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Annual Technical Progress Report I

"Analysis of the Ductile-Brittle Transition

Temperature in Fe-Binary Alloys"

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PROGRAM OBJECTIVES AND SUMMARY

The overall thrust of the program is to understand the fracture and flow mechanisms in Fe-X systems from a fundamental viewpoint. Within this scope, experimental techniques involving the recording of elastic waves emanating from a group of dislocations (acoustic emission) or from a moving crack front (stress waves) are being developed. The first year's program was addressed largely to (1) setting up test facilities, (2) preparing material and test specimens and (3) exploring various approaches to the analysis of discontinuous plasticity and fracture events. In addition several adjunct studies of a combined theoretical and experimental nature, such as a hydrogen embrittlement analysis, were initiated.

In the following report, six sections will be covered. The first three sections, I, II, III, are devoted entirely to the present program with the aim of using the acoustic emission technique as an experimental tool in understanding

- (1) dynamical dislocation processes;
- (2) discontinuous crack growth processes.

Sections IV and V are more theoretically oriented in that a basic understanding of embrittlement processes either due to hydrogen phenomena (IV) or cohesive bond energy considerations (V) is desired. Finally, section VI presents the current experimental status of the program within the context of the original proposal.

Within the first year, we have found that:

- (1) studies of the Portevin Le-Chatelier effect with the acoustic emission technique may lead to establishment of quantitative parameters associated with dislocation dynamics. This could prove invaluable when applying the technique to the study of such processes as low temperature solute softening in BCC alloys.
- (2) the quantitative jump distance of a microcrack process, such as non-propagating cleavage microcracks, may be theoretically analysed in terms of a compliance analysis.
- (3) an experimental comparison involving relationship (2), elastic stress waves and the load drops occurring during crack growth, allows the stress wave technique to follow slow crack growth processes with much greater accuracy than has been previously possible.
- (4) the ductile fracture process can be described in terms of dislocation dynamics.
- (5) the total cohesive bond energy is not the major consideration in establishing the ductile-brittle transition of transition-metal binary alloy systems.

I. Dynamical Dislocation Processes Associated with Acoustic Emission

W. W. Gerberich and G. Martin

I-1 INTRODUCTION

As discussed above, there are at least two levels of acoustic emission, those associated with actual formation of surfaces as in a discontinuous cracking event and those associated with a discontinuous plastic deformation event. If acoustic emission is to be meaningful with respect to interpreting dislocation dynamics, it is best to start with a system that has some degree of understanding. Some^(1,2) have made detailed studies of dislocation events in single crystals of LiF, NaCl, Al and Zn while others^(3,4) have attempted an analysis for more complicated aluminum alloy systems. Although the former are perhaps more amenable to analysis, the later are preferred because their polycrystallinity and the magnitude of their dislocation densities are similar to those anticipated for the Fe-binary studies. The aluminum system is also of interest because its dilute substitutional alloy systems exhibit the Portevin-Le Chatelier effect.

In the following, we will first consider what an acoustic emission event represents and then see how this might apply to dislocation dynamics. During a tensile test of an aluminum alloy at 95db gain, acoustic emission count rates of 10^2 to 10^5 /second might be observed depending upon the strain, strain rate, material condition, etc. We will first discuss the frequency and

energy content of a single event and then address ourselves to the large count rates observed.

I-1-1 Frequency Content

As pointed out by Liptai, et al.,⁽⁵⁾ the frequency content of an event, associated with a slip occurring over a 10^{-3} inch diameter grain, might be about 2 to 20 MHz. This is well beyond the range of commercial transducers. Nevertheless, the 100 - 300 KHz pass-banded transducer we are using has the advantage of eliminating mechanical noise while still picking up the ringdown of the acoustic pulse of interest. In fact, for the relatively large single acoustic emission or stress-waves (SWE) produced by cracking events, a spring-mounted piezoelectric (commercial accelerameter) is adequate. These transducers have a resonant frequency near 30 KHz and can pick up very small events from the background when pass-banded between 3 and 40 KHz.

I-1-2 Energy Content

With respect to acoustic emission sources, probably most important is the energy content of the event. First consider the elastic energy approximation of a slip event. The elastic energy density, w , in a grain undergoing deformation is

$$w = \frac{1}{2} \tau \gamma = \frac{1}{2} G \gamma^2 \quad (1)$$

where τ , γ , G are shear stress, strain and modulus, respectively. If the incremental slip distance is ΔS , then over a grain of length, l , and cross-sectional area, A , the strain would be $\Delta S/l$ and the volume, V , would be lA .

Since the total energy in the event would be the volume of the grain times the energy density, then the total energy change, ΔW , would be

$$\Delta W = Vw = \frac{1}{2}G\left(\frac{\Delta S}{l}\right)^2 lA = \frac{G(\Delta S)^2 A}{2l} \quad (2)$$

One may note that as elasticity breaks down this estimate is not reasonable. Actually, one would have to consider the local energy field about each dislocation and/or dislocation array and obtain the work involved in moving those across the crystal. A simple approach is to consider the virtual work done by moving a dislocation a distance l across the grain which would give

$$\Delta W = N_m \tau b l^2 \quad (3)$$

where N_m = number of dislocations moving a distance l ; τb = force on the dislocations; l = length of dislocation line. Since $N_m b$ would represent the incremental slip, ΔS , and $\gamma = \Delta S/l$ as before, if elastic stresses are assumed as before so that $\tau = G\gamma$, then eq. (3) becomes

$$\Delta W = \Delta S G \gamma l^2 = \frac{G(\Delta S)^2 A}{l} \quad (4)$$

Note that this is the same as eq. (2) except now the energy density is taken as $\tau\gamma$ as would be the case for perfectly plastic deformation. Although these are first approximations, they are reasonable for small strains. For example, in high strength aluminum, steel and titanium alloys, elastic strains of 0.5 to 1% are common so that for a 1% shear strain, which would be mostly elastic, the estimate of eq. (2) would not be seriously in error. Doing this for aluminum

with a spherical grain of 10^{-3} in diameter, a slip step of 10^{-5} in, and a shear modulus of 4×10^6 psi, eq. (2) gives ΔW as 2×10^{-7} in-lb.

One might compare this to what is obtained for a commensurate event associated with fracture. It has been previously shown that a single SWE associated with a single fracture event could be correlated to the change in the elastic strain energy.⁽⁶⁾ This change in strain energy is

$$\Delta U = \frac{K^2 \Delta A}{E} \quad (5)$$

where K is the applied stress intensity factor. It has been shown⁽⁷⁾ that cleavage of mild steel grains about 10^{-3} inches in diameter occur at stress intensity levels on the order of $30,000 \text{ psi-in}^{\frac{1}{2}}$. This, in conjunction with a ΔA of 10^{-6} in^2 and a modulus of 30×10^6 psi gives ΔU as 300×10^{-7} in-lb. Since the amplitude of the acoustic emission is also proportional to ΔA (see section II), it follows that the transducer must be at about 100 times the sensitivity to pick up a plastic deformation event that completely separates the crystal.

Of course, if the energy density increases in the plastic event due to gross number of dislocations moving simultaneously, a larger energy from eq. (3) would be predicted. It is perhaps significant that a plastic event representing 100 percent shear would give an energy that is 100 times that estimated above since it is largely plastic. Thus, it would be of similar magnitude to the energy associated with a fracture event. Such large local plastic strains are probably not likely, but ones approaching 10 percent

deformation, as might occur in the propagation of a Luders band, will be discussed in a subsequent section.

The relevant point for most plastic deformation and fracture processes is that for the evaluation of plastic deformation, the gain of the system must be set about 100 times higher than that for even fairly small fracture events. If during the analysis of a plastic deformation process, very large discontinuous acoustic events are noted, the possibility of microscopic fracture events such as cleavage, intergranular fracture, or the fracture of non-metallic particles such as oxides must be considered.

I-2 APPLICATION TO DISLOCATION DYNAMICS

Next, we will consider what the acoustic emission count rate means in terms of dislocations. A recent investigation on single crystals by James and Carpenter⁽²⁾ would discard the idea of acoustic emission being representative of the mobile dislocation density as had been suggested by others. However, in a recent discussion, Gillis⁽⁸⁾ has suggested that it is only the non-homogeneous dislocations, ρ_m^N , this may be a possibility. For completeness, we will still retain the Gilman concept of mobile dislocations.⁽⁹⁾

Another possibility is the rate of production of new dislocations or the breakaway of dislocations from pinning points.⁽²⁾ Although these are not the same when considering the internal stress state, they are with respect to producing plastic strain. Thus, one might consider the rate of nucleation or the rate of breakaway under the heading of rate of production of moving dislocations. Still another is the rate of nucleation of groups of dislocations.

Gillis⁽⁸⁾ has pointed out that spatially, non-uniform, time-wise discontinuous motion will produce acoustic bursts whose frequency of occurrence will depend on the initiation of motion. Thus, non-homogeneous production of dislocations might be expected to give larger acoustic bursts and one might only consider $d\rho^N/dY$. It would seem then that acoustic emission might represent:

- (1) Mobile dislocation density
- (2) Non-homogeneous dislocation density
- (3) Rate of production of moving dislocations
- (4) Rate of production of non-homogeneous dislocations.

As the Gilman analysis has been shown to represent a good fit to acoustic emission data,⁽³⁾ this will be used as a model. However, it should be emphasized that this model has serious drawbacks and in fact (2), (3), or (4) are probably more likely. These will be dealt with more extensively in the coming year.

