 항복 기준을 포함하고 있는 Perzyna의 점소성 모델이 첨가된다. 또한 Green-Naghdi 응력률이 중첩된 강체 운동하에서 응력 텐서 invariant로 사용되며, 모델링을 위하여 사각요소가 이용되고 비선형 지배 방정식을 풀기 위하여 full Newton-Raphson법에 의한 반복법이 사용된다.

본 연구를 통하여 얻은 결과는 다음과 같다.

1) 본 유한요소 프로그램은 복합재의 hygrothermal 파괴 해석에 매우 유용하게 적용될 수 있다.
2) 습기의 온도에 의한 영향을 가지는 재료의 J-적분을 정확히 예측하기 위하여는 증기 효과를 고려하여야 한다. 왜냐하면 초기단계에 균열 전파력이 가속되기 때문이다.
3) 본 해석을 위해 Uncoupled scheme에 의한 결과도 Coupled scheme에 결과에 비해 아주 타당하므로 CPU 측면에서 매우 경제적인 Uncoupled scheme이 추천된다.

1. Introduction

Interface crack between composite(dissimilar) materials with a fluid-saturated porous media under thermal loading and permeation of moisture is a major problem in the manufacturing of ceramic composites and electronics devices, in particular, plastic encapsulated ICs. For instance, there have been numerous incidents reported in the area of interface cracking between the ceramic fibers and matrix in a ceramic composite.

This kind of interface cracking is mainly caused by the fact that there are mismatch of thermal porperties and vapor pressure which may vaporize as the temperature increases.

The coefficient of thermal expansion(CTE) mismatches of the constituents of the package and permeation of moisture are the primary contributor to stresses. These stresses in concert with processing residual stresses can be sufficient to induce cracking and interfacial delamination in dissimilar materials. Delamination at these interface is a complicated function of the elastic moduli and CTEs etc..

Ceramic composites and IC packages are most often used in environments with high temperature gradients and permeation of moisture. Therefore, a better understanding of interface cracks under thermal loading and moisture conditions is needed to guide the judicious selection of materials and fabrication methods which do not lead to interfacial failure.

Recent trends pertinent to geological media have focused considerable attention on fluid-infiltrated and/or thermally induced responses. Following Terzaghi's work[1)] on one-dimensional consolidation, Biot[2)] has presented a generated three-dimensional consolidation. Nonisothermal finite-strain dynamic of a porous solid containing a viscous fluid was studied by Biot; he showed how the Lagrangian equation in the finite element methods were formulated. Rice and Cleary[3)] have reformulated Biot's equations relating strain and fluid mass content to stress and pore pressure in terms of revised material properties. McTigue et al[4)] have extended fluid-saturated porosity with temperature effects. The variational principle for fluid-coupled problems in continum mechanics was reported by Sandhu et al[5)].

The variational principle applied to the coupled--fluid and thermoelastic problem was studied by Aboustit et.[6)]. Kim[7)] extended Aboustit's work by using the Perzyna model in his viscoplastic model but his work didn't include a finite element fracture model. Lewis and Schrefler[8)] summarized investigations on coupled poroelastic and hygrothermomechancal response of geological media utilizing finite-element techniques.

The goal of this research is to develop a finite element fracture model through which the crack/delamination driving forces can be computed for representative failure mechanisms and loadings of composite materials.

2. Model Formulations

Pores in composite materials are assumed to be saturated with moisture in the liquid form at the room temperature, which may may vaporize as the temperature increases. For study these phenomena, the following equations are used.

2.1 Governing equations

From the theory of mixtures along with Darcy's law, the governing balance laws are

$$\overline{\rho_s}+\overline{\rho_s}\,\mathrm{div}(V_s)=0 \quad \cdots\cdots (1)$$

$$\overline{\rho_f}+\overline{\rho_f}\,\mathrm{div}(V_f)+V_r\mathrm{grad}(\overline{\rho_f})=0 \quad \cdots\cdots (2)$$

$$\mathrm{div}(T_s)+\bar{f}_s=\overline{\rho_s}+V_s \quad \cdots\cdots (3)$$

$$\mathrm{div}(T_f)+\bar{f}_f=\overline{\rho_s}V_f+\overline{\rho_s}L_fV_r \quad \cdots\cdots (4)$$

