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DETERMINATION OF MATERIAL PROPERTIES THROUGH COMPUTER SIMULATION

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SUMMARY

It is well known that microstructural constitution like local nonhomogeneities and anisotropy influence the microstructural behaviour of a material. However, it is not easy to study these influences through classical analytical methods of solid mechanics. With the advent of the finite element method, some attempts have recently been made to simulate the microstructure of multiphase materials using displacement formulations. This method, however, is inadequate due to the inherent incapacity of displacement finite element formulations to maintain compatibility of both displacement and relevant stress components along interphase boundaries, which is essential to reflect the exact situation existing at these boundaries.

In displacement finite element formulations, continuity of the stress tensor along the interelement boundaries is not possible even for materially homogeneous problems. This discontinuity will, in general, be even more violent if the adjacent elements are materially different. Introduction of strain components as additional degrees of freedom at element nodes provides stress continuity for materially homogeneous problems, but not for materially nonhomogeneous ones. In this paper an attempt is made to overcome this difficulty by using a mixed finite element plane stress formulation based on Hellinger-Reissner's variational principle. Linear parametric functions are assumed for both the displacement and stress components for a triangular element. Four such triangular elements are combined to give a general quadrilateral element. Nodal values of the displacement and stress components are utilized as the system unknowns providing the desired displacement and stress continuities.

The method is applied to a two-phase Fe–Ni alloy (64% Fe, 36% Ni). This is simulated by a random number technique. Six different random distributions corresponding to the same volume fraction were studied using both the mixed and 4-CST elements. The values of the Young's modulus and Poisson's ratio for all the distributions were found to be almost the same; thus proving the well known experimental fact that distributions do not have appreciable effect on material properties. While the prediction of the material properties was not found to be very much affected by the improper satisfaction of traction continuity conditions, the mixed method gave much superior stress field predictions.

INTRODUCTION

In recent years considerable progress has been made in the field of multiphase materials like composite materials and metallic alloys. Most of these studies are experimental. There are, however, attempts to predict the overall material properties using classical analytical techniques on idealised microstructural models of these materials. These studies have yielded close bounds for the elastic constants. However, these methods could not consider local nonhomogeneities, anisotropy and randomness in the arrangement of constituent phases at the microstructural level, which influence the local stress and strain fields. It is well-known that phenomena like fracture, fatigue and creep are highly sensitive to and are controlled by these local fields. With the advent of the finite element method, several attempts have recently been made to simulate the microstructure of multiphase materials and bridge the gap in the present state of knowledge. Jaensson and Sundström [1] have used the finite element technique to simulate the photomicrograph of two-phase WC-Co alloys. Miyamoto, Ishijima and Homma [2] have studied the mechanical behaviour of grinding wheels using the finite element method on a simulated microstructure of the wheel material. Random number technique was used to simulate the material. Purushothaman, Rao and Murthy [3] studied the behaviour of concrete-like materials using similar methods.

In all the above studies, conventional displacement finite element formulations have been used. Even though integrated quantities like material constants are predicted fairly accurately, these models are inadequate for the prediction of local stress and strain fields due to their inherent incapacity to maintain both the displacement and traction continuities along the interphase boundaries. In this paper, an attempt is made to overcome this deficiency by using a mixed finite element formulation due to Dunham and Pister [4] based on the Hellinger-Reissner's variational principle. The method is applied to a two-phase Fe-Ni alloy simulated by random numbers. Evaluation of the equivalent elastic constants and the stress fields have been made by both the standard 4-CST displacement model and the mixed model and the results are compared.

MIXED MODELS

In the conventional displacement finite element formulations, the continuity of the stress tensor along the interelement boundaries is not possible even for materially homogeneous problems. This discontinuity will, in general, be even more violent if adjacent elements are materially different. Higher order elements also cannot eliminate this undesirable feature of displacement models. Introduction of derivatives of displacements as additional degrees of freedom at the external nodes provides stress continuity for materially homogeneous problems. This model enforces continuity of strains rather than stresses and is not applicable to nonhomogeneous problems because in such problems the strains are in fact discontinuous at the interface between different materials.

One way to maintain both the displacement and stress continuities is to use a mixed finite element formulation where nodal values of both the displacement and stress components are utilised as the system unknowns providing the desired displlcement and stress continuities. In this paper, the mixed plane stress element of Dunham and Pister [4] based on the Hellinger-Reissner's variational principle has been adopted.