I-2-1 The Modified Gilman Model

As the general form of the Gilman model fits acoustic emission data, we will retain the functional form which may be representative of ρ_m , ρ_m^N , $d\rho/dY$ or $d\rho^N/dY$. Although the following discussion uses ρ_m^N , it should be understood that this does not discard the other possibilities. A second modification is that Dunegan and Harris⁽³⁾ and Gerberich and Reuter⁽¹⁰⁾ have observed that an initial plastic strain, ϵ_0 , is required prior to the initiation of large acoustic emission. One might associate this with the utilization of

homogeneous dislocations prior to the necessity of nucleating or moving non-homogeneous groups. Thus, the modified form of the Gilman analysis would be

$$\rho_m^N = M_p (\epsilon_p - \epsilon_o) e^{-\phi(\epsilon_p - \epsilon_o)} \quad (6)$$

Considering a direct proportionality between the dislocation events and the acoustic emission count rate, $\dot{N}$, then

$$\dot{N} = m_p (\epsilon_p - \epsilon_o) e^{-\phi(\epsilon_p - \epsilon_o)} \quad (7)$$

One further consideration is that of a pre-strain, ϵ_{pr} . If this effectively reduces the initiation strain for large acoustic emission, then $\epsilon_{initiation} = \epsilon_o - \epsilon_{pr}$. Thus, for a pre-strained sample, eq. (6) becomes

$$\rho_m^N = \text{const. } \dot{N} = M_p [\epsilon_p - (\epsilon_o - \epsilon_{pr})] e^{-\phi[\epsilon_p - (\epsilon_o - \epsilon_{pr})]} \quad (8)$$

An interesting feature of this is that if $\epsilon_{pr} > \epsilon_o$, then ρ_m^N is predicted to be a continuously decreasing function.

Some preliminary tests have been run on a commercial 1100 aluminum alloy that exhibits both a Portevin-Le Chatelier (P-L) effect and considerable acoustic emission activity. The material was evaluated in three conditions—annealed, pre-strained 2 percent and pre-strained 5 percent. Tensile tests were run in an Instron at a strain rate of $8.3 \times 10^{-4} \text{ sec}^{-1}$. Resulting acoustic emission records in terms of count rate versus plastic strain are given in

Figure 1. As noted in Figure 1A, the annealed sample required a plastic strain

of about 0.025 for a relatively large acoustic emission count rate to begin. If one sets $d\dot{N}/d\epsilon_p = 0$ in eq. (7), ϕ may be evaluated at the maximum count rate, which in the present case occurs at $\epsilon_p \simeq 0.0375$. Thus, $\phi = 1/(\epsilon_p - \epsilon_o) = 80$. Taking the measured value of $\dot{N}$ at this point which is $0.9 \times 10^4 \text{ sec}^{-1}$, then m_p may be calculated from eq. (7) to be 1.96×10^6 . It may be shown that this represents a reasonable fit to Figure 1A.

James and Carpenter⁽²⁾ have found that 10^4 to 10^6 breakaway events may be associated with a single count in single crystals. Gerberich and Reuter⁽¹⁰⁾ surmised that a factor of 10^5 might be a reasonable factor for comparing count rate to dislocation density events. Using the later, one obtains $M_p \simeq 10^5 m_p \simeq 1.96 \times 10^{11} / \text{cm}^2$ which gives a reasonable order of magnitude multiplication factor as compared to other data.⁽⁹⁾

Now, what happens if the material is prestrained? With $\epsilon_{pr} = 0.02$, according to eq. (8), large acoustic emission count rate should commence at a strain of 0.005 which is about right as indicated in Figure 1B. The multiplication factor, m_p , should remain the same at 1.96×10^6 . At the maximum acoustic emission count rate, $\dot{N}$ was 6×10^3 which gives

$$6 \times 10^3 = 1.96 \times 10^6 [\epsilon_p - (\epsilon_o - \epsilon_{pr})] e^{-\phi[\epsilon_p - (\epsilon_o - \epsilon_{pr})]} \quad (9)$$

Having ϵ_o and ϵ_{pr} and the fact that the exponential term is e^{-1} at $\dot{N}_{\text{max}}$, it follows from eq. (9) that ϵ_p at $\dot{N}_{\text{max}}$ is 0.0133 which is very close to the observed value. A further calculation shows that ϕ is 120. Using these values in eq. (8) and assuming the same constancy between m_p and M_p , the

calculated and observed dislocation events are shown in Figure 2. Except for the excursions due to the P-L effect, the observed data are predicted very well. Keeping in mind that all parameters for the pre-strain test were predicted from the annealed test, except for the peak emission count rate, this is a significant result.

Furthermore, one can use the same scheme to predict what happens after 5% pre-strain. As there was no peak emission (since we are not considering the P-L effect here), it is not possible to directly calculate ϕ . As a first approximation, a linear extrapolation of ϕ gives a value of 180 at 5% pre-strain. Using the same value for m_p , as before, gives a calculated $\dot{N}$ which decreases with increasing strains such that $\dot{N} \leq 0.5 \times 10^3$ counts/sec. Since for all plastic strains, the observed value of $\dot{N} \leq 0.2 \times 10^3$ counts/sec, this is probably a reasonable prediction.

One way to interpret these events would be in terms of ρ_m^N . At small strains, after the uniformly moving dislocations are eliminated as plastic strain sources, ρ_m^N increases at ϵ_o . Then, as the stress gets high enough to reactivate uniformly moving dislocations, ρ_m^N decreases. With respect to a pre-strained specimen, if some of the sources for non-homogeneous dislocations are eliminated by plastic deformation, then the magnitude of the peak emission would become less as the pre-strain increased. For example, consider precipitate particles as sources of non-homogeneous dislocations. If one deforms a specimen into the plastic range, then a large number of prismatic loops may be created about the particles to accommodate the gradient of slip. There may also be a bowing out of dislocations between pinning points

to create new dislocations. If the specimen is now unloaded, a reapplication of load to the same strain may not produce an equal number of non-homogeneous dislocations if (a) the work hardening is sufficient to provide dislocation arrays of sufficient strength to cut or fracture particles and/or (b) if an increase in the stress at low strains is sufficient to nucleate cross-slip and thereby pass the barriers.

Similar statements could be made if dp/dY were associated with acoustic emission. Clearly, more extensive evaluations of the acoustic emission data as a function of pre-strain and other testing variables such as strain rate are necessary. These should allow a more quantitative evaluation of what acoustic emission count rate means in terms of dislocation events.

I-2-2 Application to the Portevin-Le Chatelier Effect

In alloys with substitutional or interstitial solid solutions, the P-L effect can occur due to a dislocation-solute pinning, breakaway sequence. Consider the substitutional case which is the mechanism for the aluminum data under discussion. Initially, the dislocation velocity, v_p , is faster than the solute velocity v_s , and dislocations can move freely without any P-L effect. The reason $v_p > v_s$ is that solute velocities near room temperature are low due to the large thermal energy required for diffusion, i.e.,

$$D = D_0 e^{-(q_f + q_m)/kT} \quad (10)$$

where D_0 is the diffusion frequency factor; q_f and q_m are the respective energies for formation and migration of vacancies and kT is as usual.

However, with plastic deformation there is an increase in vacancy concentration, as given by

$$C_V = K\epsilon^m \quad (11)$$

with $K \sim 10^{-4}$ to 10^{-2} and $m \sim 1$ to 1.5 . This eliminates the q_f from eq. (10) and the solute velocity becomes

$$v_s = \frac{4K\epsilon^m D_0 e^{-q_m/kT}}{\ell} \quad (12)$$

where ℓ is the radius of the atmosphere being Ub/kT in size, U being the solute-dislocation binding energy. With increasing plastic deformation, the solute atoms catch up with the moving dislocations and the P-L effect may occur at a critical velocity

$$v_c = v_p = \dot{\epsilon}/\rho_m b = v_s = \frac{4K\epsilon^m D_0 e^{-q_m/kT}}{\ell} \quad (13)$$

assuming a constant strain rate, $\dot{\epsilon}$, test with a density, ρ_m , of mobile dislocations. Most investigators⁽¹¹⁾ are satisfied to write the dislocation density as

$$\rho \approx N\epsilon^\beta \quad (14)$$

where $N \approx 10^{11}/\text{cm}^2$ and $\beta \approx 1$. From eqs. (13) and (14), the critical strain for the initiation of the P-L effect should be

$$\epsilon_c^{m+\beta} \approx \frac{\ell \dot{\epsilon} e^{q_m/kT}}{4bKN D_0} \quad (15)$$

If m is taken as $3/2$, $\beta \approx 1$, $\ell \approx b$, $N \approx 2 \times 10^{11}/\text{cm}^2$, $K \approx 10^{-2}$, $D_0 = 1.3 \text{ cm}^2/\text{sec}$, and $q_m = 0.55 \text{ eV}$, then a strain rate of $8.3 \times 10^{-4} \text{ sec}^{-1}$ at room temperature gives a calculated ϵ_c of 0.038 while the actual value observed was 0.037. These values are similar to those used by Ham⁽¹²⁾ for other annealed substitutional alloy systems.