$$\rho\,\dot{\varepsilon}+\overline{\rho_f}V_r\cdot\mathrm{grad}(\varepsilon_f)=\rho\,r-\mathrm{div}(q)+T_s\cdot D_s+T_f\cdot D_f \quad \cdots\cdots (5)$$

where $\rho\dot{\varepsilon}=\overline{\rho_s}\dot{\varepsilon}_s+\overline{\rho_f}\dot{\varepsilon}_f$ and $\rho r=\overline{\rho_s}r_s+\overline{\rho_f}r_f$

$$\frac{\partial W_i}{\partial t}=-\mathrm{div}(j_{ic}+j_{id})+I_i \quad \cdots\cdots (6)$$

Equation(1) and (2) are the mass conservation equation of solid and fluid, respectively, equation (3) and (4) are the equibilium equation of solid and fluid, respectively, equation(5) is the energy conservation equation and equation(6) describes the moisture diffusion. During the deformation, the mass densities are updated by the following relations

$$\rho_s=\rho_{s_0}\left[1-3\beta_s(\theta-\theta_0)-\frac{1}{3K_s}\mathrm{tr}(\rho_s)\right]$$

$$\rho_f=\rho_{f_0}\left[1-3\beta_f(\theta-\theta_0)-\frac{1}{K_f}P\right]$$

In addition, the materials are assumed to be isotropic.

2.2 Constitutive equations

The constitutive equations for the time-temperature dependent elastic-viscoplastic fluid-saturated material are obtained by superposing the elastic, D_e, hygro-thermal, D_h, and time dependent viscoplastic, D_{vp}, strain rate components in the for

$$D=D_e+D_h+D_{vp} \quad \cdots\cdots (7)$$

where $D=\frac{1}{2}\left[\frac{\partial v}{\partial x}+\frac{\partial v^T}{\partial x}\right]$,

$D_h=\alpha\,\theta I+\beta\,\pi I$

The viscoplastic strain rate is assumed to obey Perzyna's viscoplastic flow rule defined as

$$D_{vp}=\gamma<\Phi(F)>\frac{\partial F}{\partial\sigma} \quad \cdots\cdots (8)$$

The total objective stress rate is defined by

$$\dot{T}=C\{D-D_h-D_{vp}\} \quad \cdots\cdots (9)$$

where C is the conventional temperature dependent elasticity tensor.

2.3 Finite element formulations

From the weak formulations for the fluid thermal diffusion and the Lagragian formulations for the solid deformation, the coupled algebraic system equations, in terms of the unknown increment and residual vectors are obtained in the form

$$\begin{bmatrix} K_{uv} & K_{u\theta} & K_{u\pi} & K_{uw} \\ M_{vu} & M_{v\theta} & M_{v\pi}+\Delta tK_{v\pi} & M_{vw}+\Delta tK_{vw} \\ 0 & M_{\omega\theta} & M_{\omega p}+\Delta tK_{\omega p} & M_{\omega p}+\Delta tK_{\omega p} \\ M_{\psi u} & M_{\psi\theta} & M_{\psi w}+\Delta tK_{\psi w} & M_{\psi w}+\Delta tK_{\psi w} \end{bmatrix}^{t+\Delta t}_{(i)} \begin{Bmatrix} \Delta u \\ \Delta\theta \\ \Delta p \\ \Delta w \end{Bmatrix}_{(i)} =\Delta L^{t+\Delta t}_{(i)} \quad \cdots\cdots (10)$$

where

$$\Delta L^{t+\Delta t}_{(i)}= \begin{Bmatrix} \Delta R^{t+\Delta t}_{(i)} \\ Q^{t+\Delta t}_{(i)} \\ F^{t+\Delta t}_{(i)} \\ W^{t+\Delta t}_{(i)} \end{Bmatrix} - \begin{bmatrix} M_{vu} & M_{v\theta} & M_{vp} & M_{vw} \\ 0 & M_{\psi\theta} & M_{\psi p} & M_{\psi\pi} \\ M_{vu} & M_{v\theta} & M_{vp} & M_{vw} \\ 0 & M_{\psi\theta} & M_{\psi p} & M_{\psi\pi} \end{bmatrix} \begin{Bmatrix} \dot{u} \\ \dot{\theta} \\ \dot{P} \\ w \end{Bmatrix}^{t+\Delta t}_{(i)}$$