The Hellinger-Reissnerrs variational principle states the stationary property of π_R where (in the absence of body forces)

$$\pi_R = \int_V[- B(\sigma_{ij}) + \tfrac{1}{2}\sigma_{ij}(u_{i,j} + u_{j,i})]dV - \int_{S_\sigma}\overline{T}_i u_i dS - \int_{S_u} T_i(u_i - \overline{u}_i)dS \quad (1)$$

where

$$B(\sigma_{ij}) = \tfrac{1}{2}\sigma_{ij}C_{ijkl}\sigma_{kl} \quad (2)$$

In these expressions

σ_{ij} = stress tensor component

C_{ijkl} = elastic compliance tensor

V = volume

u_i = displacement

S = surface

$\overline{T}_i$ = prescribed boundary traction

$\overline{u}_i$ = prescribed boundary displacement

S_σ = portion of S over which tractions are prescribed

S_u = portion of S over which displacements are prescribed

In the finite element application of the above variational principle, the the normal and tangential displacements are required to be continuous along the interelement boundaries. The assumed stress field need not satisfy the equations of equilibrium.

We consider plane stress application of the above principle for a triangular element. For such applications, if we satisfy the displacement boundary conditions identically with our field variable models, eq. (1) becomes (matrix notation is used for convenience),

$$\pi_R(u,\sigma) = \int_V(- \lfloor\sigma\rfloor[C]\{\sigma\} + \lfloor\sigma\rfloor\{\epsilon\})dV - \int_{S_\sigma}\lfloor u\rfloor\{\overline{T}\}dS \quad (3)$$

where $\{u\}$, $\{\sigma\}$, and $\{\epsilon\}$ are the relevant displacement, stress, and strain components respectively for a plane stress problem. The brackets $\lfloor\ \rfloor$, $[\ ]$ and $\{\ \}$ are used to represent row, square and column matrices, respectively.

Linear parametric functions are assumed for both the displacement and stress components. The displacement and the stress fields are then expressed in terms of the element nodal displacements $\{q\}$ and the nodal stresses $\{\tau\}$ as follows:

$$\{u\} = [N_u]\{q\} \tag{4}$$

$$\{\sigma\} = [N_\sigma]\{\tau\} \tag{5}$$

The strains may be obtained from the strain-displacement equations in the usual manner

$$\{\epsilon\} = [B]\{q\} \tag{6}$$

Substituting eqs. (4), (5) and (6) into eq. (3), we obtain

$$\pi_R = \lfloor \tau \rfloor [S_{\tau\tau}]\{\tau\} + \lfloor \tau \rfloor [S_{\tau u}]\{q\} - \lfloor q \rfloor \{F_u\} \tag{7}$$

where

$$[S\ \ ] = - \int_V [N_\sigma]^T [C][N_\sigma] dV \tag{8}$$

$$[S\ \ ] = \int_V [N_\sigma]^T [B] dV \tag{9}$$

$$F_u = \int_{S_\sigma} [N_u]^T \bar{T}' \, dS \tag{10}$$

The stationary value of the functional yields the governing equations

$$\begin{bmatrix} [S_{\tau\tau}] & [S_{\tau u}] \\ [S_{\tau u}]^T & [0] \end{bmatrix} \begin{Bmatrix} \{\tau\} \\ \{q\} \end{Bmatrix} = \begin{Bmatrix} \{0\} \\ \{F_u\} \end{Bmatrix} \tag{11}$$

The triangular plane stress element obtained in the foregoing fashion has 15 degrees of freedom, two displacement unknowns and three stress unknowns at each of the three nodes. Four such triangular elements are combined to form an arbitrary quadrilateral plane stress element. After the elimination of the five internal degrees of freedom, this element has 20 degrees of freedom. In this paper, this element will subsequently be referred to as a 4-RLT (Reissner linear triangle) element.

STUDY OF Fe-Ni ALLOY

A strip of a typical twophase Fe-Ni alloy (64% Fe, 36% Ni) under a uniform uniaxial tensile load of 100 kg/cm^2 was studied with a 8x11 rectangular mesh (Fig. 1). Random numbers from 0 to 1 with a uniform probability of distribution were generated by a subroutine. These decimal fraction numbers were converted in a simple manner to yield element material numbers 1 (for Fe) and 2 (for Ni). Even though models of this nature do not correspond to any actual microstructure, they are adequate for the purpose of our study. An important assumption was made that across the direction of thickness, the strip has uniform material properties; thus approximating the strip under study as a plane stress problem.

