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MECHANICAL ENGINEERING DEPARTMENT

SCHOOL OF ENGINEERING
THE UNIVERSITY OF CONNECTICUT
STORRS, CONNECTICUT

BIAXIAL CONSTITUTIVE EQUATION DEVELOPMENT
FOR SINGLE CRYSTALS
Semi-Annual Status Report
Grant No. NAG-3-512
January 6, 1984 - July 6, 1984

Submitted to:

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National Aeronautics and Space Administration
21000 Brookpark Road
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Introduction

Current production gas turbine engines utilize large single crystal superalloy components in the hot section. Structural analysis of these components requires a valid stress strain temperature constitutive equation. Currently no such equation exists. The goal of the program described is to create one or more models and verify these models. The program will involve an integrated effort of a theoretical, experimentalist and metallurgist. The equations will be developed with guidance provided by experimental results, knowledge of metallurgical phenomon and principals of mechanics.

This report is the first semi-annual status report on this effort done under NASA Grant NAG3-512 from the period of January 6, 1984 to July 6, 1984. The main progress made during this reporting period is the formulation programming and debugging or a constitutive equation based on an assumed slip behavior on a single slip system and design work, or on some experimental systems and delivery of others. Specifically the basic theory for a model based on aggraviting slip behavior on individual slip systems has been formulated, programmed and some simulations have been run during assumed values of constants. In addition a formulation allowing strain controlled simulations has been completed. An approach to structural analysis of the specimen has been developed. This approach uses a long tube consistancy conditions and finite elements specially formulated to take advantage of the symmetry of 100 oriented specimens.

On the experimental format an induction heater has been delivered and is nearly installed. A specimen grip configuration has been designed and several specimen have been machined and awaiting vacuum brazing. A jig for residual stress by hole drilling has been designed and is in machining. An integrator to be used in the control system has been built and works well. Several other systems have been designed. Testing will start soon after the specimens are delivered. These various developments will be described in detailed in the following report beginning with the theoretical developments and ending with description of the status of the experimental program.

Special Consideration Due To Anisotorpy

In order to understand the need for finite element analysis of the specimen, residual stress determination by hole drilling, and the measurement of extra components of strain it is essential to understand complications created by anisotorpy when determining stress from measured loads in the specimen. In general for an anisotropic tubular specimen the load-stress relation is only known when the constitutive equation is known because it can no longer be assumed that stress distribution is uniform. Since the purpose of the testing is to determine the constitutive equation this creates a uniqueness problem in testing the validity of the consitutive equation as well as the necessity of solving for the stress distribution in the specimen. Three steps are being taken in addressing this problem.

First in order to compare measured load displacement records with constitutive behavior written in terms of stress and strain it is necessary to calculate the load displacement of the specimen the proposed constitutive equation. A special finite element code is being written for this.

Second to make the experiments more discriminating in terms of the correctness of constitutive equations extra specimen displacements will be measured.

Finally to further make the testing more discriminating hole drilling to look for residual stresses will be conducted. A special jig is being designed for this purpose.

Basic Theory

As in the enclosed NASA paper. Note the negative sign in the definition of $\underset{\sim}{n}_4=\underset{\sim}{n}_5=\underset{\sim}{n}_6$ etc.

Simulations

The single crystal model described in the preceding section has been coded as a FORTRAN subroutine on the IBM PC-XT computer. A 8087 math co-processor chip is used to increase the speed of floating point arithmetic operations. Each integeration increment takes approximately 0.5 seconds of computer time when an Euler forward difference method is used to advance the time step.

Simulations with the constitutive model to date have concentrated on verification of the computer program, rather than exploring its behavior under different loading conditions. The effect of the anisotropy of a single crystal bar specimen on its cyclic stress-strain hysteresis loops is depicted in Figure 1. This bar specimen is put into tension and compression by the application of specified loads along its axis. Figure 2 shows that the angular orientation of the bar with respect to the crystallographic axes is determined by the two Euler angles θ and ψ. The curves labelled 1 to 7 on Figure 1 represent the cyclic hysteresis loops obtained with the computer program when the bar is loaded into tension and compression by the application of a fully reversed cyclic load of $\pm$30MPa to its ends. Curves 1 to 6 in Figure 1 represent the fully reversed load control loops obtained at points 1 to 6 in Figure 2, where the points are located at $\theta=0^{o}$, 9^{o}, 18^{o}, 27^{o}, 36^{o} and 45^{o} along the [001]-[011] face of the stereographic triangle where $\psi=0^{o}$. Curve 7 depicts the hysteresis loop at point [T11] in the stereographic triangle (the top most point) where $\theta=45^\circ$ and $\psi=35.26^\circ$. According to Schmid's law the yield stress decreases from $\theta=0^\circ$ to 22.5° and increases from 22.5° to 45° along the baseline, viz. [001]-[011], of the stereographic triangle. In the viscoplastic model the increased plasticity corresponding to the Schmid yield stress minimum at $\theta=22.5^\circ$, $\psi=0^\circ$ is reflected in the increased widths of the cyclic hysteresis loops at $\theta=18^\circ$ and $\theta=27^\circ$. The variation in the Schmid yield stress is symmetric about its minimum value at $\theta=22.5^\circ$, but the hysteresis loops do not exhibit this symmetric due to the fact that the elastic Young's modulus increases monotonically from the [001] vertex of the stereographic triangle to the [011] vertex, and from the [011] vertex to the [T11] vertex. This increase can be seen in the steepening of the hysteresis loops from curve 1 to curve 7.