A similar calculation can be made for the sample with two percent pre-strain. If it is assumed that no vacancies would be lost during the time interval between the pre-strain and the following test, then a calculated value of $\epsilon_c = 0.018$ would result. This compares to an observed value of 0.015 for the onset of the P-L effect. However, this is probably fortuitous to a degree since some time did elapse. Without making further a priori assumptions, the data from the acoustic emission was treated directly as a measure of ρ_m . The velocity of dislocations was then determined from the first relationship in eq. (13) using $\rho_m = 10^5$ count rate from Figure 1B. The velocity of the solute atoms was taken from the second relationship in eq. (13) using a K value that gave a v_s equal to v_p at a plastic strain of 0.02. The calculated values of v_s and v_p as shown in Figure 3, at least qualitatively confirm the type of velocity-breakaway relationship that one would anticipate. Except for a few of the load drops, it is seen that each time the dislocation velocity curve drops below the solute velocity, locking occurs and subsequent load drop follows.

What are the details of this process? One can presume that after the first breakaway the dislocation mobility is greatly enhanced. This allows the average velocity of dislocations to be less to maintain the strain rate. As

the velocity of many drops down to the velocity of the solute atoms, relocking occurs. Then, the remaining unlocked dislocations must increase their velocity and start multiplying to create the formation of another Luder's band and the whole process is reinstituted. If the acoustic emission spikes are relating the true character of the dislocations participating in the P-L effect, then the amplitude of the count rate above background should be meaningful. One can estimate the dislocation density participating in such an event and compare it to the emission peaks associated with the P-L effect. The observation was that a 2 Lb. load drop occurred at 500 Lbs in these specimens. A calculated strain of 2×10^{-4} can be associated with this event. If the volume of material participating in the event is about 1/100 of the sample, this would represent a local strain of 0.02. This strain, occurring in a grain of 10^{-3} inches, gives a mobile dislocation density of $2 \times 10^9/\text{in.}^{-2}$ or about $3.2 \times 10^8/\text{cm}^2$. However, if only 1/100 of the sample is contributing to what is observed over the background, then one might expect an excursion of $3.2 \times 10^6/\text{cm}^2$ to show up during a P-L event. In fact, the actual events implied values of $2.8 - 9 \times 10^7/\text{cm}^2$ which is more than an order of magnitude greater. Nevertheless, such calculations and additional observations, including some microscopy, should allow considerable insight into the dislocation mobility question.

Now, the dislocation mobility approach is not the only one possible. Other interpretations considering $\dot{N}$ as rate of dislocation breakaway or rate of formation of new dislocations might also be used to interpret these initial

findings. The salient point is that such approaches should promise to provide much needed information about dynamical dislocation processes.

I-3 CONCLUSIONS

1. The acoustic emission technique may be applied to dynamical dislocation processes occurring in polycrystalline metal systems.
2. A consistent relationship between the major acoustic emission count rate peak and some dislocation mobility parameter seems to exist.
3. Such effects as pre-strain on dislocation mobility and/or rate of creation or breakaway may also be investigated with the acoustic emission technique.
4. A tentative model analogous to the Gilman analysis fits the data but does not elucidate the mechanism.
5. Secondary peak emission events gave a one-to-one correspondence to the load drops of the Portevin Le-Chatelier (P-L) effect.
6. Dislocation and solute velocity estimates can qualitatively explain all load drops but additional studies must be made to establish the detailed character of the dislocation events.
7. Concurrent analyses of total acoustic emission count rates and the transient events associated with the P-L effect should allow separation of the multiplication, drag and hardening coefficients associated with dislocation dynamics.

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FIGURE 1. ACOUSTIC EMISSION AS A FUNCTION OF STRAIN
FOR THREE CONDITIONS OF 1100 ALUMINUM

FIGURE 2. FIT OF THE MODIFIED GILMAN MODEL TO ρ_m^N INFERRED FROM ACOUSTIC EMISSION DATA

FIGURE 3. COMPARISON OF DISLOCATION AND SOLUTE VELOCITIES ASSOCIATED WITH PORTEVIN-LE CHATELIER EFFECT

II. Analysis of Incremental Cracking by the Acoustic Emission Technique

J. D. Desai and W. W. Gerberich

II-1 INTRODUCTION

Fundamental to the present program is the ability to detect the micro-cracking phenomena that precede final crack instability. In the proposal, it was suggested that the emission of an elastic stress wave from a discontinuous crack growth event could be correlated to a load drop. Furthermore, this load drop may be interpreted via a theoretical compliance analysis in terms of a crack area swept out by the advancing crack. Thus, it was proposed that any discrete stress-wave emission (SWE) associated with the fracture process could be interpreted in terms of an incremental fracture area by⁽¹⁾

$$g \approx \frac{2 \Delta A K^2}{C_1 E L} \quad (1)$$

where g was the amplitude of the emission, ΔA was the area swept out, K was the applied stress intensity, E was the modulus of elasticity, L was the distance between grips, and C_1 was a constant equal to $0.02 \text{ Lb-sec}^2/\text{in.}$ Three problems were found with respect to this derivation and its application.

- (1) Except for three data points, the load drops and corresponding areas associated with the crack jumps and the resulting SWE were

somewhat ambiguous. Furthermore, the pertinent data had only been established at large load drops and, hence, large crack increments.

- (2) There was a transcription error in the derivation of eq. (1) and g should have been proportional to both K and ΔA as was suggested in two previous publications.^(2,3)
- (3) Even if eq. (1) had been correct, it was derived for the infinite plate case while the present study involved a crack-line loaded sample which requires a completely different compliance analysis.

For these reasons, it was first essential to perform an experimental correlation of relatively small discontinuous jumps to small amplitude acoustic emission (SWE). In this way a relationship appropriate to the small discontinuous steps associated with nonpropagating cleavage microcracks could be evolved. Secondly, it was necessary to rederive the compliance analyses for the infinite plate consideration and the specimen of this investigation. These experimental and theoretical studies are discussed in the following two sections.

II-2 EXPERIMENTAL

Crack-line loaded (sometimes referred to as compact tension) specimens of 7075-T6 aluminum were used for the experimental investigation. This specimen type is gaining wide spread use for plane-strain fracture toughness testing (e.g. ASTM E 399). Although some modifications have been made due to material limitations, the design is essentially that shown in

Figure 1. Specimens of about 0.073 inch thickness were fatigue pre-cracked at an applied stress intensity range of $20,000 \text{ psi-in}^{\frac{1}{2}}$ in about 10,000 cycles. This produced approximately 0.1 to 0.2 inches of fatigue crack growth at the end of the notch. The specimens were then tested in a 10,000 pound capacity Instron testing machine at increasing load. The Instron was continuously zero suppressed so that the load range was on maximum sensitivity. In this way, accurate measurement of load drops could be ascertained even at relatively high applied loads.

Besides measuring load drops associated with small and large discontinuous crack extensions, the amplitude of the corresponding single elastic stress wave (SWE) associated with this event was measured. The circuit used to measure SWE amplitude in terms of acceleration, g , is shown in Figure 2. A pass-band frequency range of 3,000 to 40,000 Hz was used to record the SWE since this has been shown to allow reasonable noise suppression and yet allow the minor resonant frequency of the transducer to be recorded.⁽¹⁾ As is shown in Figure 3, the recorded SWE amplitude is linear with the recorded load drop over about two-orders of magnitude of observation. This is essentially identical to what was found before⁽¹⁾ except that the proportionality constant is slightly lower. The important consideration is that for relatively small crack jumps, the proportionality holds. Thus, on the average, this relationship should give meaningful data on the average "micro-load drops" and hence the microcrack extension process.

To obtain experimental verification of the following theoretical analysis, it is also essential to measure the crack steps associated with the larger load

drops and SWE.⁺ This can be accomplished by measuring the displacement at some position behind the crack opening with a gage placed in the knife-edges of Figure 1. The result is that for a relatively constant load, the displacement increases as the crack increases. Calibration of the load-displacement curve as a function of known crack length leads to a reasonably accurate determination of crack length having a measured displacement. The appropriate curve relating non-dimensionalized displacement to non-dimensionalized crack length is given in Figure 4. That is, displacement may be non-dimensionalized by multiplying by thickness, B , modulus, E , and dividing by load, P . As to why this has meaning will be seen under the theoretical discussion. The important point is that for a given crack length or crack length to width ratio, a/W the measured displacement should always be the same for a given specimen configuration and a given load. Conversely, knowing the displacement from a displacement gage, the crack length may be determined from Figure 4.

Now this may be a fairly accurate way of measuring uniform crack extension but its accuracy is limited to several orders of magnitude above what we are attempting for discontinuous crack extensions. Presently, a number of displacements have been measured and are under analysis. The data discussed in the following section, however, are from relatively large "pop-in" crack extensions wherein the large crack length changes were measured directly under a traveling microscope.

⁺ It is not possible to make accurate discontinuous crack jump measurements for small SWE less than about 1 g in amplitude.

II-3 THEORETICAL CONSIDERATIONS

The theoretical derivations will be done in two steps, one for a center-notched plate using an infinite plate approximation and an exact analysis for the specimen configuration of the present investigation.

II-3-1 Center-Notched Plate

The compliance, C_s , of a specimen under tension is given in terms of the plate extension, δ , and load, P , by

$$C_s = \delta/P \quad (2)$$

From load-extension considerations, it follows that the elastic strain energy of the plate is

$$U = \frac{1}{2}P\delta = \frac{1}{2}P^2C_s = \delta^2/2C_s \quad (3)$$

For the fixed-grip condition, the change in the strain energy for an incremental crack extension is given by

$$-\Delta U = \delta^2/2C_{s(a_0)} - \delta^2/2C_{s(a_1)} \quad (4)$$

where a_0 is the crack dimension before extension and a_1 is that afterwards; thus $C_{s(a_0)}$ is the compliance at crack dimension, a_0 . Combining eqs. (2) and (4) gives

$$\begin{aligned}
 -\Delta U &= \frac{[C_s(a_1) - C_s(a_0)]}{2C_s(a_0)C_s(a_1)} \cdot P_0^2 C_s^2(a_0) \\
 &= \left(\frac{\delta}{P_1} - \frac{\delta}{P_0}\right) \frac{\delta/P_0}{\delta/P_1} \cdot \frac{P_0^2}{2} \\
 &= \frac{\delta(P_0 - P_1)}{2} = \frac{\Delta P \delta}{2}
 \end{aligned} \tag{5}$$

The sign is negative since this is elastic energy that is given up as the crack advances. Here, ΔP is simply the load drop associated with incremental crack growth in a specimen being pulled by a very stiff testing machine.

