

N89 - 17334

**HIGH TEMPERATURE CONSTITUTIVE AND CRACK INITIATION
MODELING OF COATED SINGLE CRYSTAL SUPERALLOYS***

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The purpose of this program is to develop life prediction models for anisotropic materials used in gas turbine airfoils. In the base portion of the program, two coated single crystal alloys are being tested. They are PWA 286 overlay coated and PWA 273 aluminide coated PWA 1480 and PWA 286 overlay coated Alloy 185. Viscoplastic constitutive models for these materials are also being developed to predict the cyclic stress-strain histories required for life prediction of the lab specimens and actual airfoil designs. This report highlights some of the accomplishments of the program this year. Refer to Reference 1 for more information.

SINGLE CRYSTAL CONSTITUTIVE MODEL

Two candidate constitutive models have been developed for single crystal materials. A "microscopic" model computes inelastic quantities on the crystallographic slip systems and achieves the required directional properties as a consequence of resolving the slip system stresses and strains onto the global coordinate system. The second model, the "macroscopic" model, uses anisotropic sensors operating on the global quantities directly to achieve the required directional properties. Material constants from 427C (800F) to 1038C (1900F) have been obtained for both models based on cyclic tests. Additional tests are being conducted to obtain model constants up to 1149C (2100F).

Each model has been encoded in a format consistent with that required in the MARC (Ref. 2) finite element program (via user subroutine HYPELA). Significant reduction in computing time is achieved by formulating and inverting the structural stiffness matrix only once in an analysis using elastic constants at a "reference temperature" (Ref. 3). During the incremental structural analysis, any elastic stress change due to change in temperature from the reference temperature is added to the incremental inelastic stress vector.

Simple finite element analyses are being conducted to verify proper operation of the models in the MARC program.

* Work performed under NASA contract NAS3-23939.

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COATING CONSTITUTIVE MODEL

PWA 1480 turbine airfoil TMF cracks originate from a coating crack. Thus, for airfoil life prediction, it is important to model the coating mechanical behavior as well as that of the PWA 1480. In this program, viscoplastic constitutive models are being developed for two fundamentally different coating types which are commonly used in gas turbines to provide oxidation protection: 1) PWA 286 plasma sprayed NiCoCrAlY overlay and 2) PWA 273 NiAl diffusion.

Walker's isotropic formulation (Ref. 4) was chosen as the overlay coating constitutive model based on its ability to reproduce isothermal and thermal mechanical hysteresis loop data.

MARC (Ref. 2) finite element computer program user subroutine HYPELA has been developed for the overlay coating to permit analysis of coated specimens and components.

Aluminide diffusion coating constitutive model development is continuing. Because diffusion coating properties depend on the substrate material, tests are conducted on two thicknesses of coated PWA 1480 material. Subsequently, the "effective" aluminide coating material constants will be determined by applying the overlay coating Walker model formulation to both specimen thicknesses and extrapolating to zero substrate thickness. Isothermal stress relaxation testing of the 0.25mm (0.010") thick specimens was completed. The observed specimen response at 871C (1600F) is presented in Figure 1. Testing of the 0.13mm (0.005") thick specimens and model constant determination is pending.

LIFE PREDICTION TESTS

Over 45 TMF tests of coated PWA 1480 specimens have been completed. Although many different strain-temperature cycle conditions were investigated, the bulk of TMF tests were out-of-phase. All four orientations ($\langle 001 \rangle$, $\langle 011 \rangle$, $\langle 111 \rangle$, and $\langle 123 \rangle$) initiated cracks at sites where coating cracking had occurred. This initiation mode is consistent with previously conducted experiments and turbine airfoil experience.