$$
-\begin{bmatrix} K_{vu} & K_{v\theta} & K_{vp} & K_{vw} \\ K_{vu} & K_{v\theta} & K_{vp} & K_{vw} \\ 0 & K_{\omega\theta} & K_{\omega p} & K_{\omega w} \\ K_{\psi u} & K_{\psi\theta} & K_{\psi p} & K_{\psi w} \end{bmatrix} \begin{Bmatrix} u \\ \theta \\ P \\ w \end{Bmatrix}_{(i)}^{t+\Delta t}
$$

Two point explicit time marching scheme with time rate steps and the full Newton-Raphson method are utilized. The unknown increments are solved using equation, and the total solution increments, mass densities and mesh configuration after i^{th} iteration are updated during each time step Δt.

For implicit time marching scheme, the following equations are used.

$$
\begin{bmatrix} K_{uv} & K_{u\theta} & K_{u\pi} & K_{uw} \\ M_{vu} & M_{v\theta} & M_{v\pi}+\Delta tK_{v\pi} & M_{vw}+\Delta tK_{vw} \\ 0 & M_{\omega\theta} & M_{\omega p}+\Delta tK_{\omega p} & M_{\omega p}+\Delta tK_{\omega p} \\ M_{\psi u} & M_{\psi\theta} & M_{\psi w}+\Delta tK_{\psi w} & M_{\psi w}+\Delta tK_{\psi w} \end{bmatrix}_{(i)}^{t+\Delta t} \begin{Bmatrix} \Delta u \\ \Delta\theta \\ \Delta p \\ \Delta w \end{Bmatrix}_{(i)} = \Delta L_{(i)}^{i+\Delta t} \cdots\cdots\cdots\cdots (11)
$$

where

$$
\Delta L_{(i)}^{t+\Delta t} = \Delta t \begin{Bmatrix} (1-\beta)R_{(i)}^{t} + \beta R_{(i)}^{t+\Delta t} \\ (1-\beta)Q_{(i)}^{t} + \beta Q_{(i)}^{t+\Delta t} \\ (1-\beta)F_{(i)}^{t} + \beta F_{(i)}^{t+\Delta t} \\ (1-\beta)W_{(i)}^{t} + \beta W_{(i)}^{t+\Delta t} \end{Bmatrix} - \left(\begin{bmatrix} M_{vu} & M_{v\theta} & M_{vp} & M_{vw} \\ 0 & M_{\psi\theta} & M_{\psi p} & M_{\psi\pi} \\ M_{vu} & M_{v\theta} & M_{vp} & M_{vw} \\ 0 & M_{\psi\theta} & M_{\psi p} & M_{\psi w} \end{bmatrix}_{(i)}^{t+\Delta t} \right.
$$

$$
\left. + \beta\Delta t \begin{bmatrix} K_{vu} & K_{v\theta} & K_{vp} & K_{vw} \\ K_{vu} & K_{v\theta} & K_{vp} & K_{vw} \\ 0 & K_{\omega\theta} & K_{\omega p} & K_{\omega w} \\ K_{\psi u} & K_{\psi\theta} & K_{\psi p} & K_{\psi w} \end{bmatrix}_{(i)}^{t+\Delta t} \right) \begin{Bmatrix} u \\ \theta \\ P \\ w \end{Bmatrix}_{(i)}^{t+\Delta t} + \left(\begin{bmatrix} M_{vu} & M_{v\theta} & M_{vp} & M_{vw} \\ 0 & M_{\psi\theta} & M_{\psi p} & M_{\psi\pi} \\ M_{vu} & M_{v\theta} & M_{vp} & M_{vw} \\ 0 & M_{\psi\theta} & M_{\psi p} & M_{\psi w} \end{bmatrix} \right.
$$

$$
\left. -(1-\beta) \begin{bmatrix} K_{vu} & K_{v\theta} & K_{vp} & K_{vw} \\ K_{vu} & K_{v\theta} & K_{vp} & K_{vw} \\ 0 & K_{\omega\theta} & K_{\omega p} & K_{\omega w} \\ K_{\psi u} & K_{\psi\theta} & K_{\psi p} & K_{\psi w} \end{bmatrix}_{(i)}^{t} \right) \begin{Bmatrix} u \\ \theta \\ P \\ w \end{Bmatrix}_{(i)}^{t}
$$