Now, how can equation (5) be related to the strain energy release rate per unit thickness in terms of the applied stress and crack length during any particular increment of growth? Irwin⁽⁵⁾ has shown that strain energy release rate, G , is related to either the stress intensity factor, K , or the stress, σ , and half-crack length, a , by

$$G = K^2/E = \sigma^2 \pi a/E \tag{6}$$

for an infinitely wide plate. In the context of infinitesimal crack extensions, the increment of energy released from (6) can be equated to that in eq. (5).

Taken per unit thickness, B , this becomes

$$\frac{\Delta U}{B} = - \int_{a_0}^{a_1} \frac{\sigma^2 \pi a}{E} da = - \frac{\Delta P \delta}{2B} \tag{7}$$

Given that $\Delta a \ll a$, the approximation used previously⁽²⁾ gives

$$\frac{\pi \sigma^2}{E} [a_1^2 - a_0^2] \simeq \frac{\pi \sigma^2}{E} [2\Delta a a_0] \quad (8)$$

It follows from eqs. (6), (7) and (8) that

$$\Delta P = \frac{2 B \pi \sigma^2}{6 E} [2\Delta a a_0] \quad (9)$$

Writing this in terms of the stress intensity factor and compliance from eqs. (1) and (5), this becomes

$$\Delta P = \frac{2 \sigma K \sqrt{\pi a_0} \cdot 2 \Delta a B}{E P C_s(a_0)} \quad (10)$$

It is seen that if the compliance can be resolved at the beginning of the crack jump, then a direct relationship between ΔP and Δa emerges since all other parameters are known. For center-notched plates of finite-width dimensions, Greenspan⁽⁶⁾ has given the compliance analysis in terms of the specimen length, L , specimen width, W , and other parameters described above by

$$C_s = \frac{L}{W B E} \left[1 + \frac{4 \pi a^2}{W L \left(2 - \left(\frac{2a}{W} \right)^2 - \left(\frac{2a}{W} \right)^4 \right)} \right] \quad (11)$$

For $a \ll W$, this reduces to the term outside the brackets. This in conjunction with replacing load in eq. (10) by σ/BW gives

$$\Delta P \simeq \frac{2 K \sqrt{\pi a_0} \cdot 2 \Delta a B}{L} \quad (12)$$

This result can be utilized by recognizing that $2 \Delta a B$ is an incremental area, ΔA , and the load drop is correlated to the acceleration level as shown in Figure 3. These give

$$g \simeq \frac{2mK\sqrt{\pi a_0} \Delta A}{L} \quad (13)$$

which is essentially identical to the empirical expression utilized previously for assessing stress-corrosion-cracking in titanium base alloys except for a small constant. ⁽³⁾

This analysis is not exact since some of the assessment has been done in terms of the infinite plate solution and several approximations have been made. Nevertheless, as a first approximation for center-notched plates with $a \ll W$ and $\Delta a \ll a$, it is reasonable. It is also useful from a dimensional analysis standpoint as will be seen in the following section where treatment of the specimen type used in the present investigation is considered.

II-3-2 Crack-line-loaded (Compact Tension) Specimens

As was shown in Figure 1, the compact tension specimen that we have chosen for the main body of this investigation is eccentrically loaded and has several boundary conditions. Obviously, an infinite plate analysis is not suitable for describing a load drop in this relatively compliant specimen. However, from eqs. (2) and (7), one can see that if the strain energy release rate and compliance could be written in exact terms, that a viable expression should result for any specimen configuration. The specimen compliance can be determined from the Irwin-Kies ⁽⁷⁾ relationship which is

$$G = \frac{K^2}{E} = \frac{P^2}{2} \frac{dC_s}{da} \quad (14)$$

The stress intensity for the specimen configuration in Figure 1 is given by

$$K = \frac{P(a)^{\frac{1}{2}}}{BW} \cdot Y \quad (15)$$

where⁽⁸⁾ $Y = [29.6 - 185.5(a/W) + 655.7(a/W)^2 - 1017(a/W)^3 + 639(a/W)^4]$

For a plate of thickness, B , it is seen from eqs. (14) and (15) that the compliance is given as

$$C_s = \int \frac{2aY^2}{BW^2E} da + C_0 \quad (16)$$

where C_0 is an integration constant that can be determined from a calibration experiment. Using C_0 determined previously for this specimen configuration,⁽⁴⁾ and the following values for the specimen configuration used gives:

$$\begin{aligned} B &= 0.073 \text{ in;} & W &= 2.50 \text{ in;} \\ E &= 10.5 \times 10^6 \text{ psi;} & C_0 &= 0.40 \times 10^{-4} \text{ in/Lb} \end{aligned}$$

These in conjunction with eqs. (15) and (16) after integration lead to

$$\begin{aligned} C_s &= [0.4 + 11.4(a/W)^2 - 95.5(a/W)^3 + 479(a/W)^4 \\ &\quad - 1585(a/W)^5 + 3690(a/W)^6 - 5880(a/W)^7 \\ &\quad + 6130(a/W)^8 - 3770(a/W)^9 + 1062(a/W)^{10}] \times 10^{-4} \quad (17) \end{aligned}$$

The next step is to put the load drop in terms of compliance. From eqs. (2), (7) and (15), it is seen that

$$\int_{a_0}^{a_1} \frac{P^2 a}{EB^2 W^2} Y^2 da = \frac{P \Delta P C_s}{2B} \quad (18)$$

Noting that the integral is similar to eq. (16), it follows that

$$\Delta P = P \left[\frac{C_s(a_1) - C_s(a_0)}{C_s(a_0)} \right] = P \left[\frac{C_s(a_1)}{C_s(a_0)} - 1 \right] \quad (19)$$

where $C_s(a_1)$ and $C_s(a_0)$ refer to the respective compliances at a_1 and a_0 . Thus, if one can measure a_0 and a_1 at the start and end of the crack step, ΔP can be calculated. Rather than using eq. (17) directly, however, it is simpler to use the dimensionless form as given in Figure 4. This allows calculation of the load drop having the initial value of P and the ratio of the compliances at the start and end of the "pop-in" from Figure 4. This was done for three "pop-ins" and compared to the actual values in Table 1. The calculated values from eq. (19) are seen to compare reasonably well for the first two "pop-ins" but not at all for the third "pop-in".

The main reason for the observed discrepancy is that the above analysis equates the fixed grip situation to the constant load. This, of course, is not quite correct and an appropriate assessment by area would be to equate the energy change for a fixed grip situation to that of constant load minus the energy difference illustrated schematically in Figure 5. That is, as the crack grows and a new compliance is reached, the load path may be that of fixed grip, constant load or some situation in between. First, it is appropriate to demonstrate that this simple area approach is valid. If the above approach is used, the approximate equality of fixed grip to constant

load by areas from Figure 5 gives the energy changes as

$$\frac{1}{2}(P_0 \delta_0 - P_1 \delta_0) \simeq \frac{1}{2}(P_0 \delta_1 - P_0 \delta_0) \quad (20)$$

Since by eq. (2), $\delta_0 = P_0 C_s(a_0)$ and $\delta_1 = P_0 C_s(a_1)$, it is seen that eq. (20) reduces to eq. (19). Now the situation we are evaluating is nearly fixed grip so that we should equate the diagonally marked energy increment by

$$\frac{1}{2}(P_0 \delta_0 - P_1 \delta_0) = \frac{1}{2} P_0 (\delta_1 - \delta_0) - \frac{1}{2} \Delta P (\delta_1 - \delta_0) \quad (21)$$

The term on the left represents fixed grip, the first term on the right represents constant load and the last term represents the cross-hatched area difference in Figure 5. Substituting load-compliance for δ_0 and δ_1 in eq. (21) leads to

$$\Delta P = P_0 \left[\frac{C_s(a_1) - C_s(a_0)}{C_s(a_1)} \right] = P_0 \left[1 - \frac{C_s(a_0)}{C_s(a_1)} \right] \quad (22)$$

It is seen that this is nearly the same as eq. (19) except that the compliance in the denominator is somewhat larger after crack extension. When the more exact eq. (22) is applied to the crack extension observations, use of Figure 4 as before gives the calculated values in Table 1. Here, it is seen that there is an excellent correspondence for the last two "pop-ins". The slight discrepancy in the first value is possibly due to the initially short crack length ($a/W = 0.224$) where the numerical analysis is not particularly accurate.⁽⁸⁾ The significant point is that the load drops can be predicted and that either

the estimated or the exact analysis could be used for short crack extensions. For example, the second load drop is reasonably well predicted by either eq. (19) or eq. (22) since $C_s(a_0) \simeq C_s(a_1)$. In fact these two approaches become indistinguishable for the infinitesimal crack extensions involved with slow crack growth processes or non-propagating cleavage microcracks.

