Fracture 1977, Volume 2, ICF4, Waterloo, Canada, June 19 - 24, 1977

A MODEL FOR FATIGUE CRACK INITIATION IN POLYCRYSTALLINE SOLIDS

J. W. Provan*

1. INTRODUCTION

As is well known, fatigue is a primary cause of mechanical failure in components being elastically stressed. Numerous efforts have been made to analytically describe this important phenomenon and the resulting literature is correspondingly large. A good review of the situation, especially from the applied point of view, is the recent survey [1].

Restricting attention to probabilistic techniques, the mathematical formalisms utilized in the present work, although applied in a novel manner, are common in reliability studies in design [2] and in probabilistic structural analysis [3]. Perhaps the closest work along the lines developed here is the study carried out by Murzewski [4] who described the cumulative damage in solids under random stress. Esin and Jones [5] also presented the outline of a theory of micro-inhomogenity of stresses and strains which result from the microstructural plastic properties of engineering materials. Certain aspects of their work are also allied to the present investigation.

The existence of distributions rather then deterministic values of both displacements and strains, and hence stresses, in polycrystalline materials being subjected to an externally applied load is firmly established. For example, in [6] random displacements and rotations of individual grains of aluminum embedded in an epoxy resin were observed using a combined holographic and X-ray technique, while in [7] experimental data was used to plot both probabilistic density functions and correlations of plastic deformations in quasi-isotropic polycrystalline aluminum and copper.

The most common application of probabilistic concepts in the study of fatigue is the application of specific distributions to describe the observed scatter in the number of cycles to failure. For example, Bloomer and Roylance [8] and Korbacher [9] reviewed the applicability of the log-normal, normal, Weibull [10] and extreme value [11] distributions used to describe the number of cycles to failure in polycrystalline aluminum and copper respectively. Generally they found that censored or truncated forms of these distributions give very good descriptions of the observed failure distributions especially near their "lower tails".

Recently, a probabilistic micromechanics theory, developed by Axelrad [12] and Provan and Axelrad [13] has led to the prediction of elastic microstress Gaussian probabilistic measures, $\mathcal{P}^{\xi}$, where ξ indicates the microstress, in realistic models of polycrystalline copper and aluminum subjected to uniaxial tension [14]. These distributions were obtained by investigations of: (i) the mechanical response of dislocations [15]; (ii) the computer simulation of the elastic behaviour of various grain boundaries in copper and aluminum [16]; and (iii) the displacement distributions presented in [6]. It was found in [14] that, for a specified dislocation density and

* Mechanical Engineering Department, McGill University, Montreal, Canada.

grain boundary mismatch angle distribution, the microstress distribution varied with both the mean size of the crystalline microstructure and the distribution of grain boundary orientation with respect to an external coordinate frame.

The initial results of a new probabilistic technique of generating fatigue crack initiation information based solely on polycrystalline microstructural data, without having recourse to fatigue testing, is presented in this paper. Specifically, in Section 2, each of four microstress distributions, two for copper and two for aluminum as derived in [14], is in turn considered to be the distribution of microstress amplitude existing at the first peak stress of a sinusoidal tension-compression test of such materials. Following this in Section 3, a Monte Carlo simulation of random loading histories is presented which gives more directly applicable results. These results are discussed in Section 4. Throughout this investigation, Gaussian distributions of the random variables involved are assumed to apply. These distributions are described by the pair $(\mu;V)$ where μ is the mean and V the variance of the random variable involved.

2. MICROMECHANIC FATIGUE

The major aim of this present study is to develop a model or theoretical description of fatigue damage in polycrystalline solids. The major premise is that distributions of stress and strengths exist within polycrystalline solids and that an interference between these distributions during stress cycling causes fatigue damage to accumulate within these materials.

