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Probabilistic modeling the deformation and failure in heterogeneous microstructure of Ti-6Al-4V

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Heterogeneous material is being considered as a material in which the responses vary from point to point, and thus the basic requirement for obtaining the macro-material level property is to characterize the deformation rate or the stress rate in terms of the micro-level field data [1, 2]. Statistical mechanics has enabled the macroscopic characteristics to be determined from microscopic data and therefore well-defined statistical modeling provides enhanced understanding of deformation behavior coupled with microstructual responses. In order to represent the statistical distributions in heterogeneous materials, methodologies to model materials with spatial correlation functions have been proposed over the years, and it is known that the correlation functions can be formulated by the experimentally measured probability functions [3, 4]. In spite of the success of computer simulation technologies in materials science, however, it is still not easy to represent adequately the microstructural features such as distributions of phase, morphology, and geometry related properties to the deformation behavior. Moreover modeling the deformation behavior using the reconstructed microstructural image from limited experimental data needs proper physical and statistical approximations, respectively [5].

It is well known that the $\alpha - \beta$ titanium alloys do not readily cavitate during superplastic deformation, but the materials deform inhomogeneously leading to ultimate strain localization and failure [6, 7]. Microstructural evolution, which is coupled nonlinearly with the deformation behavior, is important since it affects subsequent material properties, but in addition, contributes to the development of non-uniform failure. The $\alpha - \beta$ Ti-6Al-4V alloy is two-phase having different deformation characteristics, and thus the local deformation is strongly influenced by the heterogeneous phase distributions [8, 9]. The present paper therefore describes the efforts to develop a generic model for determining the inhomogeneous deformation and failure coupled with the heterogeneous microstructures within the statistical mechanics framework. The work essentially continues a newly developed methodology in which a probabilistic model has been presented combined with micro-level constitutive equations enabling the quantities at macro-material level to be averaged over the distributions of phase. As detailed in [10], the experimentally observed spatial correlation functions were developed, and microstructural evolutions have been investigated by means of two-point probability functions. Here, however, attempts have been extended to develop higher order probability functions such as three-point functions providing the higher order corrections for the heterogeneity of the materials [4]. The details of the statistical characteristics including phase distributions and their evolutions, therefore, can be correctly predicted using the model even though the geometry associated statistical properties of the two phases may differ. Since the quality of final microstructure depends on the properties of initial microstructure [11], Monte Carlo simulation has been used together with the probability functions developed for the reconstruction of microstructures. By imposing the precisely optimized distributions of phase on the gauge-length region using the simulation, the failure strain determined from the finite element implementation thus shows much better agreement with the experimental data.

The material used in this work is the two-phase titanium alloy Ti-6Al-4V. Experimentally measured distributions of phase size together with the volume fraction of two phases obtained from superplastic tensile tests have been used to determine the probability functions. The correlation functions then have been formulated in terms of the probability functions developed. The details of the modeling approaches for the determination of superplastic behavior using the functions may be found elsewhere [7, 10]. As the microstructure deforms, probability function is expected to change, and the function corresponds to the probability of occurrence of a certain state. Three-point probability function has been considered in the present work and the conditional probability for the function may be expressed in terms of the two-point conditional probabilities, ϕ_1' and ϕ_2', respectively as [4]

$$\phi(r' \in h_n \mid r \in h_m, h_l) = \phi_1'(r' \in h_n \mid r \in h_m, h_l) + \phi_2'(r' \in h_n \mid r \in h_m, h_2) \quad (1)$$

in which the occurrence of probability is defined by the state h_n at r', given that the state h_m, and h_l occur at r and the origin point, respectively. Either 1 or 2 can be assigned to the phase as l, m, and n for two-phase materials. It is apparent that the occurrence of probability at some point is equal to the volume fraction of the material, and thus the conditional probability, ϕ may be expressed in terms of the absolute probability, P_{lmn} with corresponding volume fraction as $\phi(r' \in h_n \wedge r \in h_m \wedge h_l) = P_{lmn}/V_1$. By employing

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TABLE I Probability parameters for the three-point probability functions of Ti-6Al-4V at 900 °C