The uniaxial loading of the bar specimen in the numerical simulations is easily accomplished by specifying the stress increment $\Delta\sigma_{zz}$ along the axis of the specimen and assuming that the other stress increments, viz. $\Delta\sigma_{xx}$, $\Delta\sigma_{yy}$, $\Delta\sigma_{xy}$, $\Delta\sigma_{xz}$, $\Delta\sigma_{yz}$, are zero under strain controlled conditions, the analysis becomes more difficult. If strain controlled loading occurs along the [001] crystallographic axis, the analysis is somewhat simplified. For example, if the z-axis corresponding to the axis of the specimen coincides with the [001] crystallographic axis, the strain increment along the axis, viz. $\Delta\sigma_{zz}$ can be specified. The two remaining strain components at the right angles to $\Delta\sigma_{zz}$, viz.

$\Delta\sigma_{xx}$ and $\Delta\sigma_{yy}$, are equal by the symmetry of the crystal. They may be determined so that the corresponding stress increments, $\Delta\sigma_{xx}$ and $\Delta\sigma_{yy}$, are zero by linear interpolation. Thus, the viscoplastic constitutive subroutine is first called with strain increments of $\Delta\varepsilon_{zz}$, $\Delta\varepsilon_{xx} = \Delta\varepsilon_{yy} = -0.25\Delta\varepsilon_{zz}$, $\Delta\varepsilon_{xy} = \Delta\varepsilon_{zz} = \Delta\varepsilon_{yz} = 0$ where no updating of the variables occurs at the end of the increment. The subroutine is then called with strain increments of $\Delta\varepsilon_{zz}$, $\Delta\varepsilon_{xx} = \Delta\varepsilon_{yy} = -0.5\Delta\varepsilon_{zz}$, $\Delta\varepsilon_{xy} = \Delta\varepsilon_{xz} = \Delta\varepsilon_{yz} = 0$, again with no variable updates. Each of these calls will give a stress increment $\Delta\sigma_{xx}$ which is non-zero. Linear interpolation then furnishes the value of λ for the strain increments $\Delta\varepsilon_{zz}$, $\Delta\varepsilon_{xx} = \Delta\varepsilon_{yy} = -\lambda\Delta\varepsilon_{zz}$, $\Delta\varepsilon_{xy} = \Delta\varepsilon_{xz} = \Delta\varepsilon_{yz} = 0$, which give a zero value for the stress increment $\Delta\sigma_{xx}$. These correct strain increments are then used in a third call to the subroutine and the variables are this time updated ready for the next increment. This method was used to produce the cyclic hysteresis loops shown in Figure 3. The four curves represent hysteresis loops carried out under fully reversed strain controlled conditions with the specimen oriented along the [001] crystallographic axis. Each curve represents the hysteresis loop obtained at strain rate magnitude, of 10^{-3}, 10^{-4}, 10^{-5}, and 10^{-6} per second.

For strain controlled tests carried out on specimens oriented at arbitrary directions θ and ψ with respect to the crystallographic axis, the preceding discussion is inappropriate. Two methods can be used for strain control of an arbitrarily oriented specimen.

The first method is the analogue of the preceding method using load control. First, the specimen is given two different load increments with no updating of the variable. Each load increment will produce a different strain increment along the axis of the specimen. By linear interpolation that load increment required to produce the required strain increment can be obtained and the third call to the subroutine uses the correct load increment and updates the variables. If only one load increment is assumed to be non-zero, viz. The load increment along the axis of the specimen, the specimen will, in general, rotate about its axis during the load increment applied to its axis. This rotation may be presented by applying torsional load increments to the specimen which prevent its rotation.

The second method which can be used for strain control of an arbitrarily oriented specimen is simply to solve for the non-specified strain components in terms of the specified components by setting the stress increments corresponding to the unspecified strain increments equal to zero. For example, if the total strain is denoted by $\underset{\sim}{\varepsilon}$ and the inelastic strain by $\underset{\sim}{c}$, and only the strain increment along the 1 axis, $\Delta\varepsilon_1$ is specified, the remaining strain increments can be found by solving the system of equations

$$\begin{matrix} D_{22} & D_{23} & D_{24} & D_{25} & D_{26} \\ D_{32} & D_{33} & D_{34} & D_{35} & D_{36} \\ D_{42} & D_{43} & D_{44} & D_{45} & D_{46} \\ D_{52} & D_{53} & D_{54} & D_{55} & D_{56} \\ D_{62} & D_{63} & D_{64} & D_{65} & D_{66} \end{matrix} \quad \begin{matrix} \Delta\varepsilon_2-\Delta c_2 \\ \Delta\varepsilon_3-\Delta c_3 \\ \Delta\varepsilon_4-\Delta c_4 \\ \Delta\varepsilon_5-\Delta c_5 \\ \Delta\varepsilon_6-\Delta c_6 \end{matrix} \quad \begin{matrix} -D_{21}(\Delta\varepsilon_1-\Delta c_1) \\ -D_{31}(\Delta\varepsilon_1-\Delta c_1) \\ -D_{41}(\Delta\varepsilon_1-\Delta c_1) \\ -D_{51}(\Delta\varepsilon_1-\Delta c_1) \\ -D_{61}(\Delta\varepsilon_1-\Delta c_1) \end{matrix}$$

In this equation D_{ij} are the elastic constants for the cubic crystal in the global (not the crystallographic) system, and the inelastic strain increment tensor $\Delta \underset{\sim}{c}$ is obtained by integration of the viscoplastic constitutive model.