Isothermal specimen tests are also being conducted. Contrary to the TMF test experience; however, many non- $\langle 001 \rangle$ oriented substrate specimens initiated cracks underneath the specimen outer surface in either the PWA 1480 or coating/PWA 1480 interfacial region, especially in the higher temperature tests. In $\langle 001 \rangle$ oriented PWA 1480 specimens, crack initiation was limited to the coating. This initiation mode shift between $\langle 001 \rangle$ and non- $\langle 001 \rangle$ specimen orientations occurred because $\langle 001 \rangle$ specimens were tested at higher strain ranges than the other orientations to obtain roughly equivalent specimen lives. The higher strains reduce the coating fatigue life below that of the PWA 1480. However, there was one exception. PWA 286 coated $\langle 001 \rangle$ specimen tests conducted at temperatures greater than 927C (1700F) generated coating cracks, but those cracks did not grow into the PWA 1480. In such cases, specimen failure was caused by crack initiation at the uncoated I.D. specimen surface.

LIFE PREDICTION MODELS

The original life prediction approach which limited the crack initiation mode to just coating cracking must be extended to include the other observed specimen cracking modes:

$$\begin{aligned} N_f &= N_c + N_{sc} + N_{sp} \\ \text{or} \\ N_f &= N_{si} + N_{sp} \end{aligned}$$

whichever is the smallest.

where: N_c = Cycles to initiate a crack through the coating.

N_{sc} = Cycles for coating initiated crack to penetrate a small distance into the substrate. Currently defined as .25 mm (.010").

N_{si} = Cycles to initiate a substrate crack due to macroscopic slip, oxidation effects, or defects.

N_{sp} = Cycles to propagate substrate crack to failure.

N_f = Total cycles to fail specimen or component.

N_c for Overlay Coating

The following modified tensile hysteretic energy model was developed for the overlay coating:

$$N_c = C W \frac{-b}{t} \nu^m$$

where: $\nu = \frac{1}{\sum_{\text{cycle}} \frac{r(T_i)}{r(T_0)} t_i^{-D_0}}$; $\nu \leq 1.0$

$r(T) = r_0 \exp(-Q/T)$ = temp. and time dependent damage rate.

$W = \frac{1}{t} \int \sigma d\epsilon$ = Tensile hysteretic energy, N-m/m³ (in-lbf/in³).

T_i = Individual temperature levels in the cycle, K (R).

t_i = Time at T_i (min), including 100% of tensile hold and 30% of compressive hold times in the cycle, if any.

To = Threshold temperature for temperature dependent damage, assumed to be 1088K (1960R).

Do = "incubation damage" = 9.985

Q = Normalized activation energy for temperature and time dependent damage.

Q = activation energy/gas constant, $\Delta H/R$
Q = 28366°K(51100°R)

The term, ν , is an extension of Ostergren's time dependent damage term (Ref. 5) that includes both temperature and time dependent damage functions to model thermally activated processes.

Model constants were determined from isothermal tests conducted at 427, 760, 927, and 1038C (800, 1400, 1700, and 1900F). Coating hysteresis loops were predicted using the PWA 286 constitutive model incorporated into a one-dimensional model. This model determines the stress-strain of the substrate and coating by imposing an equivalent displacement history. Differences in coefficient of thermal expansion are included in the model.

The life model collapses isothermal and thermal mechanical fatigue lives within a factor of about 2.5 (Fig. 2). Generally, the worst predicted test lives were limited to 1149C (2100F) max. temperature TMF tests. Prediction of these tests should improve when 1149C (2100F) isothermal tests are included in the data set used to determine model constants.

Ultimately, coated TMF life prediction must consider biaxial coating loads introduced by the thermal growth mismatch between the coating and substrate. For example, MARC finite element analysis of a simple two element structure was performed to obtain the coating hysteretic response to a uniaxial, out-of-phase TMF test conducted at 427-1038C (800-1900F), $\pm .15\%$, and 1 cpm. Predicted hysteresis loops from the finite element and one-dimensional analyses are presented in Figure 3. The coating tensile hysteretic energy was obtained from the finite element analysis by the method proposed by Garud (Ref. 6). For this test condition, biaxial coating loads increased the tensile energy 70% which reduced the predicted life by a factor of about 1.5.