P_{lmn}	α_{lmn}	β_{1lmn}	β_{2lmn}	β_{3lmn}	δ_{1lmn}	δ_{2lmn}	δ_{3lmn}	γ_{lmn}	S_{lmn}	T_{lmn}	W_{lmn}
P_{111}	0.118	0.122	0.122	0.122	0.005	0.005	0.005	−0.010	$1.750\,r^{0.942}$	$8.590\,(rr')^{-7.590}$	$0.934\,[r^{1.137}(r')^{0.799}(r'')^{0.160}]$
P_{112}	0.122	0.127	−0.122	−0.122	−0.005	−0.005	−0.005	0.500	$1.750\,r^{0.942}$	$4.688\,(rr')^{-3.688}$	$0.001\,[r^{1.584}(r')^{0.853}(r'')^{1.271}]$
P_{121}	0.122	−0.122	0.127	−0.122	−0.005	−0.005	−0.005	0.500	$2.602\,r^{0.890}$	$-0.100\,(rr')^{1.100}$	$0.001\,[r^{1.584}(r')^{0.853}(r'')^{1.271}]$
P_{122}	0.127	−0.127	−0.127	0.122	0.005	0.005	0.005	−0.010	$2.602\,r^{0.890}$	$0.234\,(rr')^{0.766}$	$0.934\,[r^{1.137}(r')^{0.799}(r'')^{0.160}]$
P_{211}	0.122	−0.122	−0.122	0.127	−0.005	−0.005	−0.005	0.500	$2.602\,r^{0.890}$	$-0.100\,(rr')^{1.100}$	$0.001\,[r^{1.584}(r')^{0.853}(r'')^{1.271}]$
P_{212}	0.127	−0.127	0.122	−0.127	0.005	0.005	0.005	−0.010	$1.502\,r^{0.879}$	$4.688\,(rr')^{-3.688}$	$0.934\,[r^{1.137}(r')^{0.799}(r'')^{0.160}]$
P_{221}	0.127	0.122	−0.127	−0.127	0.005	0.005	0.005	−0.010	$2.602\,r^{0.890}$	$0.234\,(rr')^{0.766}$	$0.934\,[r^{1.137}(r')^{0.799}(r'')^{0.160}]$
P_{222}	0.133	0.127	0.127	0.127	−0.005	−0.005	−0.005	0.010	$1.502\,r^{0.879}$	$4.135\,(rr')^{-3.135}$	$0.011\,[r^{7.471}(r')^{-5.942}(r'')^{1.925}]$

the exponential forms of three-point probability functions [3], then the absolute probability can be represented as

$$P_{lmn}(r, r', r'') = \alpha_{lmn} + \sum_{k=1}^{3} \beta_{klmn} \exp(S_{lmn} r) + \sum_{k=1}^{3} \delta_{klmn} \exp[T_{lmn}(rr')] + \gamma_{lmn} \exp[W_{lmn}(rr'r'')] \quad (2)$$

where α, β, δ, and γ are the probability parameters obtained from the limiting conditions, and the parameters, S, T, and W can be determined using the two-point probability functions through the linear regression analysis. The separation distances, r and r' are defined from the coordinate origin, and thus the remaining distance, r'' is given by the angle, θ as $r'' = \sqrt{r^2 + r'^2 - 2rr'\cos\theta}$. In two-phase material, it is apparent that eight probabilities can be found for the three-point probability function and the result of these probabilities shows that the total sum equals approximately to unity. A macro-level is defined comprising many micro-material cells in such a way that the probability functions can be represented by the experimentally measured phase distributions.

In order to measure the heterogeneous distributions of $\alpha - \beta$ phases, digital processing techniques with an image analyzer have been used [10]. A total of 560 sets of data (i.e., 20 microphotographs × 4 sections × 7 point sets) have been used for the analysis in each test specimen. Fig. 1 shows a digital image of microstructure and unit grid-point cell for the determination of the three-point probability functions. As can be seen, each point has been numbered in its respective direction with a particular angle, and then each phase within any triangle is counted sequentially (i.e., 1-2-2′, 1-3-3′, etc.). All the sets of experimental data of phase occurrences coupled with the volume fractions of each phase over a range of strain rates were employed for the determination of the probability parameters as shown in Equation 2. The parameters determined for Ti-6Al-4V at 900 °C are summarized in Table I. The predicted variations of probability using the three-point probability function are shown in Fig. 2. As can be seen, the probability changes approximately linearly with strain, and in particular, increasing strain leads to significant increasing the probability P_{111}, but gradual decreasing P_{222}. The result shows good agreement with experimentally measured volume fractions of two phases [10]. The probabilities obtained by the three-point functions have been used for the determination of aggregate stress-strain curves, and the result is shown in Fig. 3. For the two-point probability functions, the materials have been assumed initially to be statistically homogeneous and isotropic, and thus the orientation dependent probabilities were generated in further anisotropy analysis. In a current work, however, proper formulation

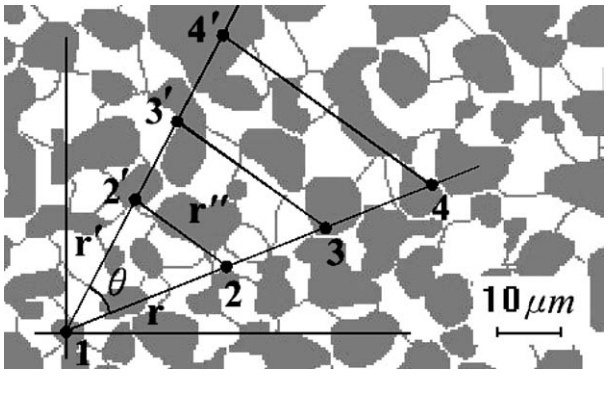

Figure 1 Diagram showing a unit grid-point cell in the digital image of two-phase Ti-6Al-4V.