The material constants chosen for the model are arbitrary values chosen to facilitate the numerical verification of the computer program. Specific values are given by:

$\alpha_{mm} = 0$

$\alpha_{nn} = 0$

$\alpha_{zz} = 0$

$\alpha_{mz} = 0$

$\alpha_{nz} = 0$

$p = 8$

$K_r^o = 10000$ (initial values of K_r for $r=1,2,\ldots,12$)

$\rho^1_{pq} = 3 \times 10^7$ for $p,q = m,n,z$

$\rho^2_{pq} = 3 \times 10^3$ for $p,q = m,n,z$

$\rho^3_{pq} = 0$ for $p,q = m,n,z$

$m = 2$

$\beta = 0$

$q = 1.4$

$h = 0$

The elasticity matrix in the crystallographic axes was taken to have the following component form:

$D^c_{11} = 32 \times 10^6$

$D^c_{12} = 22 \times 10^6$

$D^c_{44} = 15 \times 10^6$

while the $\underset{\sim}{Q}$ matrix relating the crystallographic axes to the global is given by the relation

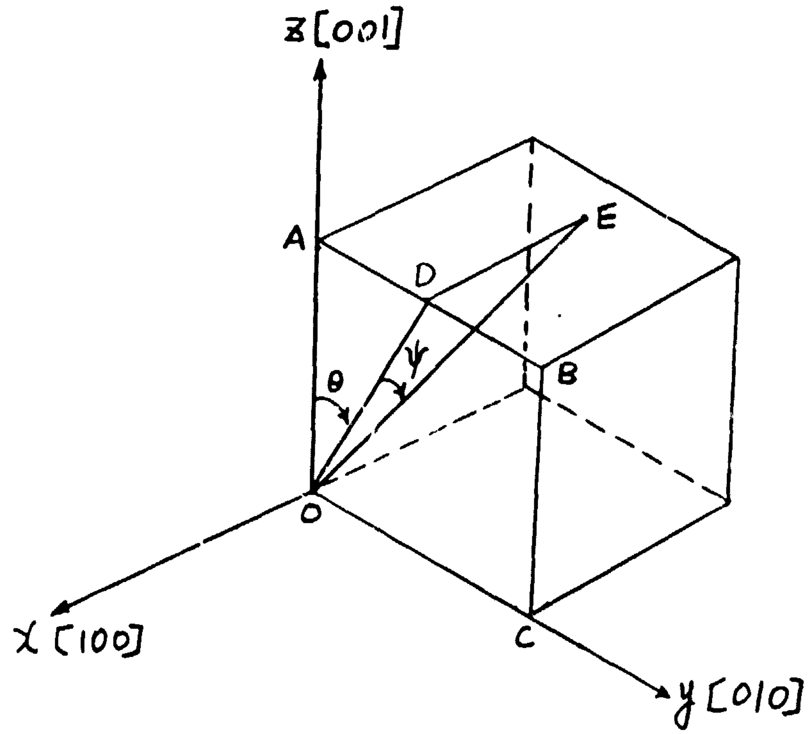
$$
\begin{matrix}
\cos\psi & 0 & -\sin\psi \\
\sin\theta\sin\psi & \sin\theta & \sin\theta\cos\psi \\
\cos\theta\sin\psi & -\sin\theta & \cos\theta\cos\psi
\end{matrix}
$$

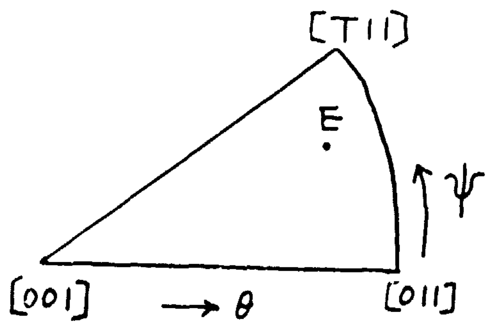
where θ and ψ are defined in Figure 2.

FIGURE 2

The Euler angle θ is in the plane ABCO

The Euler angle ψ is in the plane ODE perpendicular to the plane ABCO





Experimental Program

In the overall scope of the project the experimental program is intended to generate data for three purposes:

1. Determination of the model constants.
2. Increased understanding of the qualitative issues connected with modeling.
3. Accesses of the success of the models.

To carry out these tests a number of hardware modifications are needed to the existing test set up at the University of Connecticut. It is appropriate in this first status report to briefly describe the existing set up and then describe the additions and modifications under way.

Testing has not yet commenced due to two main factors. First difficulty was encountered in machining the specimen and as a result they are not yet available. Second the induction heater although delivered is not yet wired to the power grid. Both of these items are expected to resolved soon.

The Existing Machine

The University of Connecticut has a 50 KIP-20In-KIP tension torsion servo-hydraulic testing machine built at the University of Connecticut partially supported by NASA Grant NAG 3-160. The machine shown in Fig. 4 has been used at temperatures up to 1200 F to date. Strains are measured using a unique capacitance transducer based extensometer shown in Fig. 5. This extensometer exhibits low cross talk which is important to constitutive testing. The extensometer is able to withstand elevated temperatures without cooling. The manufacturer of the transducers recommends the tranducers for temperatures of up to (1450°F). The test temperature in the proposed program is to be 1600°F at the metal surface. Because the specimen is to be heated directly by and induction heater the temperatures at the transducers will be well within the allowed range. The testing to be done in this program requires many modifications to the existing system due to the higher test temperatures and due to the different nature of constitutive testing compared to fatigue testing previously done. The specific hardware changes and the status of each will now be described.