Nc for Aluminide Coating

Total strain range correlation of aluminide coating life at 927C (1700F) indicated that the life of this coating type depended upon the PWA 1480 substrate orientation. Fractographic analysis of the specimen crack initiation regions indicated that most of the non- $\langle 001 \rangle$ oriented PWA 1480 specimens initiated cracks under the specimen surface as discussed previously. The correlation was markedly improved by removing the substrate crack initiated specimens from consideration (Fig. 4). The square symbol points in Figure 4 were tests which exhibited PWA 1480 initiation (Nsi).

Nsc or Nsi for Single Crystal Substrate

Initial PWA 1480 life correlations evaluated the following models: Coffin-Manson, Ostergren, crack tip opening displacement (CTOD) from linear elastic fracture mechanics (LEFM), elastic modulus modified strain range model, and the modified hysteretic energy approach developed by DeLuca and Cowles (Ref. 7) which considers crystallographic effects. Each of these models was applied to the data set presented in Table 1. All the models, except CTOD, correlated the lives within a factor of about 2.5.

The elastic modulus modified strain range, Ostergren, and modified hysteretic energy models were chosen for further development based on regression analysis. Subsequently, the Ostergren model was judged to be a subset of the modified hysteretic energy model and, as such, will not be developed further. The modified strain range and modified hysteretic energy model correlations are presented in Figures 5 and 6.

The modified hysteretic energy approach was also applied to an expanded 971C (1700F) data set which included PWA 286 and PWA 273 coated PWA 1480 lives associated with both Nsc and Nsi type initiation modes (Fig. 7). This correlation indicates that the different initiation modes produce separate life trends, but that, within a given mode, lives from both coating types (i.e. overlay and aluminide) are reasonably correlated by a single expression. Also, at this temperature, the PWA 1480 cracking life from the Nsc initiation mode is less than for the Nsi mode. Lastly, for the Nsi initiation mode, greater life data scatter was observed in the overlay coated PWA 1480 lives than the aluminide coated lives. This was attributed to the fact that the PWA 1480 crack initiation in the overlay coated specimens generally occurred deeper in the specimen (i.e. farther from the O.D. surface) than that in the aluminide coated specimens. Since replication cannot monitor subsurface cracks, larger data scatter was expected from the overlay coated specimens.

FUTURE

Isothermal fatigue and TMF tests will continue. These will include preexposed (100 hr. at 1093C (2000F)) fatigue tests designed to understand long term exposure effects, biaxial fatigue tests, and coated Alloy 185 tests. Life model development will focus on prediction of PWA 1480 observed life, especially the PWA 1480 life associated with cracks originating from a coating crack (Nsc).

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TABLE I

Summary of 927°C (1700°F) Crack Initiation Information Used to Evaluate PWA 1480 Life Models