The next question is how this analysis might be used in assessing discrete acoustic emission events (SWE) associated with finite increments of crack extension.

II-4 ACOUSTIC EMISSION ANALYSIS FOR COMPACT TENSION SPECIMEN

II-4-1 Analysis

From Figure 3, the acceleration - ΔP correlation would allow $C_s(a_0)/C_s(a_1)$ to be determined from eq. (22) knowing the applied load, P_0 , at the start of the crack step and the amplitude of the stress wave. Then from the graphical representation of Figure 4, at least large steps could be calculated by taking the difference between $C_s(a_1)$ and $C_s(a_0)$ and determining Δa . However, for small crack extensions, the values must be determined from a computer calculation using eq. (17) in order to obtain any accuracy. For a somewhat more direct means of assessing the g - ΔP correlations, it was decided to curve fit the present compliance analysis to the dimensional form of the infinite plate analysis.

In section II-3-1, it was shown that the compliance could be written as

$$C_s = \frac{L}{WBE} \{ f(a/W) \} \quad (23)$$

where $f(a/W)$ is Greenspan's analysis.⁽⁶⁾ The same form can be fit to the compliance data in Figure 4 and it was found that

$$C_s \approx \frac{L}{WBE} \{0.8(a/W)^{\frac{1}{2}} Y^2\} \quad (24)$$

where Y is given in eq. (15). Now for small crack increments, we can infer from eq. (7) that

$$\frac{K^2}{E} \Delta a \approx \frac{P}{2B} \Delta P C_s \quad (25)$$

Writing P in terms of K from eq. (15) and using eq. (22) for C_s , this reduces to

$$\Delta P \approx \frac{2.5 K W^{\frac{1}{2}} B \Delta a}{Y L} \quad (26)$$

One can see this is dimensionally correct since K has $\text{psi-in}^{\frac{1}{2}}$ units and Y is dimensionless. Eq. (24) reproduces the exact calculated values in Table 1 to within about 10 percent. For use with the stress-wave emission data, it is recognized that $B \Delta a$ is the area swept out by the crack and ΔP can be related to the g amplitude in Figure 3. Applying these to eq. (26) gives

$$g \approx \frac{2.5 m K \sqrt{W} \Delta A}{L} \quad (27)$$

It is seen that this is very similar to the previous eq. (13) in that the stress wave amplitude is proportional to both stress intensity and incremental area swept out by the crack. As indicated in Table 1, this gives reasonable prediction of the actual SWE amplitudes observed.

II-4-2 Application to SWE data

It was of some use to verify the validity of eq. (27) using some previous observations of cleavage microcracking in plain carbon steels.⁽¹⁾ In particular, a 1020 steel with a fine pearlitic-ferritic structure was tested to failure at 77°K. The fracture surface, as observed by scanning electron microscopy, was seen to consist of a series of cleavage microcracks, some of which had occurred prior to the onset of fracture instability. It was previously surmised that the SWE observed up to the point of instability were associated with non-propagating cleavage microcracks. These SWE ranged from 0.002 to 0.05 g in amplitude and were considered to represent a crack jump associated with one incremental area traversing one grain. As the approximate (but nevertheless incorrect) analysis gave calculated values of 0.0015 to 0.021 g, this was reported as affirmative verification that one SWE represented one grain cleaving.

As the present investigation will derive much of its information from the ability to detect and accurately assess the character of these microcracks, it was of interest to see if the exact analysis corroborated the previous findings. The appropriate values for the specimen type used and the test data observed are:

$$K = 40,000 \text{ psi-in}^{\frac{1}{2}}, \quad Y(a/W) = 11.7$$

$$a = 0.7 \text{ in}; \quad W = 1.875 \text{ in}; \quad L = 1.25 \text{ in}$$

grain size ranging from 0.00067 in to 0.0025 in diameter

$$\Delta A \approx 0.35 \text{ to } 4.8 \times 10^{-6} \text{ in}^2$$

Using these values in eq. (27) leads to calculated values of 0.0025 to 0.036 g which are very close to the observed values of 0.002 to 0.05 g. Because of this good correlation with the exact analysis, the present approach can be used with some confidence in assessing the character of microcracking associated with the brittle fracture of Fe-base ferritic alloys.

II-5 CONCLUSIONS

1. Theoretical relationships have been derived between load drops and crack growth steps in several types of fracture mechanics test specimens.
2. Experimental observations have verified that the magnitude of a load drop, ΔP , associated with a crack jump, is linearly related to the amplitude of the resultant stress wave (SWE). For the specimen type studied, the relationship is that the acceleration amplitude is $g = m\Delta P$ with m about 0.7 in/Lb-sec^2 .
3. These two important results lead to the general conclusion that the SWE amplitude is related linearly to the applied stress intensity level, K , and the area swept out by the extending crack in any jump, ΔA .
4. Preliminary data show that SWE analyses can predict both large crack jumps on the order of 0.3 inches in length as well as small crack areas on the order of 10^{-6} in^2 , the later being associated with cleavage microcracks.
5. The range of applicability seems to extend over 5 orders of magnitude with respect to SWE amplitude observations.

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TABLE II-1

OBSERVATIONS							CALCULATIONS		
P_o	a_o	a_1	$C_s(a_o)$	$C_s(a_1)$	ΔP	g	ΔP	ΔP	g
LBS	IN	IN	Fig 4	Fig 4	LBS	in/sec ²	eq. (19)	eq. (22)	eq. (27)
820	0.56	0.86	22.6	31.0	267	179	304	222	163
605	0.86	0.96	31.0	34.9	68	85	74.5	67	53
562	0.96	1.27	34.9	57.0	208	152	354	218	162

FIGURE 1. COMPACT TENSION SPECIMEN

FIGURE 2. SET UP FOR RECORDING LARGE ELASTIC STRESS WAVES

FIGURE 3. RELATIONSHIP BETWEEN STRESS WAVE AMPLITUDE AND LOAD DROP

FIGURE 4. DIMENSIONLESS COMPLIANCE AS A FUNCTION OF CRACK LENGTH

FIGURE 5. EFFECT OF SMALL CRACK EXTENSION ON ENERGY RELEASE FOLLOWING FIXED GRIP OR CONSTANT LOAD PATHS

III. A Ductile-Fracture Instability Model Based Upon Production of Geometrically-Necessary Dislocations

W. W. Gerberich and W. Reuter

III-1 INTRODUCTION

Of late, increasing evidence points towards deformation about second phase particles as being the controlling mechanism in the ductile fracture of high strength materials. The present study was an attempt to correlate the dislocation dynamics of a tensile bar to the discontinuous crack propagation in a fracture toughness test.

III-2 EXPERIMENTAL TECHNIQUES AND RESULTS

An acoustic emission technique⁽¹⁾ recorded the low amplitude dislocation events associated with plastic flow in tensile specimens. In another set of tests, a stress-wave emission device⁽²⁾ recorded large-amplitude cracking events in 6-inch wide center-cracked plates. The material was $\frac{1}{4}$ -inch thick 7075 aluminum aged to four conditions.

From engineering and true stress-strain plots, the data for the first four columns of Table I were obtained. The acoustic emission data were found to be described by

$$\dot{N} = m_p \epsilon_p e^{-\phi \epsilon_p} \quad (1)$$

where $\dot{N}$ is the number of counts per second; m_p' and ϕ are constants; and ϵ_p is the true plastic strain. Such a plot is shown in Figure 1 for the peak-aged condition. Since $d\dot{N}/d\epsilon_p = 0$ in eq. (1) gives $\epsilon_p = 1/\phi$, ϕ is obtained directly from the peak of the $\dot{N} - \epsilon_p$ plot and m_p' is adjusted to give the best fit to the downward slope of the curve.

From eight large plate fracture tests, 12 sets of data were obtained representing fracture instabilities. About half of these were large shear instabilities in the as-quenched samples which could be directly measured. These were associated with stress intensity levels ranging from 66,400 to 102,500 $\text{psi-in}^{\frac{1}{2}}$. From the other conditions, measures of the average length of crack jump, ℓ_{OBS} , were determined from the macroscopic growth increment divided by the number of stress waves, N_{SWE} , occurring in the increment. These were associated with stress intensity levels ranging from 37,000 to 75,000 $\text{psi-in}^{\frac{1}{2}}$. The results, as given in terms of the average ℓ_{OBS} for each condition correlated with both n and ϕ , the result for ϕ being shown in Figure 2.

III-3 THEORETICAL INTERPRETATIONS

First, what does the acoustic emission data represent? One may consider two classes of interpretations, one where $\dot{N}$ represents mobile dislocation density and one where it represents rate of occurrence of dislocation events. For the first class, one might consider dislocation dynamics in the Gilman sense⁽³⁾ or for precipitation-hardening systems, Ashby's⁽⁴⁾ work-hardening model. If one considers ρ_{mD} as being the number of mobile dislocations being detected by the transducer, then one can show that as the

dislocation spacing decreases, at some point ρ_{mD} would decrease.

Interpreting this in terms of Ashby's model and invoking an effective particle radius, then $r_{eff} = r \exp(\phi \epsilon_p)$ and a modified Ashby model would give

$$\rho_{mD} \approx \frac{2f}{br} \epsilon_p^{-\phi \epsilon_p} \quad (2)$$

One might note that this is identical to the Gilman model with ϕ being a work-hardening parameter and $2f/br$ being the breeding factor as given in terms of volume fraction, f , particle radius, r , and Burgers vector, b . Each acoustic emission count rate pulse has been suggested⁽⁵⁾ to be made up of $10^5 - 10^6$ breakaway dislocation events. In a similar vein, one can use $10^5 m_p$ to give the right order of magnitude breeding factor. If one does this in Table 1 and independently calculates $2f/br$ where the parameters are approximately known, one finds a reasonable comparison between the last two columns in Table 1.