Grips and Specimen

In this program PWA 1480 single crystal specimens will be tested. The raw material for making these specimen is in the form of 1.75 in dia. cylinders 6 in long. Up to now specimen were gripped by welding on 304 stainless steel flanges that were then bolted to the machine. Unfortunately PWA 1480 does not weld readily to 304 stainless steel. An alternative gripping scheme is being developed. In this scheme Hastelloy-X extensions are vacuum brazed on to the 1480 specimen. These Hastelloy extensions serve two purposes. First the extensions make the specimen assembly long enough to provide clearance for the probes and lead wires of the extensometer. Second the Hastelloy extensions provide a Hastelloy end that may be welded to 304 stainless steel flanges as was done in earlier testing in NAG 3-160. The specimen design is a modified version of the specimen used previously. The wall thickness was reduced from 0.100 inches to 0.050 inches to get closer to a true thin walled tube behavior. This wall thickness is similar to that used by others and is expected to be thick enough to prevent buckling. The thinner wall also will make gripping easier by reducing the total loads to be handeled by the welded and by the brazed sections. The specimen, the extension and the weldable flanges are shown in Figure 6. The vacuum braze is expected to work based on advice obtained at Pratt and Whitney Aircraft. This grip is expected to work and allows existing successful techniquies to be continued. Later in the project the extensometer may be redesigned and modified allowing shorter test pieces. If this is done water cooled collect grips will be considered. It is worth noting that the enlarged opening in the base of the Hastelloy extension piece is to allow a center to be brought into engage the specimen bore so that the final assembly can be faced off square to the bore centerline.

Heating and Temperature Measurement System

To date temperatures up to 1200°F were obtained by using band heaters wrapped around the ends of the specimen and temperatures were measured by using thermocouples welded directly to the specimen. The investigation of PWA 1480 visco plastic properties requires the use of temperatures of at least 1600°F in order to begin to see the desired phenomon. The band heater technology cannot reach such temperatures as the heaters have a maximum surface temperature of 1500°F. To obtain the desired temperatures an audio frequency induction heater will be used. Such a heater was purchased on the grant and delivered. This unit is a used but guaranteed unit. It utilizes a motor generator combination to generate a 1000 hz signal for heating. This type of unit was chosen over the more common 250 KHZ RF induction heater for several reasons:

1. Motor generator units are lower frequency hence will induce less noise in other electronics.
2. The frequency of MG heaters is very constant in contrast to RF heaters with facilitates filtering of noise.
3. Audio heaters heat to a greater depth making them better at getting uniform through thickness temperature uniformity.

4. Audio heaters are much less efficient at heating small objects such as thermocouples and extensometer attachment hardware, this minimizes thermocouple measurement problems and the tenancy of the attachment hardware to heat hotter than the specimen.

Temperatures will be measured using an infrared Pyrometer which allows non contacting temperature measurement. This is essential for adjusting the induction coil to get uniform temperature in the gage length. The specimen must be soaked at temperature to stabilize the emissivity. Exerperierce at other labs shows that the emissivity is truly stable. Thermocouples must be used to calibrate the system with respect to emissivity.

At present the heater has been delivered and mounted and plumbing has been done. It is awaiting electrical hook-up. The radiation pyrometer has been delivered and tested.

Computer Control and Data Aquisition

The test system at the University of Connecticut has been fully computer controlled for several years. However, constitutive testing will place new demands on the system. In testing a history dependent material it is essential to record the whole deformation history. Further the test program is not a simple repetative one. In some cases mode switching between strain and load control is desirable. In light of the requirements the control software is being rewritten. The computer has been up graded to a faster CPU with 256 K of memory compared to the 32 K used previously. A clock board has also been added to give an output variable of time.

In the past the command signal for multiaxial tests was generated point by point by putting individual numbers out to a D/A converter. At slow strain rates this results in a visable step wise machine response which is undesirable in studying the behavior of rate dependent materials. To overcome this difficulty a very stable integrator was built. This allows computer through the D/A to command ramp rates rather than point values. With this system there are never infinite strain rates. This has the further advantage that the command signal needs to be up dated much less often as function are more readily approximated by straight line segments than by points. The circuit developed by a University of Connecticut funding has outstanding stability being able to hold a ramp for seconds and only have the voltage off by at the end of the ramp. The data collected will be stored on a floppy disk and will be available to NASA and others for modeling efforts. The format of the data will be standarized. The format will be chosen in consulation with NASA and Pratt and Whitney and if possible be common across all three.

In summary all test will have computer control and data acquisition. The nature of constitutive testing requires new machine control software which is just now being written. The information collected will if possible be put in an agreed upon format. The problem of discontinuities in the command function will be overcome using special integrator circuit which has been build and is working well.

Measurement of Additional Strains During Testing

Because of anisotropy the possiblity of change in the specimen geometry for a straight round cylinder exists. The measurements of these distortions will provide extra information very valuable in address the problem of uniqueness created by the absence of a simple load-stress relation. Some steps to develop special instrumentation to carry out these measurements have been taken.

An extensive survey of possible high temperature measurement methods was carried out by an undergraudate as a project. In this survey he identified three possible methods of making real time internal roundness change measurements. These were the nozzel flapper discussed in the proposal that relies on back pressure generator at a nozzel discharging against a wall. Capacitance probes that change capacitance as a function of the distance between a probe and the specimen wall, and an inductive probe that senses displacement by the change in inductance caused by the proximity of the wall. Design work was done on all three concepts.

The capacitance probe uses the same well established technology used in the University of Connecticut extensometer. The chief question being whether or not such probes can survive 1600°F. A test was run using two probes donated by Hi Tech Inc. One of the probes stopped working at temperature while the other continued to work. The probe that worked was rather a large one however, discussions with Hi Tech suggest that they "may" be able to make a smaller version for our application.

A nozzel flapper system was designed and heat transfer analysis showed that it was necessary to actively heat the air used as it did not pick up enough heat as it traveled down the axis of the specimen. Additional heat transfer analysis and response time analysis showed that it was possible to put the pressure transducers far enough from the heated zone to use low cost room temperature pressure probes. The use of room temperature pressure transducers reduces the potential cost of the system greatly.

