

A MODEL FOR THE INITIATION OF CAVITATION AND ITS
APPLICATION TO THE CREEP FRACTURE OF
316 STAINLESS STEEL

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ABSTRACT

A model for the cavity nucleation process based on the recent developments which have occurred in the understanding of the structure of grain boundaries is presented. The concept of grain boundary degeneracy is used to model the dynamics of high angle grain boundaries at elevated temperatures as a stochastic process on a two dimensional random Ising lattice. This model predicts a continuous grain boundary phase transition at approximately one half the absolute melting point, which is the region of most interest as far as the creep rupture of engineering alloys is concerned. In this regime the kinetics of cavity nucleation under low tensile stresses are dominated by group processes and an analytic estimate of the initiation time is made. The model is tested by its application to the creep rupture data of 316 stainless steel for which a good fit is obtained.

KEYWORDS

Creep fracture; cavity nucleation; grain boundary; phase transition; kinetic Ising model; stainless steel.

INTRODUCTION

There is a longstanding engineering problem in being able to reliably extrapolate creep rupture data which is generally measured at temperatures above the service temperatures and for shorter times. There are several methods for extrapolation of creep rupture data in current use (McLean, Dyson and Taplin, 1977; ASME, 1979), based on either reaction rate theory and assuming that the Monkman-Grant relationship holds, e.g. Larson-Miller or Manson-Haferd, or assuming a phenomenological Kachinov damage type summation, which are useful in certain circumstances. However as Ashby (1977) has recently emphasised these methods may lead to a non-conservative extrapolation of creep rupture data through an inadequate appreciation of changes in creep fracture mechanisms and/or the material's microstructure. In the majority of service applications the main creep fracture mechanism is the initiation and growth of voids, either wedge cracks

or cavities, at the grain boundaries. The diffusional growth of these defects is reasonably well documented and understood, but the problem of nucleation kinetics has received relatively little attention. This can lead to considerable difficulties in applying the predictions of mechanistic models to such important engineering materials as AISI 316 stainless steel where there are very long initiation times for void nucleation. Raj and Ashby (1975) and Raj (1978) have, with limited success, applied classical nucleation theory to estimate incubation times for void nucleation. The present investigation concentrated on developing a stochastic model for the nucleation process based on the recent developments which have occurred in the understanding of the structure of grain boundaries (Pond and Vitek, 1977a, 1977b; Smith, Vitek and Pond, 1977; Ashby and Scaepen, 1978).

A MODEL OF VOID INITIATION

It is now recognised (Pond and Vitek, 1977a, 1977b; Smith, Vitek and Pond, 1977; Ashby and Scaepen, 1978) that the structure of grain boundaries can be considered as a random close packed arrangement of atoms. More importantly though, numerical analysis combined with experimental transmission electron microscopy on symmetrical grain boundaries (Pond and Vitek, 1977a, 1977b), has shown two crucial features which shall be used in developing the model. (i) The grain boundary is very narrow with atoms in the boundary conforming to a two dimensional random close packed structure. (ii) The grain boundary structure is degenerate, i.e. there will be several atomic configurations of the same energy, and in the case of symmetrical boundaries each structure is characterised by a particular translation.

Although the above calculations refer to structures at absolute zero, i.e. entropy is not considered, and symmetrical boundaries which account for less than 1% of the grain boundaries in a typical stainless steel (Pumphrey, 1975), the conclusions can be used to develop a model for the majority of grain boundaries i.e. random high angle boundaries at temperatures up to about half the absolute melting point of the material.

Consider an interface between two crystals A and B. We define the grain boundary as the set consisting of those atoms which by a small thermally activated displacement (in a real or phase space) will assume a low energy configuration with respect to the crystals A and B. It is hypothesised that there is more than one low energy configuration (state) and is a fundamental tenet of the model which cannot at this stage be theoretically, a priori, justified but is supported by numerical analysis (Pond and Vitek, 1977a, 1977b). On the basis of the work cited above then, it is clear that the set of atoms will define an approximately two dimensional random close packed array. Thus we can say in a formal manner that atoms in this set may exist in two states and transitions between these states may be accomplished by interaction with a heat reservoir. Figure 1 schematically depicts this situation.