Before starting into the analytical developments of the present study, it is instructive to clarify certain aspects of fatigue from a micromechanics point of view. The onset of damage in a stressed ductile metal is generally associated with a free surface, and the present investigation is concerned only with metals in which the fatigue cracks are initiated at such a free surface. One of the basic concepts of micromechanics is the mesodomain. A mesodomain has three complementary interpretations. The first is that it has a Gibbsian ensemble of microelements within a region of the specimen on which the boundary conditions are assumed to be deterministically known. The second is that each mesodomain contains a large number of microelements or grains so that certain aspects of the law of large numbers may be applied. The third interpretation is perhaps the most important from our point of view. This says that the statistics of the variables involved within the mesodomain are position independent. With this in mind, the only mesodomain we are interested in, in the present study, is the surface mesodomain, which is defined as a layer of the surface material within which the statistics of the random parameters are position independent. The problem of crack propagation is not being attempted here since the mesodomain is no longer the same near a crack tip. The mesodomain contains M microelements, α, $\alpha = 1, \ldots, M$, M large. At time $t = 0$ there are no damaged, i.e., plastically deformed or fractured, microelements and all contribute to resisting the external load. Distributions exist for the microstress, yield strength and ultimate strength of the microelements. If a microelement is stressed beyond its yield strength, residual stresses remain, while if it is stressed beyond its ultimate strength it is no longer effective in resisting any externally applied stress, i.e., it ceases to exist for the purposes of this analysis.

2.1 Stress Interference with Yield Strength - The Effect of Residual Stresses

With reference to Figure 1, the residual stress effect is incorporated into the model through the interference between the i^{th} loading microstress distribution $\mathcal{P}^{\xi^i}$, with the yield strength distribution $\mathcal{P}^X$, where ${}^{\alpha}X$ indicates the yield strength of the α^{th} microelement. The probability that any microelement α be plastically deformed at any peak stress is the probability that ${}^{\alpha}\xi^i$ exceeds ${}^{\alpha}X$. Thus a new random variable, κ^i, is defined as:

$$\kappa^i = X - \xi^i \tag{1}$$

and has the Gaussian density, p_{κ^i}, provided X and ξ^i are both normally distributed, described by:

$$p_{\kappa^i}(\tau) = \frac{1}{\sqrt{2\pi V_{\kappa^i}}}\exp\left\{\frac{-(\tau-\mu_{\kappa^i})^2}{2\,V_{\kappa^i}}\right\} \;;\quad \mu_{\kappa^i} = \mu_X - \mu_{\xi^i} \;;\quad V_{\kappa^i} = V_X + V_{\xi^i} \;. \tag{2}$$

With its appropriate subscript, p, indicates the probability density function of the random variable involved. Using simple transformations the fraction of microelements which become plastically deformed on the i^{th} stress, Q_i, is given by:

$$Q_i = \int_{-\infty}^{0} p_{\kappa^i}(\tau)d\tau = \frac{1}{2\pi}\int_{-\infty}^{K^i} \exp\left\{-z^{i\,2}/2\right\} dz^i \;;\quad K^i = \frac{-\mu_{\kappa^i}}{\sqrt{V_{\kappa^i}}} \;. \tag{3}$$

The residual stress is related to the amount by which a stress exceeds the yield strength in a material. This is a manifestation of the microscopic phenomena of dislocation generation and pile up at grain boundaries resulting in an increasing amount of residual microstress and local or micro-work hardening. Although the process is macroscopically elastic, microscopically it is thermodynamically irreversible. To model this effect it is assumed that for the transition from one stress state to the next the following relations hold:

$$\left.\begin{array}{ll} {}^{\alpha}\xi^{i+1} = {}^{\alpha}\sigma^{i+1} & ;\quad 1 < \alpha < M - \sum_{j=1}^{i} m_p^i \\ {}^{\alpha}\xi^{i+1} = {}^{\alpha}\sigma^{i+1} + H^i\mu^i_{res} & ;\quad M - \sum_{j=1}^{i} m_p^i < \alpha < M \end{array}\right\} \tag{4}$$

where m_p^j is the number of microelements plastically deformed during the j^{th} loading, ${}^{\alpha}\sigma^j$ indicates the stress in α due solely to the externally applied load, $H^i = \mu_{\xi^i}/|\mu_{\xi^i}|$ and μ^i_{res} is a measure of the residual stress effect given by:

$$\mu^i_{res} = \left|\frac{1}{Q_i}\int_{-\infty}^{0} \tau p_{\kappa^i}(\tau)d\tau\right| \;. \tag{5}$$

Based on (4) and (5) it may be shown that:

$$\mu_{\xi^{i+1}} = \mu_{\sigma^{i+1}} + \mathcal{F}^i H^i \mu^i_{res} \;;\quad V_{\xi^{i+1}} = V_{\sigma^{i+1}} + (1-\mathcal{F}^i)\mathcal{F}^i \mu^{i\,2}_{res} \tag{6}$$

where $\mathcal{F}^i = Q_i$ in this case where there is no interference with the ultimate strength distribution.