An eddy current probe was designed and there is no fundamental reason why it will not work. The practical difficulty is finding a high temperature insulation that will be thin enough to allow enough turns of wire on the coils. Discussions are still going on with KAMAN Aerospace concerning a custom fabrication.

All of the above projects are presently on hole due to information recently obtained. Torsion tests of a single crystals superalloy were done at the University of Connecticut on single crystal tubes as part of a small industrial contract. Inspite of many cycles applied to these specimens at room temperature and at 1200^{o}F no shape change was detected using a micrometer. It seemed prudent to wait until the size of the shape changes that occured in the experiments under the grant could be measured. This way if changes occured the system could be designed to have the right sensitivity and if no changes take place a needless complex project could be avoided and energies and resources directed at more productive results.

A Jig for Residual Stress Determination by Hole Drilling

As mention previously the stress distribution is not expected to be uniform in the single crystal specimen tested in this program. Finite element analysis is to be done to solve for the specimen stress distribution. Determination of stresses by hole drilling will provide a direct experimental check on the correctness of the calculated results. In order to perform this hole drilling it is necessary to bring a drilling jig to a selected location and drill a radial hole. To do this accuarately requires a fixture that will allow the drill to be moved to various positions around the circumference. A jig is being built for this purpose. This jig is designed to carry the hole drilling device made by micro measurements. Drawings of the fixture for holding the drill is shown in Fig. 7.

This device will be used in two types of experiments. First room temperature hole drilling will be done while the specimen is under load to determine the applied stress distribution. Second residual stresses following an elevated temperature test will be determined by drilling holes at room temperatures after the test.

Program Status Summary

In the first six months of the program the theory has been formulated and numerical simulations have been run. Further modifications of the theory are planned to account for known non symmetric flow stress and to account for other phenomon revealed by experiments. Model constants need also to be determined.

In the experimental program a number of important equipment additions and modifications are nearly done. Considerable design effort on new measurement devices is substantially complete. Testing will begin following electrical hook of the induction heater and delivery of the first specimen. Both of the above are expected soon, certainly before the end of the next reporting period.

The sensible behavior of the model is hardening. Much work remains in revising and improving the equations to model what are expected to be both a valuminoius and complex set of experiment data. Because multiaxial testing of the material is new it is impossible to anticipate what problems may or may not arise. It is certain however that because of the complex histories often run in this kind of testing considerable time will be spend choosing programming the test program histories. The direct transfer of experimental data to the computer will allow us to pursue this challenging task of producing a useful constitutive equation for solving elevated temperature gas turbine structural analysis problems.