Spec. ID	Condition	E GPa (ksi)	σ_t MPa (ksi)	$\Delta\epsilon_{in}$ Percent	$\Delta\sigma$ MPa (ksi)	$\Delta\sigma_{[111]}$ MPa (ksi)	$\Delta\epsilon/2$ MPa (ksi)	$\sigma_t \Delta\epsilon_{in} \frac{\Delta\sigma_{[111]}}{E}$ Pa (psi)	$N_{.030 - N_{ac}}$ (cycles)	$\langle hk \rangle$
JB-23	+/- .3 percent	87.8 (12735)	280. (40.6)	.0307	556. (80.6)	185. (26.9)	263. (38.2)	181. (.0263)	8100	<001>
JB-28	+/- .34 percent	87.8 (12735)	319. (46.1)	.0337	607. (88.1)	203. (29.4)	299. (43.3)	247. (.0356)	3080	<001>
JB-31	+/- .4 percent	87.8 (12735)	384. (55.7)	.0514	720. (104.4)	240. (34.8)	351. (50.9)	539. (.0782)	2875	<001>
LB-180	+/- .25 percent	245.1 (35550)	526. (76.3)	.1065	1035. (150.1)	1035. (150.1)	613. (88.9)	2366. (.3431)	<<3941	<111>
LB-195	+/- .2 percent	245.1 (35550)	472. (68.4)	.0285	852. (129.4)	892. (129.4)	490. (71.1)	490. (.0710)	1780	<111>
LB-236	+/- .17 percent	245.1 (35550)	380. (55.1)	.0172	761. (110.4)	761. (110.4)	416. (60.4)	203. (.0294)	2.2-6.1k	<111>
KB-23	+/- .25 percent	169.3 (24550)	418. (60.6)	.0167	616. (118.4)	544. (78.9)	423. (61.4)	224. (.0325)	2440	<011>
KB-31	+/- .2 percent	169.3 (24550)	330. (47.9)	.0137	665. (96.5)	443. (64.3)	338. (49.1)	119. (.0172)	5-20k	<011>
KB-28	+/- .3 percent at +.3 percent	169.3 (24550)	299. (43.3)	.0919	903. (130.9)	602. (87.3)	508. (73.7)	975. (.1414)	1150	<011>
MB-21	+/- .25 percent	169.3 (24550)	416. (60.4)	.0315	808. (117.2)	692. (100.4)	423. (61.4)	536. (.0778)	2910	<123>
MB-18	+/- .3 percent	169.3 (24550)	505. (73.2)	.0528	973. (141.1)	834. (120.9)	508. (73.7)	1313. (.1904)	920	<123>
MB-4	+/- .3 percent at +.3 percent	169.3 (24550)	343. (49.8)	.1348	926. (134.3)	794. (115.1)	508. (73.7)	2170. (.3147)	770	<123>

NOTE: All σ_t , $\Delta\epsilon_{in}$, $\Delta\sigma$ were determined from specimen data at approximately $(N_{.030} - N_{ac})/2$ cycles.

1) $N_{.030} - N_{ac}$ = Cycles to .762mm (.030") surface crack length minus cycles to surface crack length equal to 2X coating thickness. This definition does not discriminate between N_{sc} and N_{sf} failure modes.

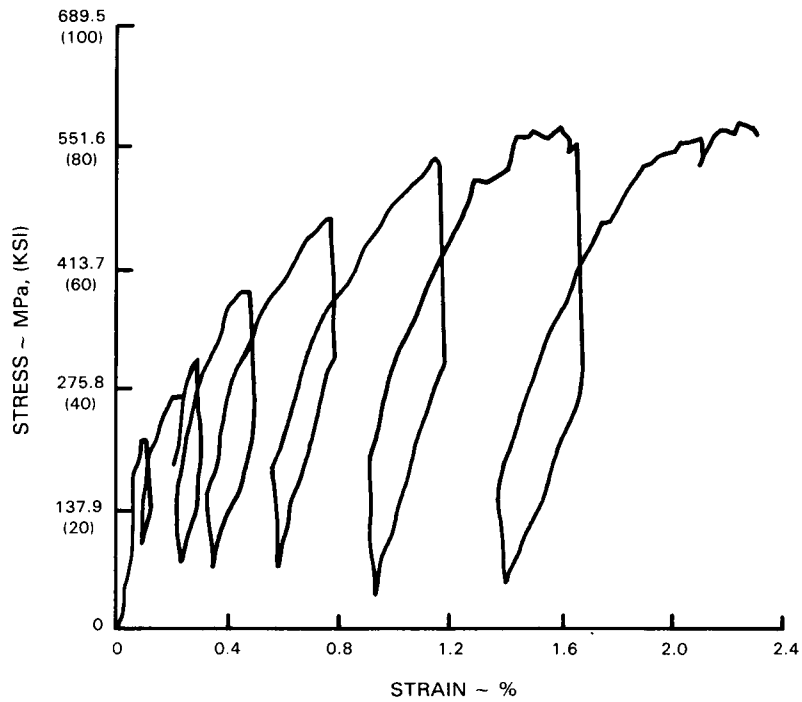


Figure 1 Stress Relaxation Test of PWA 273 Aluminide Coated 0.25 mm (0.010") <001> PWA 1480 Strip Conducted at 871°C (1600°F).

