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ESTIMATION OF FATIGUE LIFE BY LETHARGY COEFFICIENT USING MOLECULAR DYNAMIC SIMULATION

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ABSTRACT−A vehicle structure needs to be more precisely analyzed because of complexities and varieties. Structural fatigue which is generated by fluctuations of stresses during the service life of a mechanical system is the primary concern in the structural design for safety. A fatigue life is difficult to obtain in structural components during the service life of mechanical systems since the fluctuating stress contributes to fatigue. This study introduces new procedures to measure the lethargy coefficient and to predict the fatigue life of a mechanical structure by using molecular dynamic simulation. A lethargy coefficient is the total defect-estimating coefficient, which was obtained by using the results of a simple tensile test in this study. With this lethargy coefficient, fatigue life was estimated. The proposed method will be useful in predicting the fatigue life of a structurally-modified vehicle design. The effectiveness of the proposed method using lethargy coefficient measurement to predict the fatigue life of a structure was examined by applying this method to predict the fatigue life of SS41 steel, used extensively as material of vehicle structures. Two types of specimen such as pre-cracked plate and simple plate is discussed. equation of fatigue life using the lethargy coefficient and failure time, both obtained from a simple tensile test, will be useful in engineering. This measurement and prediction technology will be extended for use in analysis of any geometric shapes of modified automotive structures.

KEY WORDS : Lethargy coefficient, Molecular dynamic simulation, Fatigue life, Probability, Tensile test

1. INTRODUCTION

The failures of material structures or mechanical systems are most likely to result from the effects of direct or indirect fatigue. To best estimate the reliability of a mechanical system before designing, one must first and foremost accurately predict the failure life of material structures or mechanical systems.

In automotive engineering, many structural modifications are usually required to satisfy the design specification including demanded fatigue life and strength.

Most related literature dealing with mechanical structures has, studied the estimations of structural safety through fatigue failure tests and the fault finder system, such as the expert system using a finite element method on the initial design (Paik *et al.*, 1990; Kim *et al.*, 1996; Chu *et al.*, 1999; Hong *et al.*, 2001). Failures may occur from various factors; static strength, fatigue stress, impact load, etc.

Structural fatigue due to fluctuation of stresses generated in the service life of mechanical systems is the primary concern in structural design for safety.

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Fatigue life is difficult to obtain in structural components during the service life of mechanical systems that fluctuating stress contribute to fatigue.

It is a tendency and necessarily required that absolute results such as accurate fatigue strength and fatigue life of materials under service load are needed to minimize the cost and time of designing.

The lethargy coefficient was derived from the results of previous applications of molecular dynamics in materials research. Although molecular dynamics was considered a branch of physics until recently, it is now viewed as a valuable asset in the new field of material science (Baginski *et al.*, 2002; Pusztai *et al.*, 2002; Ward *et al.*, 2002). The lethargy coefficient is obtained from molecular dynamic simulation and is measured as a function of complete failure time and tensile stresses. In view of molecular dynamic, the inter-atomic binding energy of a stressed body is reduced in magnitude. The magnitude of tensile stress inducing thermal fluctuation strongly relates to the amount of chemical bind rupture throughout the material.

This paper presents a method for predicting the fatigue life of SS41 steel, used extensively as materialof vehicle structures, as shown in Figure 1. First, the lethargy

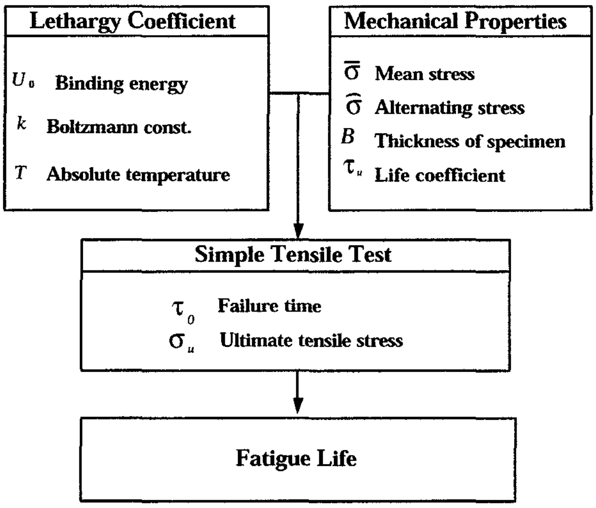

Figure 1. Determination of fatigue life in terms of cycle with lethargy coefficient using molecular dynamic simulation.

coefficient-tensile stress relationship was introduced to predict the fatigue life by using molecular dynamic simulation. Second, the lethargy coefficient of SS41 specimen was measured from a simple tensile test. Finally, the result from second step was compared to experimental data (Fatigue strength data, 1996).