Six different random distributions corresponding to the same volume fraction were evaluated by both the 4-CST and 4-RLT elements. 8x11 rectangular meshes were used in all the computations. One convergence study using a 16x22 mesh showed that the 8x11 mesh grading was adequate for the purpose for both the 4-CST and 4-RLT analyses.

One such random arrangement is shown in Figure 1. The deformations predicted by the two methods are almost the same. In fact, the deformation patterns by the two methods were so close to each other that no distinction between them was possible at the time of plotting them in Figure 2. Horizontal displacements were plotted to a scale five times larger than that for the vertical displacements. The normal stresses σ_y have been plotted along a typical cross-section in Figures 3a and 3b for the 4-CST and 4-RLT analyses respectively. It is noted that the mixed finite element model gives more even stress field than that given by the displacement model.

Prediction of Elastic Moduli

For the six different random arrangements corresponding to the same volume fraction, the values of Young's modulus (E) and Poisson's ratio (ν) for the alloy, based on average stresses and strains, were found to be almost the same; thus proving the well-known experimental fact that distributions do not have appreciable effect on the material properties. It was also seen that there was no appreciable difference in the values of the material properties computed by the mixed and the displacement models. Table I shows the evaluated values of E and ν for the six different distributions by the two methods.

CONCLUSIONS

The important conclusions are

(i) Mixed models give a better estimate of the local stress and strain fields. The local bending effects shown by the displacement models are considerably smoothered out.

(ii) The overall material properties like elastic moduli are not sensitive to the kind of elements and the interphase boundary conditions.

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Table I- Values of E and ν for Fe-Ni alloy through computer simulation

Distribution no.	$E \times 10^6$ kg/cm^2	ν
Fe	2.00	0.293
Ni	1.43	0.259
	4-CST analysis	
1	1.772	0.280
2	1.771	0.280
3	1.770	0.279
4	1.774	0.279
5	1.772	0.281
6	1.771	0.279
	4-RLT analysis	
1	1.759	0.279
2	1.760	0.279
3	1.762	0.277
4	1.760	0.279
5	1.759	0.278
6	1.759	0.278

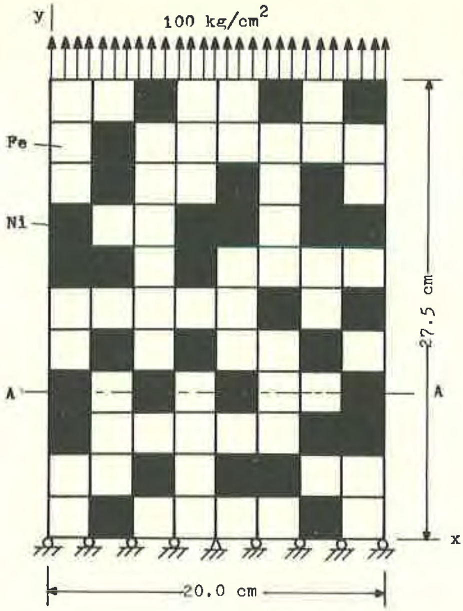
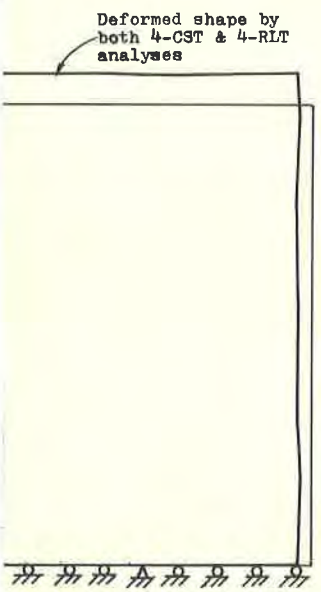


Fig.1- Random arrangement of constituent phases in Fe-Ni alloy



g.2- Shape of the deformed strip by both 4-CST and 4-RLT analyses

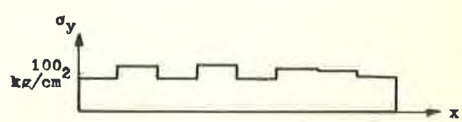


Fig.3a- Distribution of σ_y along a typical section AA by 4-CST analysis

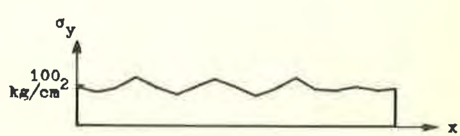


Fig.3b- Distribution of σ along the typical section AA by 4-RLT analysis