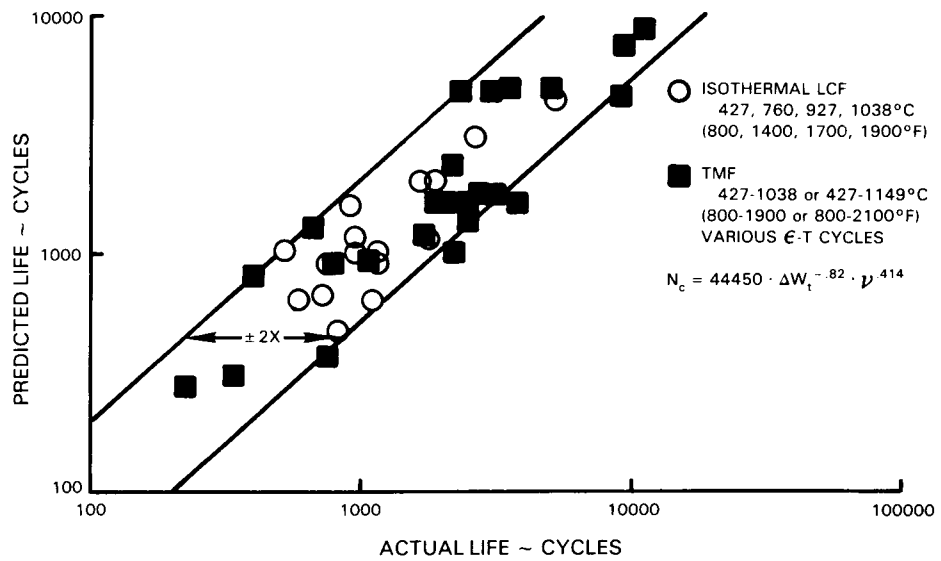


Figure 2 PWA 286 Coating Model Prediction of Isothermal LCF and TMF Life.