For the second class, one can interpret N as the rate of dislocation breakaway⁽⁵⁾ or, in the present case, the rate of production of geometrically necessary dislocations. Physically, $d\rho^G/d\epsilon_p$ could decrease to some small value when particle decohesion, shear or fracture started. Keeping the same functional form as above, then

$$\frac{d\rho^G}{d\epsilon_p} = \frac{\alpha 2f}{br} \epsilon_p^{-\phi \epsilon_p} \quad (3)$$

where α is some constant on the order of 10^3 to 10^4 . If one integrates eq. (3),

then a continuously increasing value of ρ^G with strain is found. In any event, considering the recent literature^(2,5), one may conclude that one of these approaches represents the likely source for the acoustic emission. At this point it is of value to consider possible fracture models.

Krafft⁽⁶⁾ suggested that fracture proceeded in a process zone, d_T , close to the crack tip when the strain reached a critical value, ϵ_{CR} . For a plane strain situation where Poisson's ratio is 0.3, using the conditions $\sigma_y, \sigma_x = \sigma_y$ and $\sigma_z = 2\nu\sigma_y$ leads to

$$K = \epsilon_{CR} E [8\pi d_T]^{1/2} \quad (4)$$

where K is the applied stress intensity and E is Young's modulus. Krafft suggested that ϵ_{CR} is the strain associated with a macroscopic tensile instability. However, the stress-strain relationship is also a function of dislocation density. Thus, if one considers local plastic instability between particles, then one could use the criterion that $d\rho_{mD}/d\epsilon_p = 0$. From eq. (2) this occurs at $\epsilon_{CR} = 1/\phi$ so that the Krafft criterion becomes

$$d_T = \frac{1}{8\pi} \left(\frac{K\phi}{E} \right)^2 \quad (5)$$

For the high stress intensity levels where conditions are not plane strain, eq. (5) is about two orders of magnitude too high. However, if one considers just the relatively plane strain cases, then for $K \sim 40,000 \text{ psi-in}^{1/2}$ and $\phi \sim 80$, d_T is calculated to be 0.004 in. while the observed values ranged from 0.001 to 0.004 in.

For the second model, a strain distribution based upon the tensile analogy of the elastic-plastic Mode III situation is used to define the total region in the vicinity of the particle where the fracture strain is exceeded. In this case, the condition for fracture could be that the rate of production of geometrically-necessary dislocations drops to some low value as described above. As a first approximation, let $d\rho^G/d\varepsilon_p \rightarrow \alpha\varepsilon_p$, and take the log of eq. (3) which gives $\varepsilon_p = \ln(2f/br)\phi^{-1}$. If, as the final event of microvoid coalescence, this strain is that leading to fracture, the insertion into the strain distribution gives a fractured region, l^* , of

$$l^* = \frac{\phi K^2}{3\pi\sigma_{ys} E \ln(2f/br)} \quad (6)$$

It might be pointed out that even if the estimate of $d\rho^G/d\varepsilon_p$ is off by several orders of magnitude, this only makes a factor of two difference in the estimate of l^* . Using the observed values of ϕ , K , σ_{ys} , E and the value of $10^5 m_p^{-1}$ for $2f/br$, the theoretical fit of eq. (6) to the observed crack jumps is seen in Figure 3.

In summary, it can be said that both fracture models give the right trend to the data with the latter being more accurate. However, absolute magnitudes mean relatively little here because of the approximate nature of several of the assumptions. Since ϕ is also a function of the particle characteristics, it is not possible to further differentiate between these two approaches without additional study.

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Table 1: Flow Parameters for 7075 Aluminum Alloy

Condition	σ_{ys} 1000 psi	σ_{ULT} 1000 psi	n	ϕ	$10^5 m_p$ $10^{11}/cm^2$	$2f/br^+$ $10^{11}/cm^2$
As	22.1	58.9	0.213	1820	258	140
Quenched	22.5	57.6	0.231	940	208	140
Aged 250°F	62.0	76.7	0.080	50.5	0.58	---
4 hr.	59.8	83.5	0.087	---	---	---
Aged	73.0	83.5	0.064	81.3	0.77	2.8
T6	72.0	83.3	0.057	81.3	1.55	2.8
T6 + Aged	56.1	69.3	0.072	102	1.95	---
350°F, 12 hr.	57.2	70.2	0.070	---	---	---

+ For as-quenched: $b = 2.96\text{\AA}$; $f \approx 0.05$; $r \approx 25\text{\AA}$ for G.P. zones

For T6: $b = 2.86\text{\AA}$; center-to-center spacing of $2000\text{\AA}$; $r = 500\text{\AA}$;
 $f \approx 0.02$. Based upon E-phase ($Cr_2Mg_3Al_{18}$) on fracture surface.

Fig. 1: Acoustic Emission Count Rate From Tensile Test.

Fig. 2: Crack Jumps Versus Dislocation Parameter From Tensile Tests.

Fig. 3: Actual Crack Jumps Compare To Calculations From Fracture Model.

IV. Stress-Gradient Effects on Hydrogen Phenomena

Y. T. Chen and W. W. Gerberich

IV-1 INTRODUCTION

Because of the general interest in the area of stress-corrosion cracking and hydrogen embrittlement, as associated with the power industry, it was decided that some emphasis should be placed upon such areas. Two other circumstances led to this decision, in concurrence with the technical project monitor: (a) previous success⁽¹⁾ had been obtained using the acoustic emission technique to analyse the step-wise time dependent growth processes; and (b) initial work with C. St. John at Berkeley⁽²⁾ had led to some fundamental questions concerning the exact effect of stress gradients on the long range diffusivity of absorbed gases, particularly hydrogen. This is of primary importance, whether one is considering the Zircalloy cladding of fuel elements, the stainless steel tubing in water-cooled reactors or the refractory metals proposed for fusion reactors.

IV-2 THEORETICAL

There have been several recent papers associated with hydrogen effects in a stress gradient.^(2,3,4) However, none of these have dealt with the plastic problem as must be occurring in a real material that is undergoing hydrogen cracking. Now, the sharper the crack is, the closer the region of

high triaxiality is to the crack tip. Nevertheless, it is probably impossible to avoid being in the plastic region at the incipient fracture point except in the most brittle of materials. Since the stress and strain gradients in elastic and plastic regions are of completely different character, it is of necessity to see if these gradients can be analysed.

The importance of establishing these gradients is that the flux equation is governed by the pressure gradient, dP/dx . For a uniform concentration, C , of hydrogen, the governing equation is

$$J = Cv = -\frac{DC}{kT} \nabla U \quad (1)$$

where ∇U is the gradient of the interaction energy, and D is the diffusivity of hydrogen. Since $\nabla U = -\Delta \bar{V}_H dP/dx$, where $\Delta \bar{V}_H$ is the partial molar volume of hydrogen, eq. (1) allows calculation of the velocity from

$$v = \frac{D}{kT} \bar{V}_H \frac{dP}{dx} \quad (2)$$

for the short time approximation.

It is possible to write the pressure tensor, P ,^(2,3) for the elastic fields although modifications should be included for any crack-tip radius changes due to plastic deformation. The plastic stress gradients are not so simple. A modified Hill⁽⁵⁾ analysis might be applicable if the crack tip radius blunts sufficiently with plastic deformation. There will be an experimental attempt to model this effect since initial results indicate that the crack tip radius can be represented in terms of

$$\rho = f(K, \sigma_{ys}, \epsilon, d, E) \quad (3)$$

where K is the stress intensity, σ_{ys} is the yield strength, ϵ is the crack tip strain, d is a microstructural parameter, and E is the modulus of elasticity. A preliminary treatment of the maximum principal stress gave the stresses and gradient in the elastic and plastic regions shown in Figure 1. Since the gradients are similar to the pressure gradients, it is possible to analyse the character of the resulting concentration gradient. For dP/dx negative in the elastic region, the velocity is in the negative direction and the interstitial is diffusing toward the crack tip. For dP/dx positive in the plastic region, the interstitial is diffusing away from the crack tip towards the region of high triaxiality. Thus, near some region where the σ_{yy} stress is maximum, it will also happen that the maximum concentration of hydrogen is achieved. A description of $\sigma_{yy\max}$ and $C_{\max}$ should allow analysis of current hydrogen embrittlement theories. Models based upon eqs. (2) and (3) are currently being computerized using dP/dx , $C_{\max}$, the incipient fracture point and the crack jump distance as variables.