2. EQUATION OF FATIGUE LIFE WITH LETHARGY COEFFICIENT

Zhurkov (1965) expressed the fatigue life of materials as follows

$$\tau = \tau_0 e^{\left(\frac{U_0 - m\sigma}{kT}\right)} \tag{1}$$

Where τ : life (sec)
τ_0 : life coefficient (sec)
U_0 : binding energy (kJ/mole)
m : lethargy coefficients (kJ/mole·mm^2/N)
σ : stress (MPa)
k : Boltzmann constant (kJ/mole·K)
T : temperature (K).

In the view of molecular dynamics, Equation (1) gives the probability of failure energy for mechanical materials (i.e., it represents a relationship between the life and the influence parameters for the fatigue life).

The binding energy U_0 is determined by the probability of rupture for a given strength, derived from the equation for the prediction of static failure. It is the minimum energy to separate 1 mole of any molecular compound from its stable lattice. In other words, the binding energy U_0 is equal to the binding energy of atoms within the metals lattice and corresponds to the activation energy in polymer materials.

Since the life coefficient τ_0 is based on the order of magnitude of stress as shown in figure 2, its constant value may be taken as 10^{-13} seconds for all materials that possess similar chemical characteristics as those of the vehicle structure. The Boltzmann constant k is 8.3454× 10^{-3} kJ/mole·K. In addition, the loading axial stress is generally expressed in terms of the material coefficient (Lee, 1982).

The relationship between the lethargy coefficient and the tensile stress can be explained as follows.

The failure probability of binding energy U_0 is related to the thermal fluctuations of atoms. Under tensile stress σ, the failure probability becomes $e^{\left(-\frac{m\sigma}{kT}\right)}$. In a stressed material, the inter-atomic binding energy is reduced to the magnitude of the stress of σ. The magnitude of tensile stress inducing thermal fluctuation is strongly related to the reduction in the chemical binding energy due to the thermal fluctuation.

From a statistical dynamics point of view, Equation (1) gives the probability of failure energy for a mechanical part (i.e., it represents a relationship between the life of a material or part and the parameters that influence the failure of the material or part). From Equation (1), a bond rupture could occur even if $m\sigma$=0.

As described above, the kinetic mechanism for the fracture of solids under tensile stress is directly related to the reduction of interatomic binding energy.

From Equation (1) and statistical molecular dynamics, the thermal oscillations of atoms or molecules in material lattices is written as $\Delta t/\tau_0$ during the time Δt, the probability of dislocation becomes Equation (2).

$$e^{\left(-\frac{U_0 - m\sigma}{kT}\right)} \frac{\Delta t}{\tau_0} \tag{2}$$

In the Equation (2), mechanical failures occurs when the probability of dislocation is 100%, that is, when one atom is fully dislocated from unstable zone to stable zone on the lattice. Then, the lattice is fully broken into two parts within this period so this phenomenon influences the fatigue life of materials. Equation (2) yields Equation (3) from the integration of life time L of time t. Left of Equation (3) is the probability of separation of ab atom or molecule from its lattice, which is the failure probability. When this probability is 1, mechanical failure occurrs. Because the upper limit L of the integration represents the failure time of a structure, we can estimate the life of a structure as a function of the lethargy coefficient m.

$$\int_0^L \frac{dt}{\tau_0 e^{\left(\frac{U_0 - m\sigma(t)}{kT(t)}\right)}} = 1 \tag{3}$$

The life time, L can be obtained by solving Equation (3), if loading conditions are expressed as follows;

$\sigma(t)=\bar{\sigma}+\hat{\sigma}\cos\omega t$

where $\bar{\sigma}$: mean stress

$\hat{\sigma}\cos\omega t$: alternating stress

and time dependant temperature is constant as $T(t)=T$

The parameters of Equation (3) could be replaced by the fatigue cycle N with vibrating frequency f:

$$L=\frac{N}{f}=\frac{2\pi N}{\omega} \tag{4}$$

where $\omega=2\pi f$, $\omega t=x$ and $dt=dx/\omega$.