2.2 Stress Interference With Ultimate Strength - Accumulation of Damage

Again with reference to Figure 1, accumulation of damage at each load is due to the interference between ξ^i and the ultimate-strength distribution, Ξ, where ${}^{\alpha}\Xi$ indicates the ultimate strength of the α microelement. The probability that any microelement, α, be fractured, thereby becoming ineffective, is the probability that ${}^{\alpha}\xi^i$ exceeds ${}^{\alpha}\Xi$. Again a new random variable defined as follows may be introduced:

$$\zeta^i = \Xi - \xi^i \ . \tag{7}$$

The equations already introduced, namely (2) and (3), are again applicable with ζ^i replacing κ^i, Ξ replacing X, P_i replacing Q_i, and Z^i replacing K^i, with the understanding the P_i is the fraction of the effective microelements which are permanently damaged at the i^{th} stress.

Cumulative fatigue damage is modelled mathematically as follows. Consider the first loading. There are no permanently damaged microelements and hence the mean and variance of the microstresses in the surface mesodomain are:

$$\mu_{\xi^1} = \mu_{\sigma^1} \ ; \ V_{\xi^1} = V_{\sigma^1} \ . \tag{8}$$

At the first loading, a fraction P_1 of the microelements become permanently damaged. Hence, the number of damaged microelements and effective microelements, after the first load is respectively:

$$m^1 = P_1 M_e^1 = P_1 M \ , \ M_e^2 = M - m^1 \ . \tag{9}$$

Since M_e^2 is less than or equal to M the average stress in the microelements before the second externally applied load is increased by an amount:

$$\mu_{\xi^2} = \mu_{\sigma^2}/(1-P_1) + \mathscr{F}^1 H^1 \mu^1_{res} \ ; \tag{10}$$

the first term being the Robotnov damage term of fracture mechanics. Similarly, since the number of microelements rendered ineffective during the second load is: $m^2 = P_2 M_e^2$, the mean stress at the third load becomes:

$$\mu_{\xi^3} = \mu_{\sigma^3}/\prod_{j=1}^{2}(1-P_j) + \mathscr{F}^2 H^2 \mu^2_{res} \ . \tag{11}$$

Extending this to the i^{th} load then:

$$\mu_{\xi^i} = \frac{\mu_{\sigma^i}}{\prod_{j=1}^{i-1}(1-P_j)} + \mathscr{F}^{i-1} H^{i-1} \mu^{i-1}_{res} \quad \text{where} \quad \mathscr{F}^i = 1 - \frac{\prod_{j=1}^{i}(1-Q_j)}{\prod_{j=1}^{i}(1-P_j)} \ . \tag{12}$$

Concerning the criterion for fatigue failure, the surface mesodomain is assumed to fail when the mean stress in the microelements exceeds the mean of their ultimate strengths, i.e., if:

$$\mu_{\xi^i} > \mu_{\Xi} \ . \tag{13}$$

Using the above equations, an iterative computer programme was devised which had as inputs the Gaussian pairs: $(\mu_{\xi^0}; V_{\xi^0})$, (μ_χ, V_χ), and $(\mu_\Xi; V_\Xi)$. Restricting attention to a sinusoidal loading, the index i identifies the peak stress, i = 1, ..., 2N, N being the number of cycles to either fatigue crack initiation or to the failure of the surface mesodomain. With this interpretation the curves shown in Figure 2 were obtained for the idealized polycrystalline solids discussed in [14]. Here, κ is inversely related to the average size of the microelements and $\mathscr{P}\phi$ is the probabilistic measure of grain boundary orientations. The values of $(\mu_\chi; V_\chi)$ and $(\mu_\Xi; V_\Xi)$ are taken from [1] and modified as indicated in [4], by utilizing the coefficient of variation (C.O.V.).