One analytical approximation assumes that the pressure gradient driving the hydrogen is approximately the same in both elastic and plastic regions. Consider Figure 1 with the pressure gradient being approximated by $d\sigma_{yy}/dx$. From eq. (2), it is seen that the greater the gradient, the faster hydrogen travels. Since $d\sigma_{yy}/dx$ increases from the fracture site toward the crack tip in the plastic region, then the gradient at the fracture point underestimates the average value within the plastic zone. This may be expressed as

$$\left. \frac{d\sigma_{yy}}{dx} \right|_{x_{CR}}^{pl} < \overline{\frac{d\sigma_{yy}}{dx}}^{pl}$$

where the pl stands for the plastic region. In the opposite sense, however, $d\sigma_{yy}/dx$ decreases from the fracture site into the elastic region so that the gradient at the fracture site overestimates the average value within the elastic region, el , or

$$\left. \frac{d\sigma_{yy}}{dx} \right|_{x_{CR}}^{el} > \overline{\frac{d\sigma_{yy}}{dx}}^{el}$$

These two results are fortuitous in that, if the elastic and plastic stress gradients are similar in magnitude, then a good first approximation of the average gradient contribution to the hydrogen sink is

$$\left. \frac{d\sigma_{yy}}{dx} \right|_{ave} \simeq \frac{1}{2} \left[\left. \frac{d\sigma_{yy}}{dx} \right|_{x_{CR}}^{el} + \left. \frac{d\sigma_{yy}}{dx} \right|_{x_{CR}}^{pl} \right] \quad (4)$$

In Figure 1, for example, the average gradient is 0.8×10^8 psi/in while that given by eq. (4) is 0.88×10^8 psi/in. This type of approximation for the pressure tensors and associated gradients will be made and compared to numerical solutions.

This type of first approximation was assumed for the pressure gradient. In addition, if one assumes that the crack jump is related to the stress intensity factor as was originally observed by Gerberich and Hartbower,⁽¹⁾ then the crack growth rate becomes

$$da/dt = 2.5 \left(\frac{C_o}{C_{CR} - C_o} \right) \frac{K D \bar{V}_H \sigma_{ys}}{\pi E \epsilon_f k T d \sqrt{2 \pi d}} \quad (5)$$

where C_{CR} is the critical hydrogen concentration for incipient cracking and C_o is the initial uniform concentration. Details of the model will not be presented at this time but will be the subject of a forthcoming paper. (6)

If a concentration gradient is initially present, as in the case of hydrogen gas being adsorbed at the crack tip from an atmosphere, then the analysis changes. Here, the flux equation would be

$$J = -D \left(\nabla C + \frac{C \nabla U}{kT} \right) \quad (6)$$

This can also be solved numerically, once the elastic and plastic gradients have been solved. The initial emphasis, however, will be on the experimental verification of gradients and crack growth rates associated with an initially uniform concentration of hydrogen.

IV-3 EXPERIMENTAL

The initial material to be evaluated is AISI 4340 since this is a typical high strength steel that has been shown to be susceptible to hydrogen embrittlement and stress corrosion cracking. Five tempered conditions from 200°C to 550°C have resulted in hardness levels ranging from 52 R_C down to 40 R_C or an ultimate strength range of about 270,000 psi down to 200,000 psi. This variation in strength level will give us a means to establish the effect of degree of plane strain. That is, at the same stress intensity level,

$(K/\sigma_{ys})^2$ will vary by a factor of two over the tempering range considered.

As the stress tensor varies considerably between plane stress and plane strain, the effect on the pressure gradient and the concomitant embrittlement process should be considerable. This is not completely unambiguous, however, because the microstructure varies with the strength level. Thus, various thicknesses will also be evaluated, ranging from 0.15 inches to 0.75 inches, representing a wide range of states of stress. These two sets of data will allow separation of the relative effects of yield strength, microstructure, stress intensity and state of stress on the susceptibility to hydrogen embrittlement.

For all tests, crack-line-loaded samples similar to the one shown in Section II have been prepared. About 40 of these fracture mechanics test coupons have been prepared, pre-fatigue cracked and tempered. Several trial specimens have been evaluated with a hydrogen charging procedure, to obtain uniform concentrations of hydrogen. These have produced rapid slow crack growth at stress intensities as low as $25 \text{ ksi-in}^{\frac{1}{2}}$. However, the crack growth shape was slightly accelerated towards the outside surfaces as compared to the center of the specimen thickness. This meant that a hydrogen gradient existed, being more concentrated at the surfaces. This is not surprising for the $3/4$ inch thick specimens charged, since the time and temperature of charging was barely sufficient to allow diffusion of hydrogen half way through the specimen. For this reason, subsequent tests will involve cadmium plating and baking after hydrogenation to ensure as uniform a concentration as possible. Other trial tests have documented that the

acoustic emission technique and tape-recording system for analysing time-dependent, slow-crack growth is in order.

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FIGURE 1. STRESSES AND STRESS GRADIENTS IN THE ELASTIC-PLASTIC REGIONS AT THE TIP OF A CRACK

V. Correlation of Atomic Structure and Cohesive Energy with Changes in Ductile-Brittle Transition Temperature

D. G. Atteridge

V-1 INTRODUCTION

It has been suggested recently that a given alloying element will decrease the ductile-brittle transition temperature (TT) if it has a higher cohesive energy than the bcc metal to which it is added.⁽¹⁾ Those elements with cohesive energies less than that of the given bcc metal, when added as alloying elements, are assumed to increase the TT. A possible relationship between electronic structure and cohesive energy for the transition elements has also been mentioned in the literature; it is that the cohesive energy increases as the number of valence electrons increases.⁽¹⁾

With the advent of the Engel-Brewer Correlation (EBC) between solid state crystal structures and s,p valence electrons per atom (e/a) concentrations it is now possible to theoretically calculate the solid state cohesive energies for the transition metals. It is therefore possible to determine if, indeed, the cohesive energies of alloying elements can be correlated with changes in TT.

V-2 COHESIVE ENERGY CORRELATION

The EBC sets relatively fixed s,p e/a concentration limits for each crystal structure, and has been shown to be surprisingly successful in

predicting both the correct sequence of phase changes in a given alloying system and the approximate composition stability ranges of the phases.⁽²⁾

The phase stability proceeds from bcc to hcp to fcc as the number of s,p e/a increases; the predicted phase stability ranges as a function of s,p e/a are given below.

<u>Phase</u>	<u>Composition Range (s,p e/a)</u>
bcc	1.0 - 1.5
hcp	1.7 - 2.2
fcc	2.5 - 3.0

The simplified integer approximations of 1 s,p e/a for bcc, 2 s,p e/a for hcp, and 3 s,p e/a for fcc will be used in the calculations for cohesive energy presented in this report.

Once one has decided to use the integer s,p e/a approximations one can immediately determine the solid state electronic configurations for the transition elements exhibiting only one solid state crystal structure; the given crystal structure determines the number of s,p e/a, and the rest of the valence electrons are therefore d shell electrons. The structure used for the elements exhibiting allotropic phase transformations was the structure predicted to be stable in dilute solution with the given bcc metal. This was determined through the use of the phase stability rules, for elements exhibiting allotropy, pointed out in the explanation of the application of the EBC.⁽²⁾

The cohesive energies for the various transition elements can be calculated, after the electronic structures are determined, through the use of the graphs of cohesive energy per bonding electron given by Brewer.⁽³⁾

These graphs present the cohesive energy per valence electron as a function of electron type and shell number designation.

A plot of the cohesive energy per s,p electron as a function of shell number and element is given in Figure 1. The cohesive energy attributed to the d electrons is also plotted in Figure 1 as a function of shell number, and both the total number of d shell e/a and the number of bonding d shell e/a. The determination of the number of bonding d e/a is made from the fact that the d shell can accommodate only 10 electrons, and that once it is half full the added electrons must form non-bonding pairs. The formulas for calculating the number of bonding d e/a is given below.

For the total number of d e/a ≤ 5 ,

$$\text{No. of bonding d e/a} = \text{total No. of d e/a.}$$

For the total number of d e/a > 5 ,

$$\text{No. of bonding d e/a} = 10 - \text{total no. of d e/a.}$$

These graphs were used to calculate the cohesive energies of the elements whose effect upon the TT of bcc Fe, Cr, Ta and Nb was reported in the proposal for this study. The results were then plotted, Figures 2 and 3, as a function of the effect of the element on the respective TT. These results show that the change in TT is not a direct function of the change in cohesive energy upon alloying. Both elements decreasing and increasing the TT are found to exhibit larger cohesive energies than the matrix metals. It is also evident that the increase in cohesive energy is not a function of the increase in total valence electrons, as Fe and Cr are in the middle of the Periodic

Table and elements on either side of them exhibit cohesive energies of much larger magnitudes.

This lack of direct correlation between TT and cohesive energy is not too surprising if one assumes that the observed TT in bcc metals is due to the large covalent character of their bonds. It is well known that the relatively open bcc structure would transform spontaneously into one of the close packed structures if it were not stabilized by strong directional bonds between atoms.^(4,5) As dislocation induced slip requires "bending" of atomic bonds as the dislocation travels down the slip plane, it is postulated that the strong directionality of the bcc bonds makes slip increasingly difficult as the temperature is decreased. This would be due to an increase in the applied energy required to "bend" bonds as the thermal vibration component decreased. This effect would be similar to that found in Si, where one is able to propagate dislocations in a covalent material at sufficiently high temperature where the thermal vibrations of atoms becomes significant.⁽⁶⁾

Strong directional bonding is not found in either the hcp or fcc metals, as evidenced by their lack of strong temperature dependence of yield strength upon test temperature as found in bcc metals. Their close packed structure also indicates their lack of directional bonds, as this is the maximum packing density one can achieve with spherically symmetrical balls. In addition, most of these metals do not exhibit a TT.

This reasoning leads to the assumption that the over-riding consideration in determining the effect of a given substitutional alloying element on dislocation mobility would be the amount of covalent bond character it exhibited.

The cohesive energy would be a secondary consideration, if it is assumed that the ability of a given atom to retain its innate bonding characteristics in a foreign environment increased as its cohesive energy increased.