Substituting these variables into Equation (3), we can rewrite Equation (3) as

$$\int_0^{N\left(\frac{2\pi}{\omega}\right)} \frac{dt/\omega}{\tau_0 e^{\left(\frac{U_0-m(\bar{\sigma}+\hat{\sigma}\cos(x))}{kT(t)}\right)}}=1 \tag{5}$$

$$\frac{2N}{\tau_0 e^{\left(\frac{U_0-m\bar{\sigma}}{kT(t)}\right)}}\int_0^{\pi}\left(e^{\left(\frac{U_0-m\bar{\sigma}}{kT}\right)}\right)\frac{dx}{\omega}=1 \tag{6}$$

From the relationship between the integral and the Bessel function as shown in Equation (7), the above equation yields Equation (8).

$$\int_0^{\pi}\left(e^{\left(\frac{U_0-m\bar{\sigma}}{kT}\right)}\right)dx=\pi I_0\left(\frac{U_0-m\bar{\sigma}}{kT}\right) \tag{7}$$

$$\frac{2N\pi}{\omega}\frac{I_0\left(\frac{m\hat{\sigma}}{kT}\right)}{\tau_0 e^{\left(\frac{U_0-m\bar{\sigma}}{kT(t)}\right)}}=1 \tag{8}$$

and then reduces to life time L,

$$L=\frac{\tau_0 e^{\left(\frac{U_0-m\bar{\sigma}}{kT}\right)}}{I_0\left(\frac{m\hat{\sigma}}{kT}\right)} \tag{9}$$

where I_0 is the Modified Bessel function of the first kind of order 0.

The lethargy coefficient, m represents a material dependent property; therefore, many tensile tests are needed to determine m. In this paper, to determine m, results from simple tensile tests performed by Yang *et al.* (1997) and Song *et al.* (1998) were used. Yang *et al.* computed the lethargy coefficients and fatigue life with the ultimate stress, σ_u and failure time, τ_u at constant loading speed condition.

$$m=\frac{U_0}{\sigma_u}(1-\eta) \tag{10}$$

Where

$$\eta=\frac{\ln\left(\frac{\tau_u}{\tau_0}\right)}{\frac{U_0}{kT}}\left(1-\frac{\ln\left[\frac{U_0}{kT}-\ln\left(\frac{\tau_u}{\tau_0}\right)\right]}{\ln\left(\frac{\tau_u}{\tau_0}\right)\left[1-\frac{U_0}{kT}-\ln\left(\frac{\tau_u}{\tau_0}\right)\right]}\right)$$

Lethargy coefficient m is proportional to the binding energy over the tensile strength range and reduces to η, expressed in failure time, life coefficient, and loading time. These terms can be obtained from a simple tensile test.

Then, the fatigue life in terms of cycles can be obtained by the multiplication of life time L and frequency f.

$$N=L\cdot f \tag{11}$$

3. MEASUREMENT OF LETHARGY COEFFICIENT FROM SIMPLE TENSILE TEST

This section describes the measurement of lethargy coefficient from the results of a simple tensile test of SS41 steel plates, widely used as vehicle structural materials. As described in the previous section, fatigue life could be calculated from the results of a simple test, because this Equation (9) is the only function of the complete failure time.

Specimens were made for the tensile test as shown in Figure 2 with a SS41 steel plate. Two types of specimen such as pre-cracked plate and simple plate in Table 1 were used.

Type I: Simple plates

To verify the proposed Equation (9) incorporating the lethargy coefficient, we compared with the results from Equation (9) the data of JIS [8]. Thickness of the plate specimen was 3.2 mm. The input data are shown in Table 2.

Type II: Pre-cracked plates

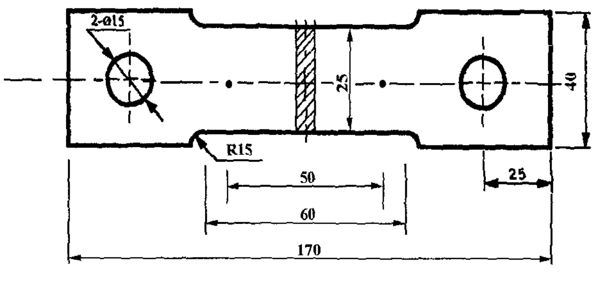

Figure 2. Simple tensile test specimen.

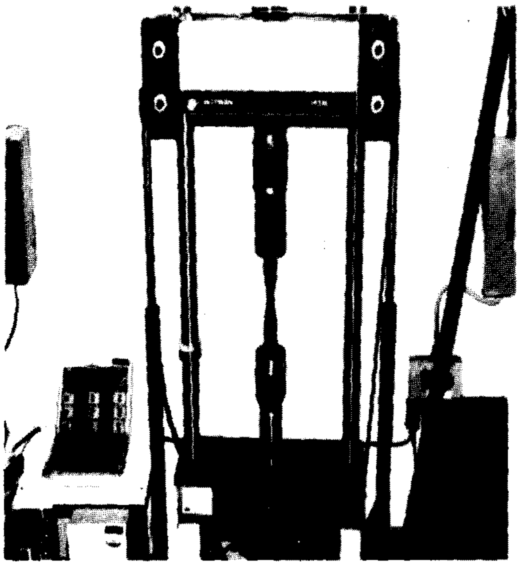

Figure 3. Universal tensile tester: tensile test specimen performed at room temperature at loading speed 0.2 mm/sec.