3. MONTE CARLO SIMULATION OF RANDOM LOADING HISTORIES

Instead of subjecting the mesodomain to a sinusoidal loading a more realistic and certainly more practical situation would be to consider a polycrystalline solid subjected to a random stress history. Such stress histories can be digitized using standard techniques and histograms, plotted as indicated on the ordinate of Figure 3, may easily be devised. Such histograms were curve fitted, in this case to form Gaussian density distributions defined by $(\mu_\sigma; V_\sigma)$ from which Monte Carlo methods were used to generate various external loads, σ^i. In this case, i = 1, ..., N identifies the Monte Carlo simulated load and again, for each such load, the relations presented in Section 2 were invoked. This process was repeated 50 times and results similar to those indicated on the abscissa of Figure 3 were obtained.

Figure 4 shows the results for the idealized copper and aluminum introduced in [14]. Using the values of $(\mu_\chi; V_\chi)$ and $(\mu_\Xi; V_\Xi)$ given in [4] and a more realistic C.O.V. of the microstress distribution of 0.1, the graph indicated in Figure 5 is obtained for steel.

4. DISCUSSION AND CONCLUSIONS

The results indicated in Figure 2 clearly show that changes in the microstructure of polycrystalline solids have, by the method presented in this paper, a quantifiable influence on the number of sinusoidal loading cycles to crack initiation. Furthermore, the results shown in Figures 4 and 5 indicate the wide variety of loading situations that may be covered by this procedure. Finally, Figure 5 shows that for real materials the technique gives the same characteristics as those obtained by experimentation.

The above information has been obtained from microstructural information *only* and not from macroscopic fatigue experimental investigations. Their qualitative agreement strongly motivates further investigations of the microstructural influences on the fatigue characteristics of polycrystalline solids.

ACKNOWLEDGEMENTS

The help obtained from Messrs. G. Thouret, H. Ghonem and W. Kernisan during the formulation of this report is gratefully acknowledged. So is the financial assistance of the National Research Council of Canada through their Grant No. A7525.

REFERENCES

1. FROST, N. E., MARSH, K. J. and POOK, L. P., "Metal Fatigue", Clarendon Press, Oxford, 1974.
2. HAUGEN, E. B., "Probabilistic Approaches to Design", John Wiley, 1968.
3. FREUDENTHAL, A. M., GARRELTS, J. M. and SHINOZUKA, M., J. Struct. Div. Proc. ASCE, 92, 1966, 267.
4. MURZEWSKI, J., Engrg., Fracture Mech., 8, 1976, 131.
5. ESIN, A. and JONES, W. J. D., J. Strain Anal., 1, 1966, 415.
6. KALOUSEK, J., Ph. D. Thesis, McGill University, 1973.
7. ASATUROV, A. A., KOMOROVA, V. A., RYBALKO, F. P. and VOLKOV, S. D., Fiz. Metal. Metalloved, 17, 1964, 744.
8. BLOOMER, N. T. and ROYLANCE, T. F., Aeronaut. Quar., 16, 1965, 307.
9. KORBACHER, G. K., Exp. Mech., 11, 1971, 540.
10. WEIBULL, W., "Fatigue Testing and Analysis of Results", Pergamon Press, 1971.
11. GUMBEL, E. J., "Statistics of Extremes", Columbia University Press, New York, 1958.
12. AXELRAD, D. R., "Micromechanics of Solids", PWN-Elsevier, 1976.
13. PROVAN, J. W. and AXELRAD, D. R., R. Deform. Behaviour Matls., 3, 1976.
14. PROVAN, J. W. and AXELRAD, D. R., Arch. Mechaniki Stos., 28, 1976.
15. AXELRAD, D. R., PROVAN, J. W. and EL HELBAWI, S., Arch. Mechaniki Stos., 25, 1973, 801.
16. PROVAN, J. W. and BAMIRO, O. A., Acta. Met., (Accepted for Publication).