Consider now one of the crystals, say A, and let the state in which a grain boundary atom is "bonded" preferentially to B be defined as 0 and to A be defined as 1. We define the parameter Z as the concentration of thermally activated sites in state 0. In the low

temperature limit Z must tend to zero. Further consideration shows that there must also be a high temperature limit. This arises since under equilibrium conditions we could define the system entirely equivalently with respect to B rather than A. The value of Z must be invariant with respect to the choice of reference system. This leads to a value of Z restricted to $\frac{1}{2}$. The presence of a tensile stress across the boundary will destroy the symmetry and as shown below lead to correlated grain boundary decohesion.

An applied tensile stress of magnitude σ normal to the boundary will give rise to a change in chemical potential of $\sigma\Omega$, where Ω is the atomic volume. Therefore Z becomes $Z \exp(\sigma\Omega/kT)$, where k is Boltzman's constant and T is the absolute temperature.

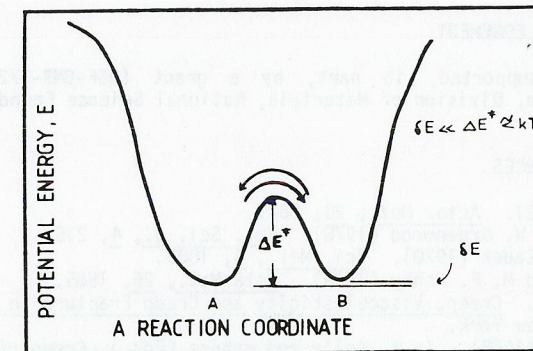


Fig. 1. Degenerate energy levels of grain boundary atoms.

Even though the potential surface shown in Fig. 1 is not well known, we can estimate the rate of transitions at high temperatures using absolute rate theory (Christian, 1975), viz. $\nu \approx kT/h$, where ν is the rate and h is Planck's constant. The solution to this dynamical model would be trivial were it not for the strongly interacting nature of the grain boundary set. It is clear that this must be a positive ferromagnetic-type interaction between neighbours, thus damping the transitions. If the interaction were limited to nearest neighbours, then the model conforms to the kinetic Ising model on a random close packed lattice (Glauber, 1963; McCoy, 1972; Kawasaki, 1972). Consequently there must of necessity be a phase transition, and furthermore the transition temperature will be at $0.5x$ the absolute melting point of the material T_m (Wang and others, 1965). This confirms Hart's (1968, 1970, 1972) predictions but with a fundamental distinction. The grain boundary phase transition is not first order as Hart suggested, but is continuous (high order). Since this phase transition is continuous we can in principle make predictions across the transition.

Much of the current theoretical work (Stanley, 1971; Ma, 1976; Pfeuty and Toulouse, 1977) has used renormalisation techniques to the extract critical exponents which characterise the singular divergences of thermodynamic parameters. Here we use renormalisation (Ma, 1976; Pfeuty and Toulouse, 1977) to estimate the incubation time for a cavity nucleation event.

The application of a tensile stress across the boundary defines a stable void of radius $r=2\gamma/\sigma$, where γ is the surface energy. The number of atom spaces in the void will be

$$(1) \quad N=8F_V\gamma^3/\sigma^3\Omega$$

where F_V is a geometrical shape factor. We then partition the boundary set in blocks of size n and hence analytically derive a probabilistic estimate for the expectation time t_i for a correlated region of atoms in state 0 of size n within a larger block of size N to appear (Boyd, 1980).

$$(2) \quad t_i = \tau N^{-1} (Z \exp \sigma \Omega / kT)^{-n}$$

where $\tau = \nu^{-1}$. This procedure involves a scale change of $s = n^{1/2}$ and providing we are sufficiently close to the transition temperature ($\frac{1}{2}T_m$) we can use the concepts of universality to identify $n^{1/2}$ as a correlation length ξ and furthermore the time to form a correlated region will be the rate determining step for cavity initiation. There are in principle therefore three nucleation regimes (Boyd, 1980),

- (a) $N^{1/2} \gg \xi$ No nucleation (low stress; low temperature)
- (b) $N^{1/2} \ll \xi$ Immediate nucleation (high stress; high temperature)
- (c) $N^{1/2} \sim \xi$ delayed nucleation (intermediate stress; $T \sim 0.3-0.5T_m$).