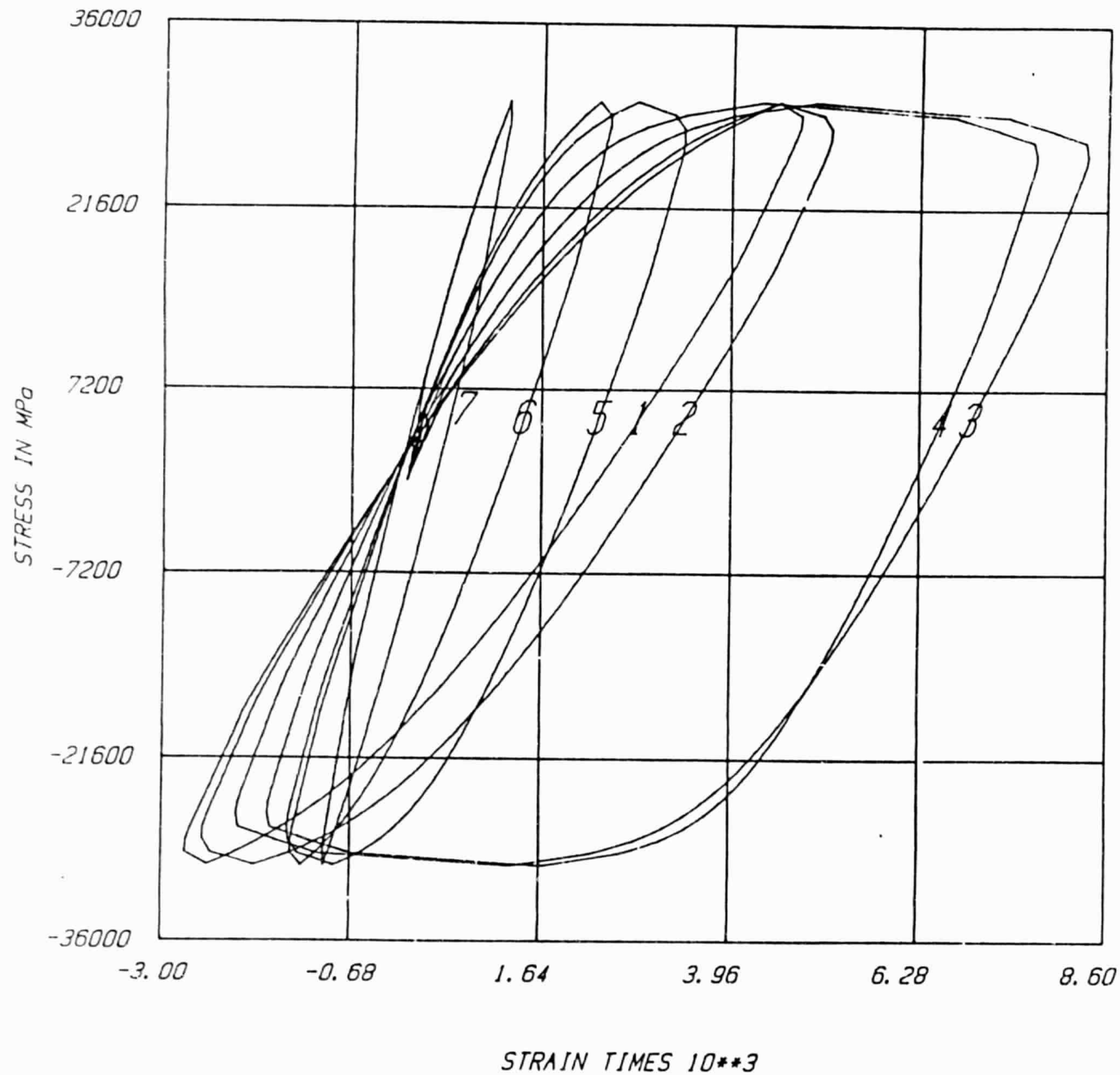


Figure 1. Orientation Dependence of Hysteresis Loops

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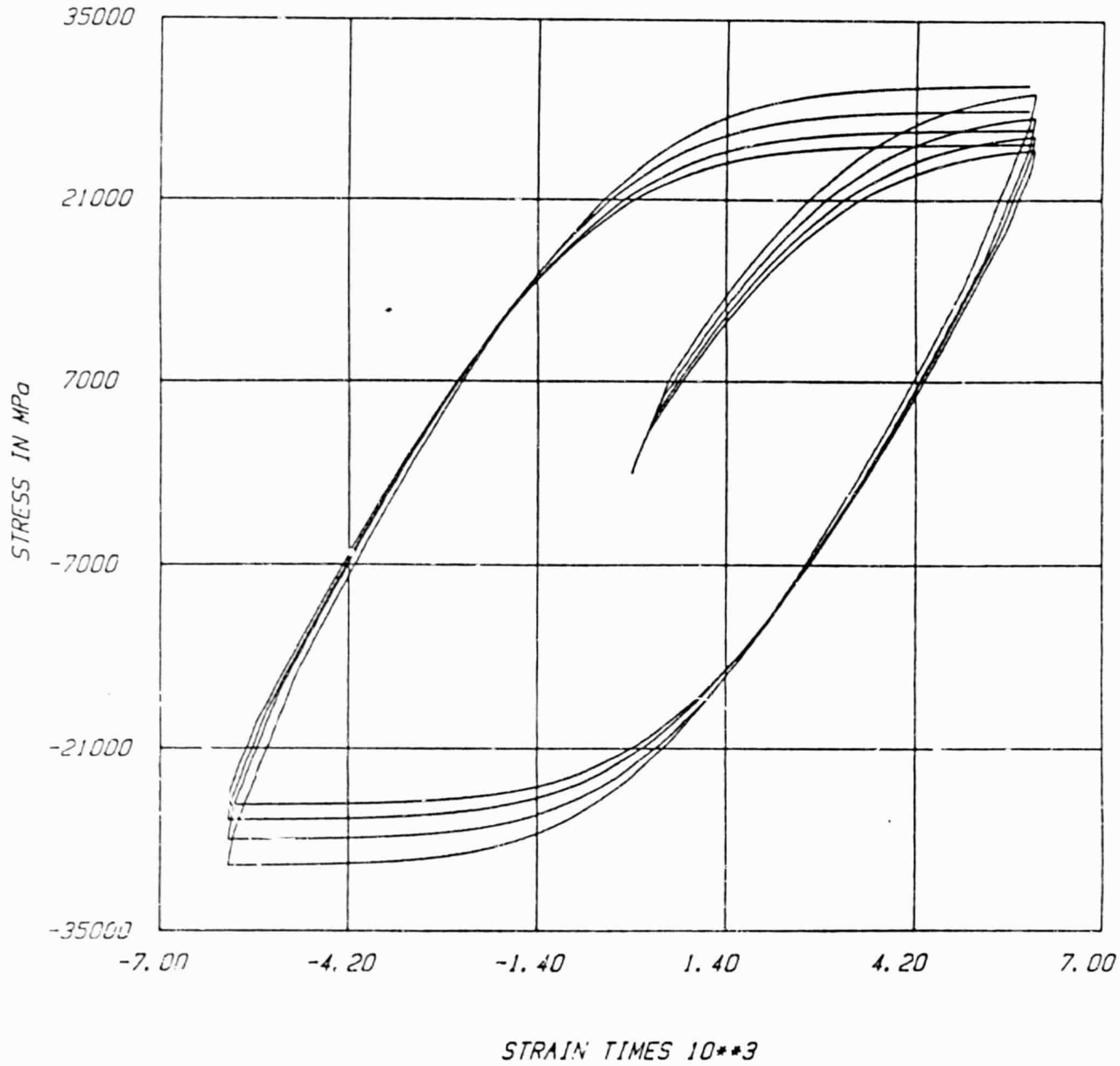