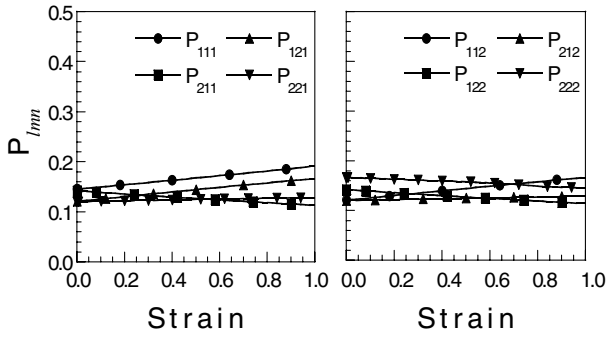

Figure 2 Graph showing the evolutions of probability with strain for Ti-6Al-4V at 900 °C at a strain rate of $1 \times 10^{-3}\ s^{-1}$.

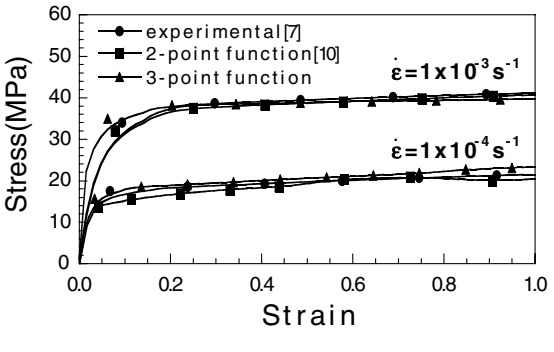

Figure 3 Comparison of the stress-strain curves using the two-point and three-point probability functions with experimental data.

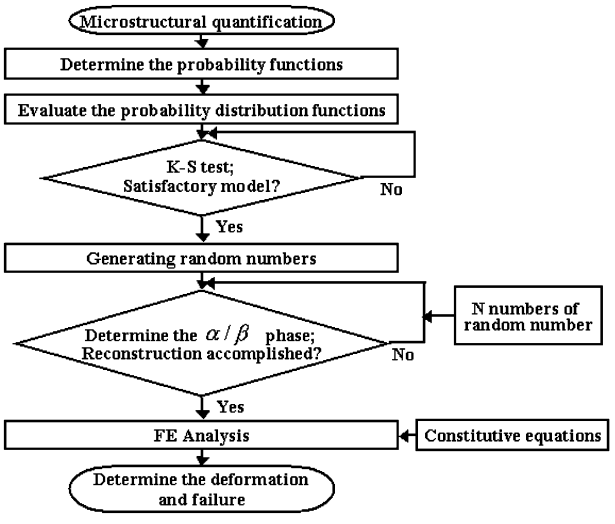

Figure 4 Flow diagram showing the procedure for the determination of failure strain.

incorporating the directional dependence of statistical characteristics using the three-point probability functions has been presented. It is known that $\alpha - \beta$ titanium alloys do not readily cavitate, and failure processes are governed by inhomogeneous deformation rather than cavitation [6]. Usually the heterogeneity of phase distributions can be observed in an undeformed material and this initial non-uniformity may influence deformation and failure. The probabilistic model developed has been implemented into the FE software to predict the failure strain over a range of strain rates. As detailed in previous work [7], failure strain was determined at which the rapid decrease in average stress to lead to strain localization. It is apparent that the initial microstructure is the most important factor that influences deformation characteristics, and thus the material model using the microstructure obtained from limited experimental data requires more accurate statistical representations [5, 11]. The overall process developed for the analysis is shown in Fig. 4 in which the Monte Carlo simulation, together with the probability functions determined are used to reconstruct the initial microstructures. The Monte Carlo simulation provides the most effective microstructural image followed by the K-S (Kolmgorov-Smirnov) test through the comparisons with the probability distribution functions assumed [12]. The results obtained are shown in Table II in which three failure strains are indicated. By imposing the precisely determined phase distributions on the gauge-length region, the failure strain determined from current work, therefore shows that good agreement with experimental data is achieved for both strain rates. The accuracy of the simulation depends on the quality of random numbers [13, 14], and the probabilistic model enabling the phase occurrence to be represented provides much better agreement with experimental data.

In summary, a robust probabilistic model is presented for the determination of heterogeneous phase distributions of Ti-6Al-4V alloy. The effect of initial microstructures, and their evolutions on the superplastic deformation can be correctly predicted using the model. Since no considerable anisotropy is indicated for the material at this temperature, the results have shown that the probabilities change approximately linearly with deformation, and similar stress-strain curves are obtained from both two- and three-point functions. For the case in which different statistical characteristics should be considered, however the three-point probability functions can be thought as an effective formulation for the orientation dependent probabilities. The FE analysis using the reconstructed microstructures achieved by the Monte Carlo simulation shows better agreement with experimental data of failure strain. The unified probabilistic model therefore provides a step towards the practical methodology for the determination of random heterogeneous microstructure and deformation behavior.

TABLE II Comparisons between experimental and predicted failure strains for Ti-6Al-4V at 900 °C

$\dot{\varepsilon}$	Experimental [7]	Two-point functions [10]	Three-point functions with MCS
$1 \times 10^{-3}\,s^{-1}$	1.55	1.46	1.48
$1 \times 10^{-4}\,s^{-1}$	1.72	1.82	1.67

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