2.4 Boundary and initial conditions

The region, Ω occupied by the saturated solid is subjected to applied traction t, prescribed displacement $\hat{u}$. The boundary of Ω, $\partial\Omega$ may also be divided into portions of boundary of temperature $\partial\Omega_h$, moisture $\partial\Omega_w$, pore-pressure $\partial\Omega_\pi$. The domain $\overline{\Omega}$ is composed of the interior Ω and the boundary $\partial\Omega$. All of the functions defined in the domain are the product of the spatial domain with a non-negative time interval, i.e. $\overline{\Omega}\times[0, \infty)$.

2.5 J-integral

The J-integral by virtual crack extension(VCE) method[9] is

$$
J=-\int_{v_0} \left\{ w\frac{\partial p_n}{\partial x_i} - \sigma_{kl}\frac{\partial u_k}{\partial x_i}\frac{\partial p_n}{\partial x_i} + \sigma_{mm}\beta_t\frac{\partial T}{\partial x_i^n}p_n \right\} |J|\,dV \cdots\cdots\cdots\cdots (12)
$$

In the influence of hygro-thermal stress, J-integral is

$$
J=-\int_{v_0} \left\{ w\frac{\partial p_n}{\partial x_i} - \sigma_{kl}\frac{\partial u_k}{\partial x_i}\frac{\partial p_n}{\partial x_i} + \sigma_{kk}\beta_t\frac{\partial T}{\partial x_i^n}p_n + \sigma_{kk}\beta_w\frac{\partial W}{\partial x_i^n}p_n \right\} |J|\,dV \cdots\cdots\cdots\cdots (13)
$$

where β_t and β_w are coefficients of thermal, hygral expansion, respectively, p_n is the element shape function.

3. Application on Composite Materials

A typical shape of crack problem is shown in Figure 1.

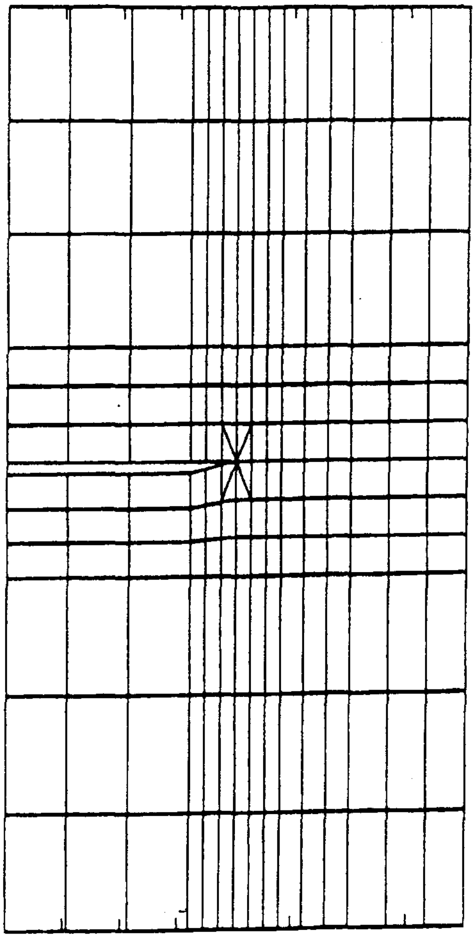

Fig. 1 Finite element discretization of this model

This is composed of two materials : Silicon and Encapsulant.

The initial moisture content, mass density and porosity of the encapsulating material are estimated to be W=0.25%, ρ_s=4.925(kg/m^3) and ϕ=0.005, respectively.

Ideal gas equation (Pv=RT) is valid in this case, R=461.6(J/kg°K) for vapor. Increased vapor pressure is due to the heating of entrapped moisture.

Only the encapsulant can absorb moisture.