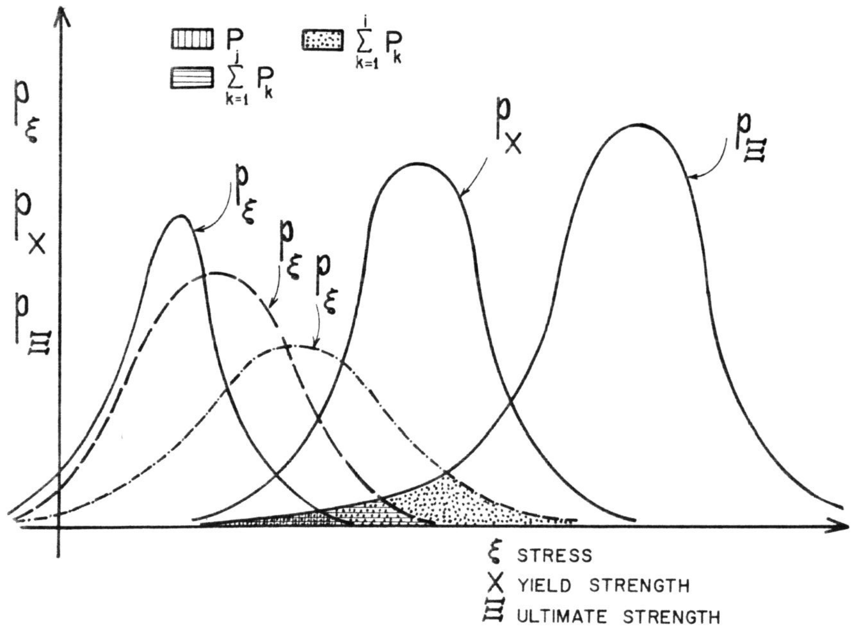

Figure 1 Schematic of Interferences Between the Stress Distribution and the Distributions of Yield and Ultimate Strengths

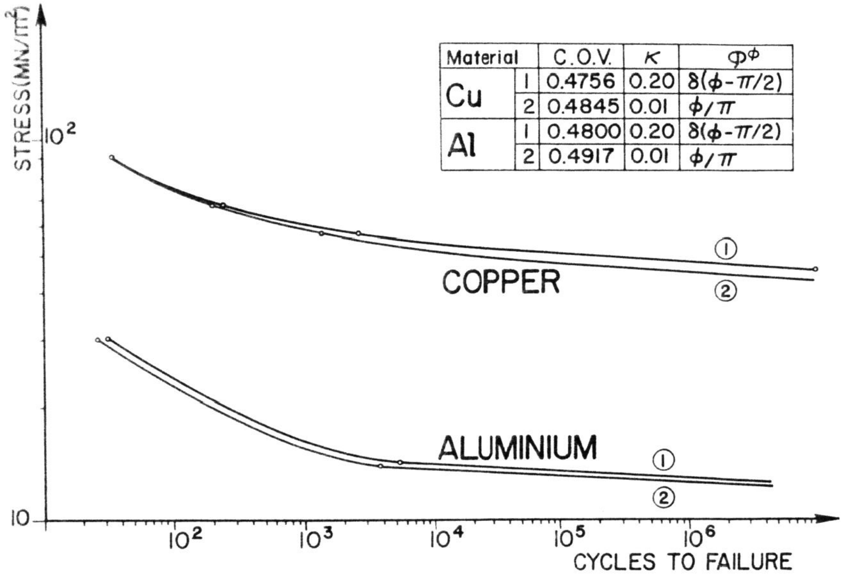

Figure 2 Theoretical S-N Curves for Various Microstructurally Different Coppers and Aluminums