Table 1. Descriptions of specimens.

Type I	Simple plate	Pre-crack length : 0 mm Thickness : 10 mm
Type II	Pre-cracked plate	Pre-crack length : 4 mm Thickness : 3.2 mm

To calculate the fatigue life of the pre-cracked plate specimen by using Equation (9), we used the input data in Table 2. The pre-crack length of the specimen was 4 mm and the thickness 3.2 mm.

A series of tensile tests was performed on the universal tensile tester, in which maximum tensile load was 25 tons at room temperature. Since the loading speed is 0.2 mm/sec and data-measuring cycle is 15 Hz by A/D converter and data acquisition system, the complete fracture times were obtained automatically as shown in Figure 3. Failure time of each specimen is listed in Table 2. Using Equation (9) and failure time, we can calculate the fatigue life. However, the failure times were the same for each type and this is due to the difference in the sizes of the specimens. Because Equation (9) is the function of tensile stress and failure time, these specimens have different failure times despite the same failure time.

4. RESULT OF FATIGUE LIFE PREDICTION AND DISCUSSION

To calculate the fatigue life of the tensile specimen by Equation (9), we used the input data in Table 1 and Table 2. The failure life of Type I was calculated with Equation

Table 2. Input data to Equation (9).

Binding energy	418.4 (kJ/mole)	
Life coefficient	10^{-13} (sec)	
Boltzmann constant	*(kJ/moleK)*	
Plastic deformation Energy	6.02×10^{-3} (kJ/moleK)	
Temperature	300 (K)	
Frequency	15 (Hz)	
Crack length	See Table 1	
Thickness	See Table 1	
Specimen type	Type I	Type II
Tensile strength	472.36	450.8
Alternating stress	183.26	132.3
Mean stress	262.64	299.39
Fracture time	103 sec	103 sec

Table 3. Fatigue life (cycle).

	Experiment	Prediction	Error (%)
Type I	5.35×10^5	5.03×10^5	6.36
Type II	2.30×10^4	1.99×10^4	15.60

(9). This result was validated by comparing it with the data of JIS, as shown in Table 3.

For the Type I simple plate, the predicted fatigue life is 5.03×10^5 cycles from Equation (9) with tensile strength 472.36 MPa and failure time 103 sec. The error to JIS data 5.35×10^5 cycles is 6.36%. Therefore, the presented method can predict the fatigue life of a steel plate. The equation of fatigue life that ues the lethargy coefficient and failure time obtained from asimple tensile test can be applied in engineering.

The fatigue life of the type II plate, the pre-cracked plate, is 2.30×10^4 cycles in JIS. Fatigue life from Equation (9) was 1.99×10^4 cycles, which is 15.6% in error from JIS data. This difference may be due to the difference of the lethargy coefficient between the pre-cracked plate and simple plate. To reduce this error, the lethargy coefficient must be modified according to the type of pre-cracked. That is, the lethargy coefficient must be corrected with the result obtained from the simple tensile test for pre-cracked plates instead of simple plates, which are used for any case.

5. CONCLUSION

The lethargy coefficient is introduced for total defect estimation coefficient in terms of tensile test results. The lethargy coefficient is based on the results obtained from previous applications of molecular dynamics in materials research. Lethargy coefficient is proportional to the ration of binding energy over tensile strength and reduced to the terms of tensile test results such as failure time, life coefficient, and loading time.

Whether or not the proposed method of lethargy coefficient measurement could predict the fatigue life of structure was examined by comparing the fatigue life obtained from the proposed method with JIS data. From this lethargy coefficient by simple tensile test, fatigue life was estimated and compared to the experimental data. Since the error was 6.36% for the simple plate case, we know that the equation of fatigue life that uses the lethargy coefficient and failure time obtained from a simple tensile test can be applied in engineering. For the pre-cracked plate case, the error was as large as 15.6%. This error could be reduced by a series of tests with a pre-cracked specimen.

The proposed procedure can be extended to the analysis of structural modification and geometric shape in structure. Since the proposed method can identify the fatigue life, it can serve as the fatigue life prediction method for design and structural modification of an automotive structure. The presented method would be very useful for predicting the fatigue life resulting from the structural modification in vehicle design. This method will reduce the cost and time consumed for design of vehicle and making of a prototype.

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