So a probabilistic estimate can be made for (i) $\sigma \lesssim kT/\Omega$, (ii) $T \sim 0.3-0.5T_m$, and (iii) $N^{1/2} \sim \xi$ as follows:-

$$(3) \quad t_i = \frac{h\sigma^3\Omega}{kT8F_V\gamma^3} (Z \exp \sigma \Omega / kT)^{-n}$$

The physical interpretation of the above analysis leading to equation (3) is that at high temperatures (greater than about $\frac{1}{2}T_m$) the boundary is fully activated and grain boundary sliding will predominate. At temperatures less than $\frac{1}{2}T_m$ the boundary tends to be pinned by unactivated sites but at sufficiently long times correlated grain boundary decohesion will occur leading to nucleated cavities which can grow by plasticity and/or diffusion. These time dependent processes are dominated by the continuous phase transition which occurs at about $\frac{1}{2}T_m$. Further extension of the model will require renormalisation group concepts (Ma, 1976; Pfeuty and Toulouse, 1977) and/or Monte-Carlo simulation methods (Penrose, 1978; Binder, 1979), and work is in hand in this direction.

EXPERIMENTAL

An AISI 316 stainless steel was chosen for this study because of its actual and potential uses in structures operating at elevated temperatures i.e. $\lesssim \frac{1}{2}T_m$ and low stresses $\sigma \lesssim kT/\Omega$. The composition is given in Table 1. The heat treatment of the 316 prior to testing was solution treating in vacuo at 1323K for 1 hour followed by air cooling. The microstructure was precipitate free with an average linear intercept grain size of $14\mu\text{m}$. Creep rupture data were obtained using pin-loaded specimens of cross-section 4mm x 4.5mm and gauge length 16mm. Specimens were tested using constant load creep machines at 909K. Selected tests were interrupted prior to failure for destructive metallographic examination.

TABLE 1 Chemical Composition of Steels (in weight per cent)

	Cr	Ni	Mo	C	B	N	Mn	S
AISI 316	16.9	12.5	2.4	0.03	<0.001	0.028	1.66	0.013
BSCC 316	17.0	11.7	2.4	0.04	0.0001	-	1.65	0.024

	P	Si	Al	Sb	Sn	V	Nb
AISI 316	0.032	0.27	0.007	0.002	0.018	0.08	0.01
BSCC 316	0.024	0.30	-	-	-	-	-

RESULTS AND DISCUSSION

Metallographic examination (Boyd, 1980) has shown that the creep fracture of AISI 316 stainless steel between 800K and 1000K is generally dominated by the initiation phase (i.e. $t_i/t_f \sim 0.8$) with grain boundary voids evident only in the very late stages of creep. Figure 2. shows a scanning electron micrograph of the section of a specimen which was interrupted just prior to failure ($t_f \sim 4 \times 10^6$ s, interrupted time $\approx 0.99t_f$).

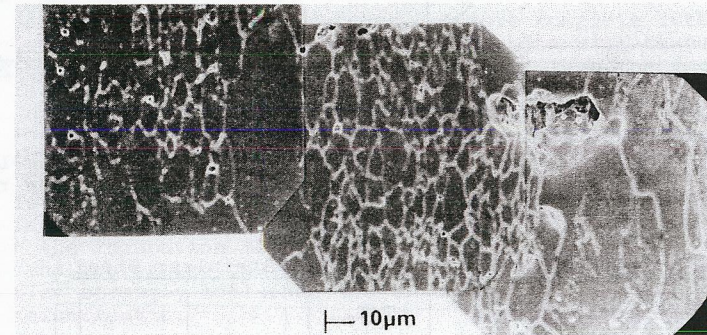


Fig. 2. A SEM micrograph of the interrupted test

On the basis of this observation we can strongly argue for the replacement of t_i by t_f in equation (3) which can now be written as

$$(4) \quad \ln(t_f/\sigma^3) = \ln(A) + B\sigma$$

where

$$A = \frac{h\Omega Z^{-n}}{kT8F_V\gamma^3} \quad \text{and} \quad B = \frac{-n\Omega}{kT}$$

For 316 stainless steel $T_m=1810K$, $\Omega=1.21 \times 10^{-29} m^3$, and $\gamma=2.0 Jm^{-2}$ (Frost and Ashby, 1975). $F_v=4/3\pi$ was taken for a spherical void. This and other approximations made are reasonable because of the strong exponential dependence of the parameters Z and n . By plotting $\ln(t_f/\sigma^3)$ as a function of σ we can obtain the two temperature dependent parameters Z and n (Fig. 3, Table 2.). Figure 3b shows that using equation (4) can lead to conservative extrapolation of data.