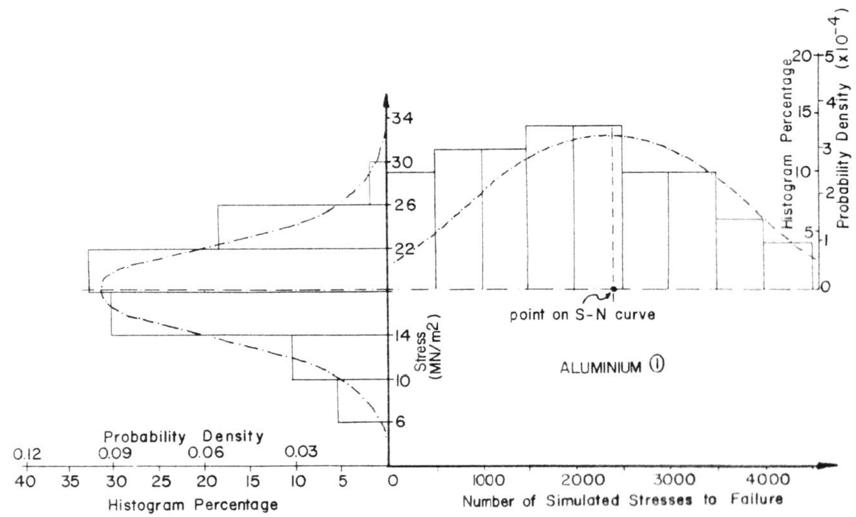

Figure 3 Random Loading Histogram and Its Resulting Distribution of Numbers of Simulated Stresses to Failure in Idealized Aluminum With a C.O.V. of 0.48

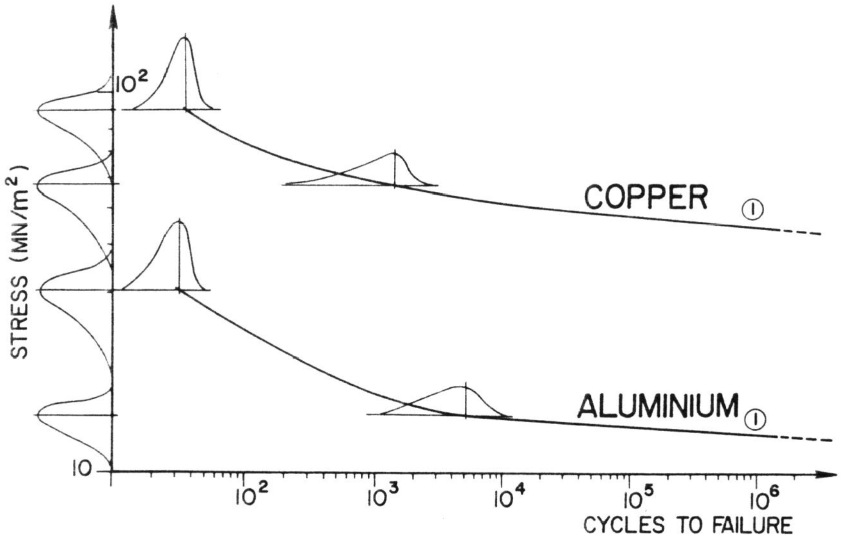

Figure 4 The Monte Carlo Simulated S-N Curves for Idealized Copper and Aluminum

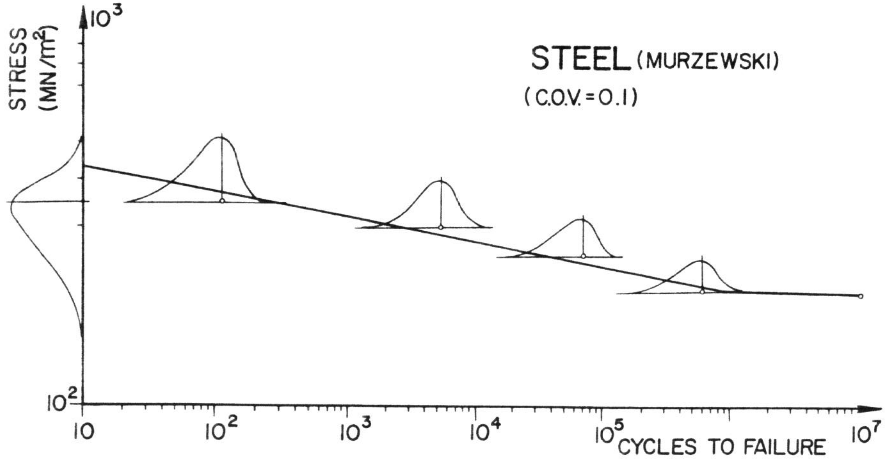

Figure 5 The Monte Carlo Simulated S-N Curves for Steel