It is not expected that all changes in TT can be explained as a function of alloying element crystal structure and cohesive energy. Other effects such as size difference, solubility, microstructural changes, reactions with impurities and segregation to grain boundaries certainly effect the TT as well as the purely solid solution effect. However, an attempt at an empirical correlation between electronic structure and cohesive energy and the change in TT has been made and is presented below.

V-3 PROPOSED ELECTRONIC STRUCTURE FACTOR

If the atomic bond structure and characteristics are dependent upon the number of s, p e/a , as the EBC states, and alloying elements in dilute solution essentially exhibit their pure metal bonding characteristics, one can hypothesize a model for decreasing the TT as one adds hcp or fcc alloying elements to bcc metals. This decrease in TT is postulated to be due to a localized region around the alloying atom having its directional bonding characteristics reduced due to the localized increase in the number of s, p e/a associated with the alloying element. If this is so, one can assume as a first approximation that the size of the localized region affected would be related to the number of s, p e/a associated with the alloying element and available for interaction with the bcc matrix atoms. This model predicts

that fcc metals, with 3 s,p e/a, would be more effective in lowering the TT than hcp metals, with 2 s,p e/a, as is seen in the data presented in this study's proposal.

The assumption is also made that two secondary effects are important. The first is that the cohesive energy of the given alloying element is, as mentioned above, expected to increase the retention of the bond characteristics of a given bond configuration as the cohesive energy increases. This quantity is entered into the calculation as a normalized cohesive energy ratio; the cohesive energy ration, R_{CE} , is normalized for each structure and each Group in the Periodic Table. This is done by dividing the cohesive energy for a given element in a given structure by the cohesive energy of the element in Period IV in the same Group and with the same electronic configuration; this procedure was used as the cohesive energy was found to increase as the Period number increased.

The other factor deemed to be important is the change in the relative number of valence s,p e/a to bonding d e/a between the alloying element and the bcc matrix element; this relative number of electrons, R_e , is expressed as a ratio of s,p e/a to bonding d e/a for a given atom in a given crystal structure. The basic ratio is introduced due to d electrons exhibiting essentially directional short range bonding and not directly influencing the long range bonding characteristics.^(7,8) It is postulated that the higher the ratio of s,p e/a to bonding d e/a an element has the more effective the increase in cohesive energy will be in increasing dislocation mobility. The difference between the R_e of the alloying element and that of the given matrix

element is assumed to be proportional to the effectiveness of the given element in a given electronic configuration in decreasing the TT.

All the various stability factors mentioned above were then combined into an electronic structure factor, e_F , given below.

$$e_F = S^A (R_e^A - R_e^M) (R_{CE}^A)^3$$

e_F = electronic structure factor

S^A = # of s, p e/a for alloying element

R_e^A = alloying element electronic ratio

R_e^M = matrix element electronic ratio

R_{CE}^A = alloying element cohesive energy ratio

This electronic structure factor was then plotted in figure 4 versus the experimental data for Fe and Cr of the decrease in TT per atomic percent of alloying element as given in the background section of the proposal for this study. The values of the factors used in the calculation of e_F are given in Table 1.

The approximately linear correlation found between an increase in the electronic structure factor and a decrease in TT, as a function of alloying element, indicates that the solid solution effects of alloying additions may well be explained as a direct function of solid state electronic configurations.

V-4. CONCLUSIONS

A TT model was proposed, based upon the change in electronic configuration of alloying elements as a function of crystal structure. A first-approximation electronic structure factor was developed as a function of the

alloying element's crystal structure, its relative change in electronic configuration as compared to that of the bcc matrix element, and its cohesive energy. The magnitude of this electronic structure factor was found to relate to the magnitude of the decrease in TT caused by a given alloying element in a given bcc matrix.

Prior to this, we compared alloy element cohesive energy, as calculated through the use of the EBC, with the element's effect upon the TT of a given bcc matrix. The results demonstrated that there was no direct relationship between the element's cohesive energy and its effect on the TT. It was also found that the cohesive energy did not increase with the total number of valence electrons.

These results indicate that the change in localized electronic structure in a bcc matrix due to the addition of alloying elements is a more important factor in understanding property changes due to the addition of alloying than alloy element cohesive energy. In fact this type of change may be the controlling factor for changes in TT in substitutional solid solution alloys.

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Table V-1 Factors Used In The Calculation Of e_F

Element	Structure	#s, p e/a	R_e	Cohesive Energy	R_{CE}
Ag	fcc	3	3/2	246	1.04
Cu	fcc	3	3/2	237	---
Pt	fcc	3	1	296	1.25
Ni	fcc	3	1	237	1.00
Ir	fcc	3	3/4	314	1.40
Rh	fcc	3	3/4	272	1.21
Co ¹	fcc	3	3/4	225	1.00
Fe ¹	fcc	3	3/5	191	1.00
Os	hcp	2	1/2	255	1.90
Ru	hcp	2	1/2	216	1.61
Fe	hcp	2	1/2	134	---
Re	hcp	2	2/5	259	1.96
Mn ¹	hcp	2	2/5	132	1.00
Fe	bcc	1	1/3	114	---
Cr	bcc	1	1/5	75	---

1. Allotropic form predicted to be stable in dilute solution with bcc Cr

Note: R_{CE} values only given for elements plotted in Figure 4

FIGURE 1. COHESIVE ENERGY AS A FUNCTION OF ELECTRONIC STRUCTURE

FIGURE 2. COHESIVE ENERGY OF ALLOYING ELEMENT VERSUS EFFECT OF ELEMENT ON THE TT OF bcc Fe AND Cr

FIGURE 3. COHESIVE ENERGY OF ALLOYING ELEMENT VERSUS EFFECT OF ELEMENT ON THE TT OF bcc Nb AND Ta

FIGURE 4. RELATIONSHIP OF e_F TO DECREASE IN TT

VI. Experimental Alloy Test Program

D. G. Atteridge and W. W. Gerberich

VI-1 INTRODUCTION

The alloys to be investigated in the test program consist of three bcc binary alloys of iron plus a "pure" iron control alloy. The compositions of the alloys in this study are listed below:

Fe-1 at. % Ni	Fe-1 at. % Si	Fe-1 at. % Pt
Fe-2.5 at. % Ni	Fe-2.5 at. % Si	Fe-2.5 at. % Pt
Fe-4 at. % Ni	Fe-4 at. % Si	Fe-4 at. % Pt

Each alloy will also contain 0.18 at. % Ti added to getter interstitials from solid solution.

All three alloying elements are expected to exhibit a solute softening effect when alloyed with Fe. The difference between elements comes in their expected effect on the TT of Fe and in their respective volume misfit factors. The Ni, with a relatively small ϵ_{Ω} , is expected to lower the TT; the Pt, which is in the same Group in the Periodic Table as Ni but with a large ϵ_{Ω} , is also expected to lower the TT. The Si, on the other hand, has a large ϵ_{Ω} and is expected to raise the TT.

The test program is designed to allow comparison of tensile, charpy and fracture toughness properties on either side of the experimentally determined TT for each of the given alloys, and for the comparison of these

respective properties as a function of alloy concentration and alloying element. The "pure" iron alloy is to be used as a standard. The status of the experimental test program is given below.

VI-2 ALLOY FABRICATION

All of the alloys, except the Pt alloys, have been fabricated. The as-cast ingots for these alloys were first cut in half; one half was processed so that it could be utilized for tensile and Charpy specimens, while the other half was processed for fracture toughness specimens. The following processing procedures were followed:

(a) Tensile and 1/2 — thickness Charpy specimens

1. Upset forge the 2" x 3" ingot to 1-1/2" x 2.8" pancake at 1100°C.
2. Cross forge at 1100°C to ~2" x 2" x 2.4".
3. Hot roll at 1050°C to ~2" x 1" x 4.8", air cool.
4. Split into two equal sections.

Section 1 for tensile specimens: Continue to hot roll to

2" x 0.2" x 12". Austenitize at 1250°C for one hour, air cool.

Cold roll 50 percent to 2" x 0.1" x 24".

Section 2 for Charpy specimens: Austenitize at 1250°C for two

hours, air cool. Cold roll 50 percent to 2" x 0.2" x 13".

(b) Fracture toughness specimens

1. Upset forge the 2" x 3" ingot to 1-1/2" x 2.8" pancake at 1100°C.
2. Cross forge at 1100°C to ~2" x 2" x 2.4"

3. Hot roll at 1050°C to ~2" x 1" x 4.8", air cool.
4. Austenitize at 1250°C for two hours, air cool.
5. Cold roll 50 percent to 2" x 1/2" x 9.6".

The Fe-Si alloys were cold rolled at 300°C to assure that deformation took place well above the ductile-brittle transition temperature.

The Fe-Pt alloys have exhibited cracking during processing due to the presence of small voids in the as-cast ingot; it is felt that these voids are due to gases trapped during solidification. This has resulted in the need for the development of special melting procedures for this alloy series. It is believed that this problem has now been overcome, and the alloys are now in the process of being remelted with the new vacuum melting procedure.

VI-3 RECRYSTALLIZATION

The as-received wrought material has been cut up into specimen blanks and is ready for recrystallization, which will be done prior to final machining. We are currently heat treating test sections of each alloy at the recrystallization parameters outlined in the proposal to determine if these do indeed give the expected grain sizes. An ASTM grain size of 6-8 is desired for all alloys, and the proposed recrystallization heat treatments are as follows:

Fe and Fe-Si Alloys		1 hour at 750°C
Fe-Ni Alloys and Fe-Pt Alloys	1 at. %	1 hour at 750°C
	2.5 at. %	8 hours at 680°C
	4 at. %	500 hours at 580°C