Figure 3 Strain Rate Dependence of Hysteresis Loops

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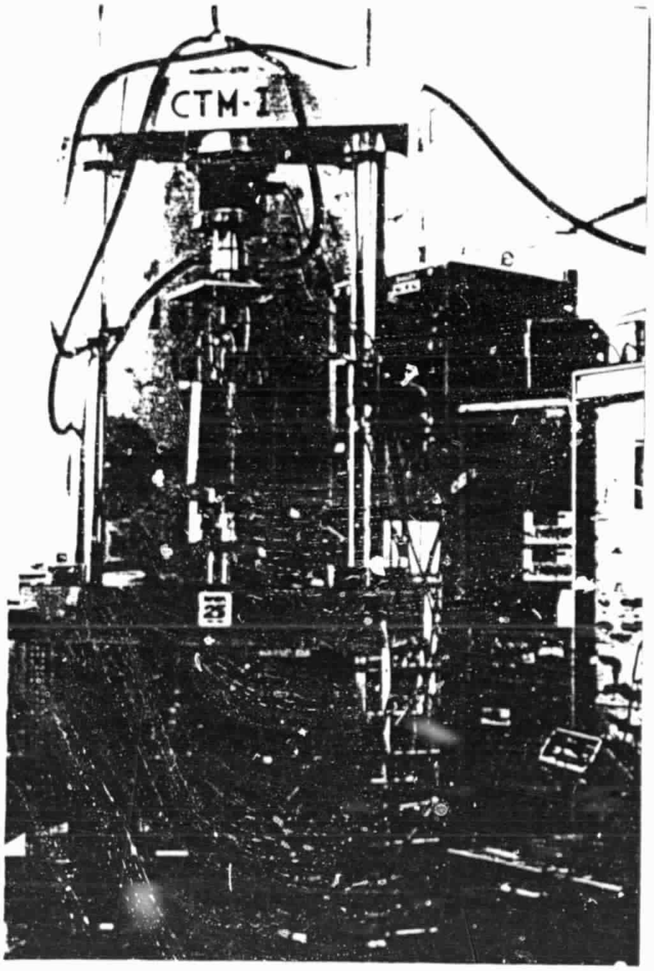

Figure 4: Tension-Torsion Servo-hydraulic Testing Machine

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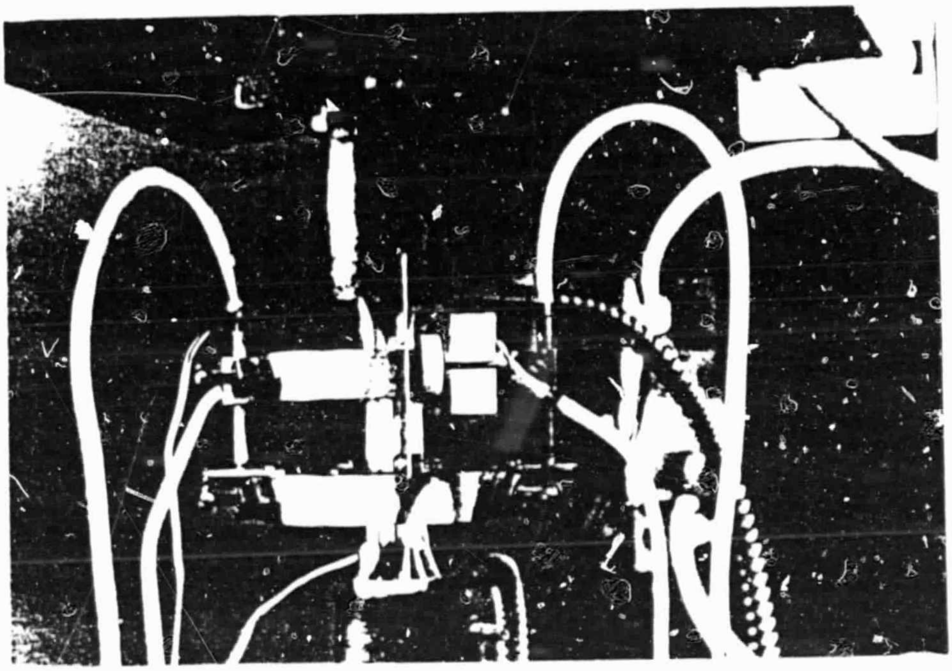