Initial conditions :

- Encapsulant with moisture 4.925(kg/m^3), ϕ=0.005
- Initial temperature 26℃
- No strains and stresses
- This bimaterial has an initial crack length 4mm (2mm in the half meshed model) in the center

Boundary conditions :

- This bimaterial is heated from 26℃ to 220℃ for 200sec. at the upper boundary
- No moisture flux at the boundaries

4. Results and Discussion

Two methods(coupled system and uncoupled system) of solving the heat and moisture transient problem are compared. Coupled solutions are obtained directly by solving the problem with assumption that the displacements, temperature and moisture are fully coupled. Uncoupled solutions are obtained by solving each field separately. The solution sequence made in the uncoupled system is moisture, temperature, displacement and stresses. With such sequence, the vapor pressure is determined by the moisture content and current temperature(Pv=RT).

The deformation of this model is influenced by the moisture, temperature and vapor pressure. For this case, the J-integral histories are shown in Figure 2. As this figure shows, the energy release rates by these two schemes in consideration of hygrothermal or thermal effect are compared.

The comparison of the principal stress distribution of these schemes are shown in Figure 3 and Figure 4. Figure 5 shows the representative principal stress distribution.

From this comparison, we can see that the developed program is accurate because results between the coupled solution and uncoupled solution in Figure 2~4 are almost similar and maximum values of these two results are almost equal to those of ABAQUS. Therefore, the use of uncoupled solution is recommended because the coupled

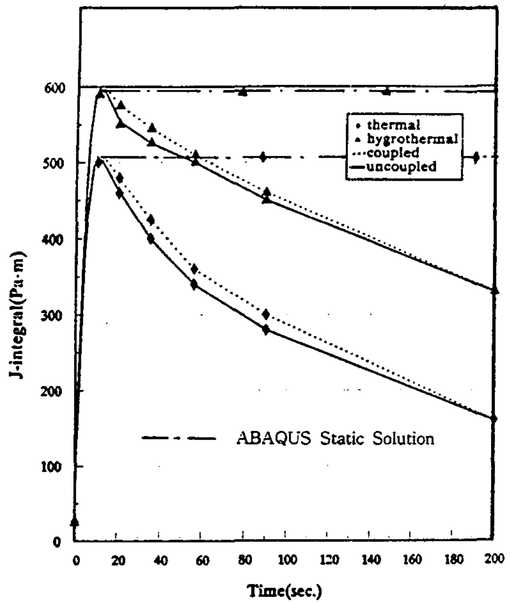

Fig. 2 J-integral histories

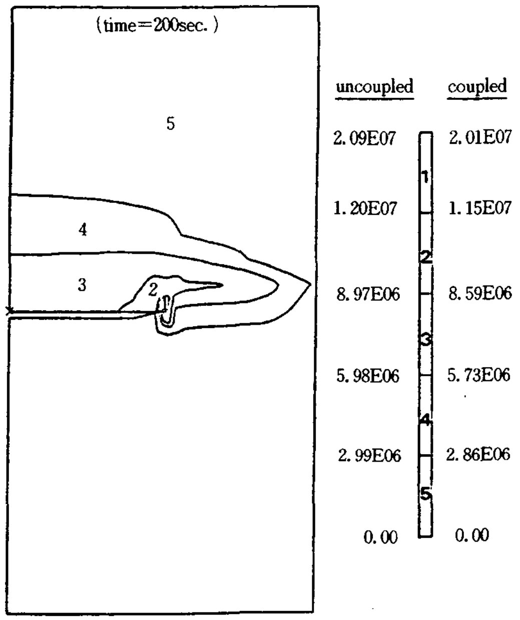

Fig. 3 The comparison of the principal stress by two schemes in consideration of thermal effect

case is expensive to run (5 times larger than uncoupled case).