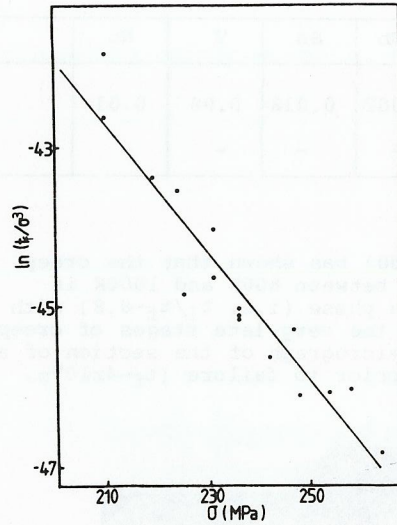


Fig. 3a Results for AISI 316 plotted according to the model.

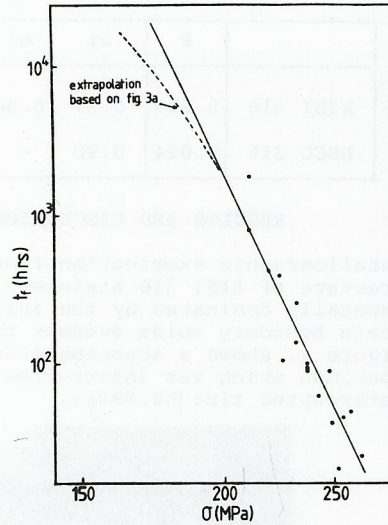


Fig. 3b Conventional log-log plot of the same results as Fig. 3a.

TABLE 2. Summary of Results on 316 Stainless Steel

Data Source	T	T/T _m	Z	n
Boyd, (1980)	909K	0.49	0.399	83.8
BSCC, (1971)	823K	0.45	0.178	41.8
" "	873K	0.48	0.357	74.2
" "	898K	0.50	0.424	89.6
" "	923K	0.51	0.382	75.9
" "	948K	0.52	0.436	86.9
" "	973K	0.54	0.521	112

The values of the temperature dependent parameters $Z=0.398$ and $n=84$ for the steel considered in this work satisfy the predictions of the theory with Z below but close to the restricted value of $\frac{1}{2}$ and n indicating a reasonable correlation length of about 9 atoms. As an

additional test for the model BSCC (1971) data on another cast of AISI 316 stainless steel (Table 1.) is considered in Fig. 4. The values of Z and n obtained are shown in Table 2. and clearly satisfy the predictions of the model.

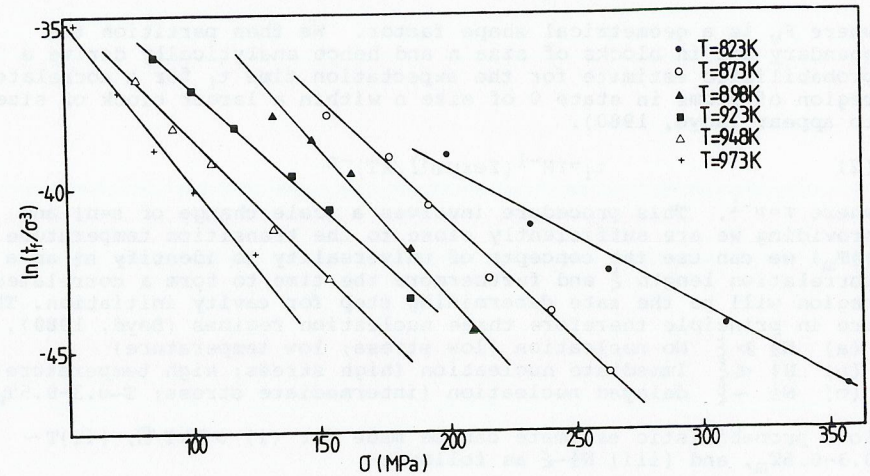


Fig. 4. BSCC data at temperatures between 823K and 973K

These results confirm that the mechanism of cavity nucleation described above is probably correct. A more complete interpretation of the temperature dependent parameters Z and n will be published elsewhere (Boyd, 1980). We emphasize however that the foregoing analysis is perhaps more useful in characterising the mechanisms in cavity nucleation and it is still too early to say whether this analytical model can be used in its present form for prior prediction of rupture times. It is anticipated that the work in hand using Monte-Carlo computer simulation methods will prove to be more useful for this purpose. Nonetheless some of the implications of the analysis will be examined. Precipitates and plastic flow tend to shorten the incubation time by respectively reducing the interfacial energy and increasing the local stress across the boundary, while impurities strongly influence the time dependent behaviour of the correlation length.