Figure 5: Capacitance Probe Based High Temperature Biaxial Extensometer

A	HASTELLOY - T
B	PWA - 1480
C	304 STAINLESS STEEL

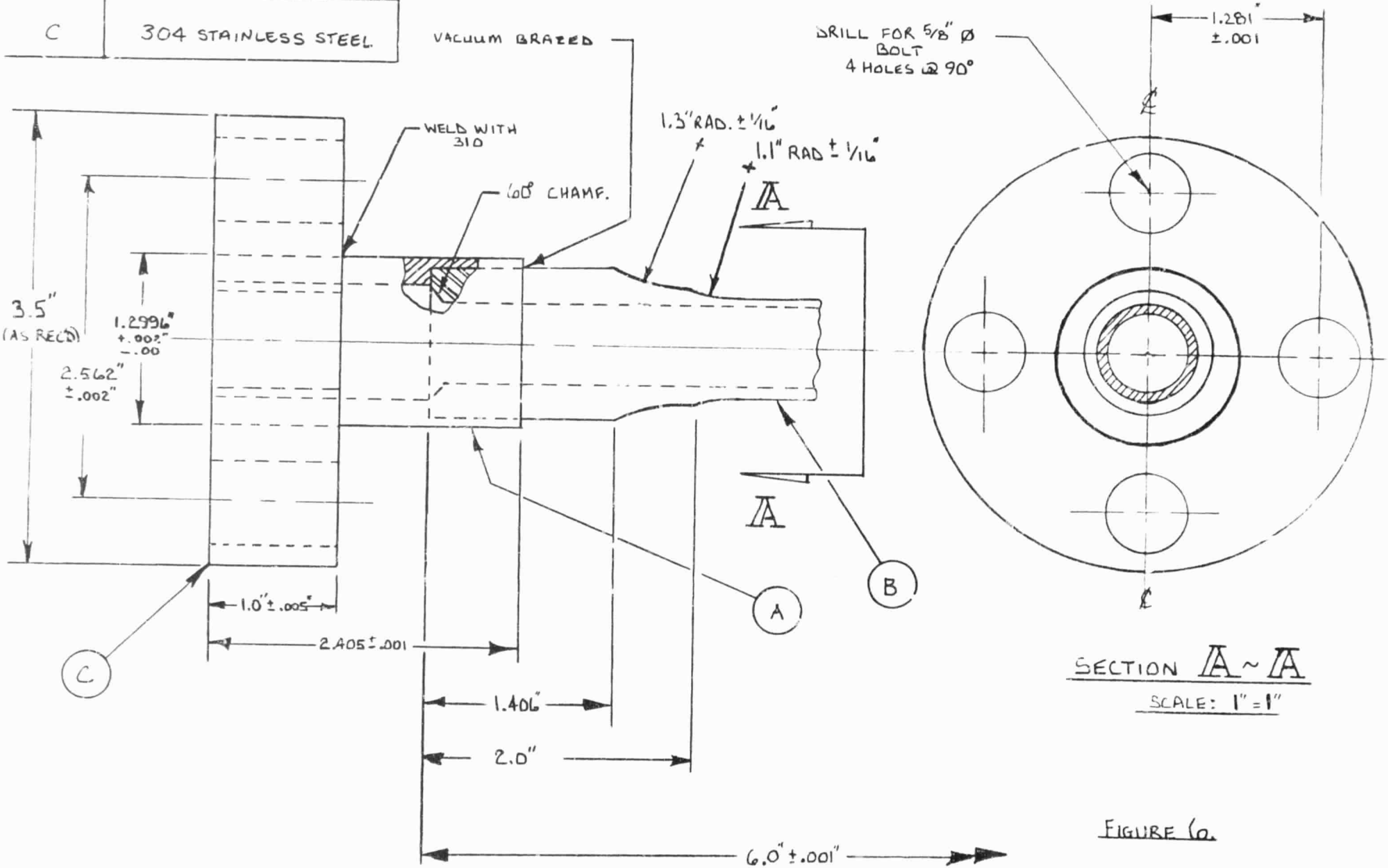

FIGURE 6.

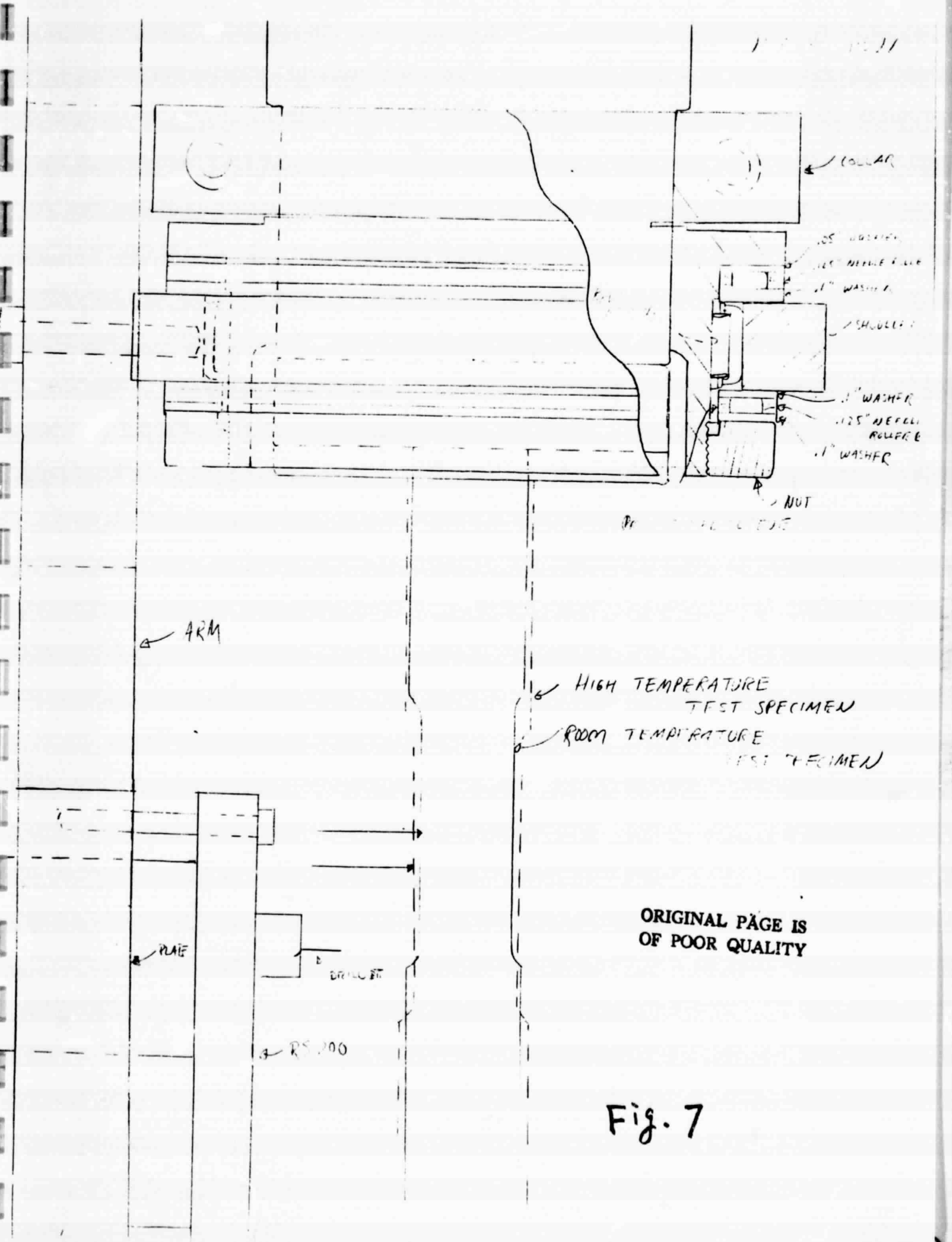

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Fig. 7