And the Maximum J-integral value by the effect

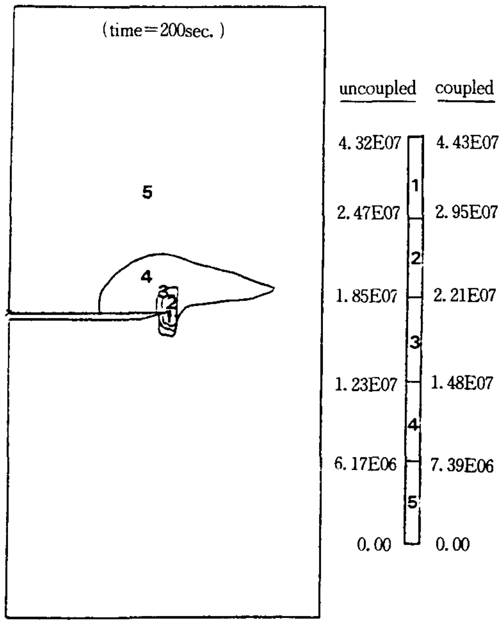

Fig. 4 The comparison of the principal stress by two schemes in consideration of hygrothermal effect

of vapor pressure(hygrothermal) is about 20% larger than that by the effect of thermal.

The entrapped moisture and its vapor pressure (hygrothermal effect) create larger spreading force on the delamination surfaces, causing the J-integral value to increase quickly to the maximum value at time=10 sec. After this time the J-integral is decreased to zero slowly.

5. Conclusions

Through the finite element analysis for hygrothermal fracture in composite materials, we obtained the following conclusions :

1) This finite element program is very reasonable to apply to hygrothermal fracture analysis of composite materials.
2) To predict J-integral accurately, the vaporization effect has to beconsidered because it is accelerate the crack driving force at an early stage.
3) The use of uncoupled solution in this analysis

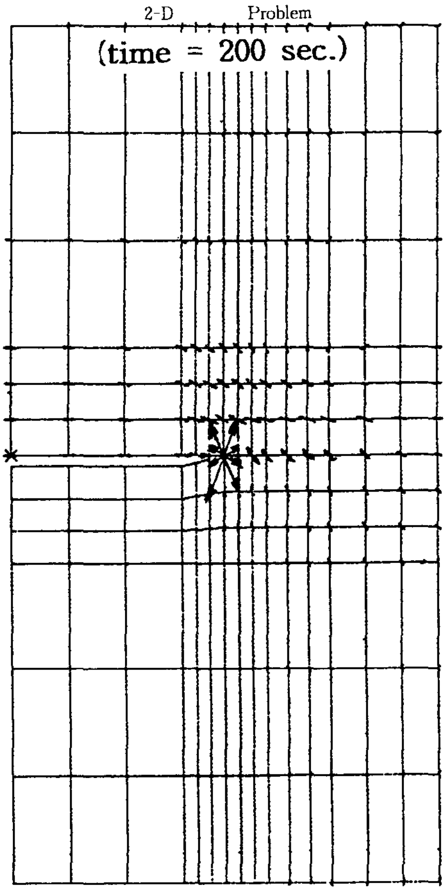

Fig. 5 The principal stress distributions

is recommended because the result by this scheme is reasonable and CPU time is not costly.

4) This procedure is also applicable to problems related to structureresponse evaluations associated with various porous materials, including ceramics, polymers, thin film and plastic encapsulated ICs etc..

Nomenclature

Subscripts

s : solid constituent

f : fluid constituent

Roman symbols

D_e, D_h, D_{vp} : elastic, hygrothermal, viscoplastic strain rates, respectively

F, F_s, F_f : deformation gradient tensors

f, f_f, f_s : body forces

J : J-integral

k, k_f, k_s : heat conduction coefficients

q : heat flux vector

r, r_s, r_f : specific energy supply rates

T, T_f, T_s : Cauchy stresses

t, t_f, t_s : surface tractions

t : time

$u, \hat{u}, u_0$: displacement vector and its boundary and initial values

ν_s, ν_f, ν_r : velocities

v_0 : volume

w : weight function

W : moisture content

Greek symbols

β, β_s, β_f : thermal expansion coefficients

γ : viscosity constant of viscoplastic material

ϵ : symmetric part of displacement gradient tensor

$\theta, \hat{\theta}, \theta_0$: temperature, its boundary and initial values

$\Omega, \partial\Omega$: domain and boundary

$\pi, \hat{\pi}, \pi_0$: pore pressure, its boundary and initial values

$\rho, \overline{\rho}$: true and apparent mass densities

$\sigma, \overline{\sigma}$: Cauchy and effective stresses, respectively

ϕ : porosity

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