CONCLUSIONS

On the basis of the limited success of the model applied to 316 stainless steel we can draw a number of conclusions as follows:-
 (i) The grain boundary undergoes a phase transition at about $\frac{1}{2}T_m$.
 (ii) At temperatures close to the transition temperature correlated grain boundary decohesion can occur due to large scale stress induced fluctuations.
 (iii) The nucleation mechanism below $\frac{1}{2}T_m$ is qualitatively and quantitatively different from above $\frac{1}{2}T_m$ because of complicated divergences in certain thermodynamic parameters.
 (iv) Extrapolation on a log-log plot can overestimate creep rupture lifetimes.

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REFERENCES

- ASME, (1979). Trans. ASME J. of Eng. Mat. and Tech., 101, No.4. Goldhoff Issue : Materials at elevated temperatures.
- Ashby, M. F. (1977). Proc. ICF4 (1977), Waterloo, Canada.
- Ashby, M. F., and F. Scaepen (1978). Scripta Met., 12, 193-195.
- Binder, K. (1979). (Ed) Monte-Carlo Methods in Statistical Physics., Springer-Verlag, Berlin.
- Boyd, G. A. C. (1980). To be published.
- BSCC (1971). High Temperatur Data, Iron and Steel Institute, 1971.
- Christian, J. W. (1975). The Theory of Transformations in Metals and Alloys., Pergamon Press, Oxford.
- Frost, H. J. and M. F. Ashby (1975). CUED Report. July 1975.
- Glauber, R. (1963). J. Math. Phys., 4, 294-307.
- Hart, E. W. (1968). Scripta Met., 2, 179-182.
- Hart, E. W. (1970). Intergranular Failure. In J.J. Burke and V. (Eds) Ultrafine-Grained Metals., Syracuse Univ. Press, N.Y.
- Hart, E. W. (1971). Grain boundary phase transformations. In H. Hu (Ed) The Nature and Behaviour of Grain Boundary Symposium, Detroit. Met. Soc. of AIME proc.
- Kawasaki, K. (1972). Kinetics of Ising Models. In C. Domb and M. S. Green (Eds) Phase Transitions and Critical Phenomena, Vol 2, Academic Press, New York. pp443-501.
- Ma, S-K, (1976). Modern Theory of Critical Phenomena, W. A. Benjamin Inc., Reading, Mass.
- McCoy, B (1972). Exact Calculations of a Random Ising System, In C. Domb and M. S. Green (Eds) Phase Transitions and Critical Phenomena, Vol 2, Academic Press, New York. pp 161-195.
- McLean, D., B.F. Dyson and D. M. R. Taplin (1977). The Prediction of Creep Fracture in Engineering Alloys. Proc. ICF4 (1977), Canada.
- Penrose, O. (1978). Kinetics of Phase Transitions. In L. Garrido, P. Seglar and P. J. Shepherd (Eds) Stochastic Processes in Nonequilibrium Systems. Proc. Sitges 1978. Springer-Verlag, Berlin, pp 211-234.
- Pfeuty, P. and G. Toulouse (1977). Introduction to the Renormalization Group and Critical Phenomena, J. Wiley & Son.
- Pond, R. C., and V. Vitek (1977a). Proc. R. Soc. (London) A357, 453-470
- Pond, R. C., and V. Vitek (1977b). Idem. 471-483
- Pumphrey, P. H. (1975). Phys. Status Solidi, A28, 545-553.
- Raj, R., and M. F. Ashby (1975). Acta Met., 23, 653-666.
- Raj, R., (1978). Acta Met., 26, 995-1006.
- Smith, D. A., V. Vitek, and R. C. Pond (1977). Acta Met., 25, 475-483.
- Stanley, H. E. (1971). Introduction to Phase Transitions and Critical Phenomena, Clarendon Press, Oxford.
- Wang, Y., T. Ree, T. S. Ree, and H. Eyring (1965). J. Chem. Phys. 42, No. 6, 1926-1930.