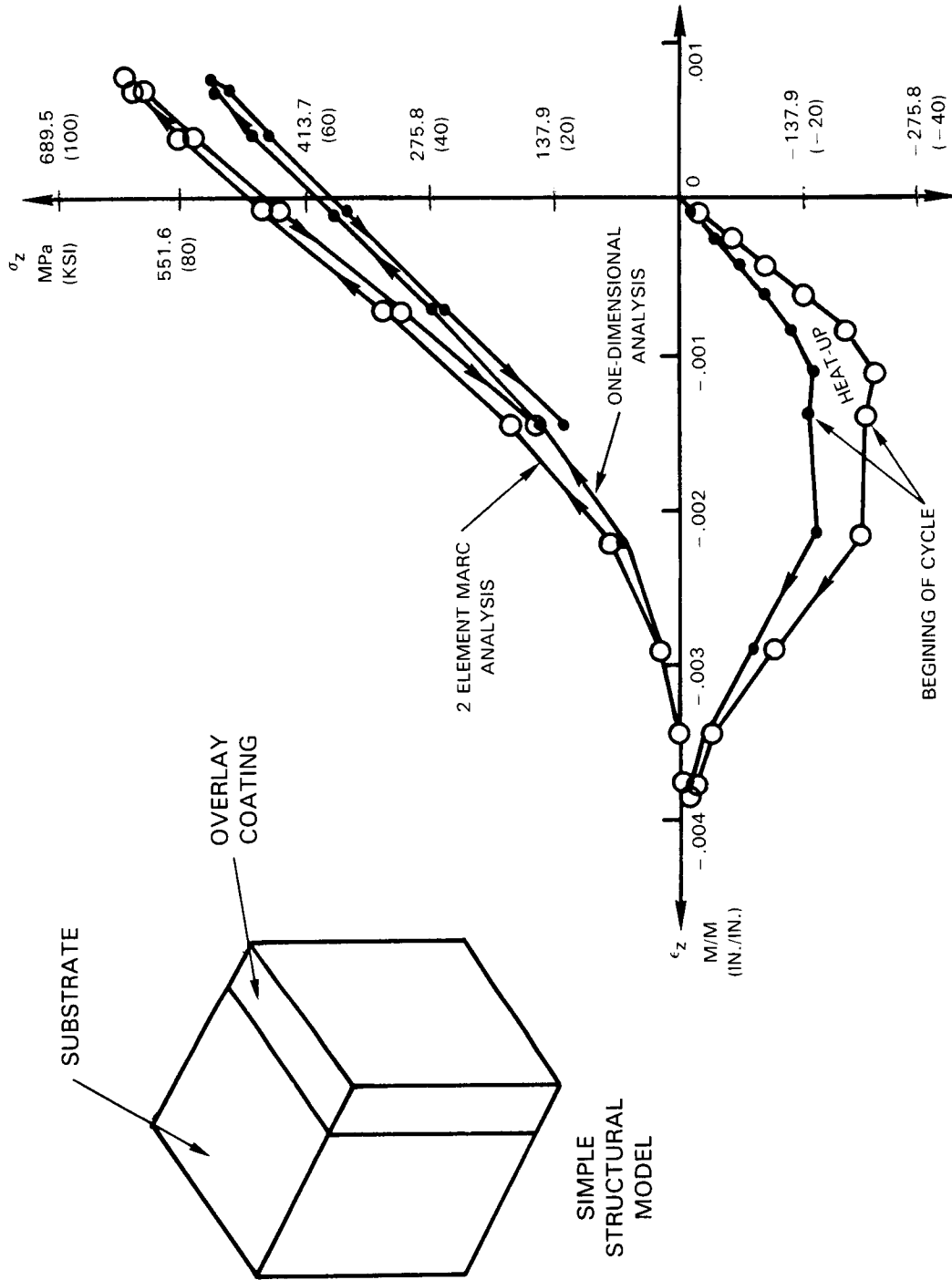


Figure 3 Predicted PWA 286 Coating Response to 427-1038C (800-1900F), \pm .15%, 1 CPM, Out-of-Phase Uniaxial TMF Test.

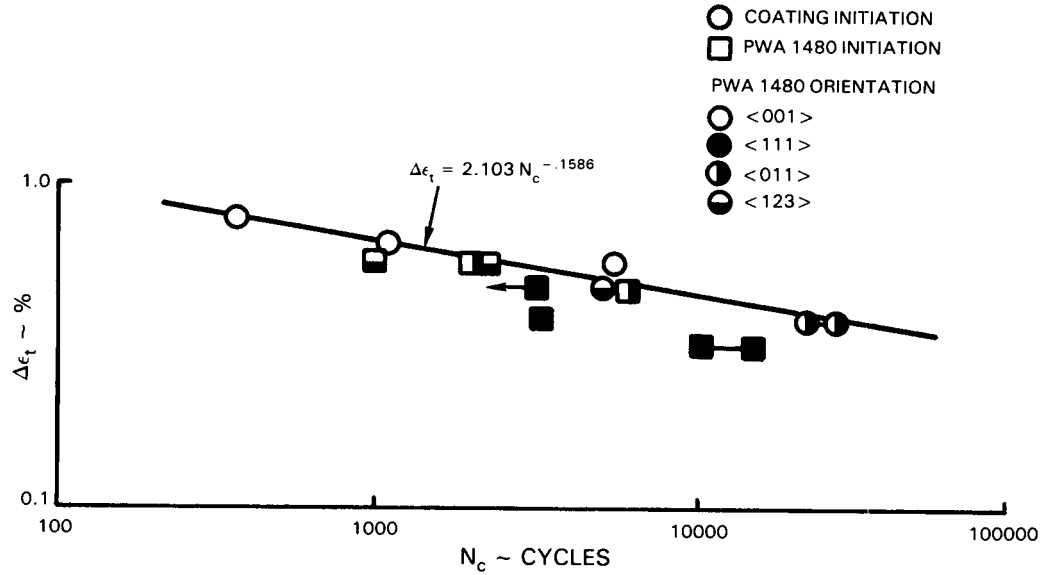


Figure 4 Total Strain Correlation of PWA 273 Aluminide Coating Cracking Life at 927C (1700F).

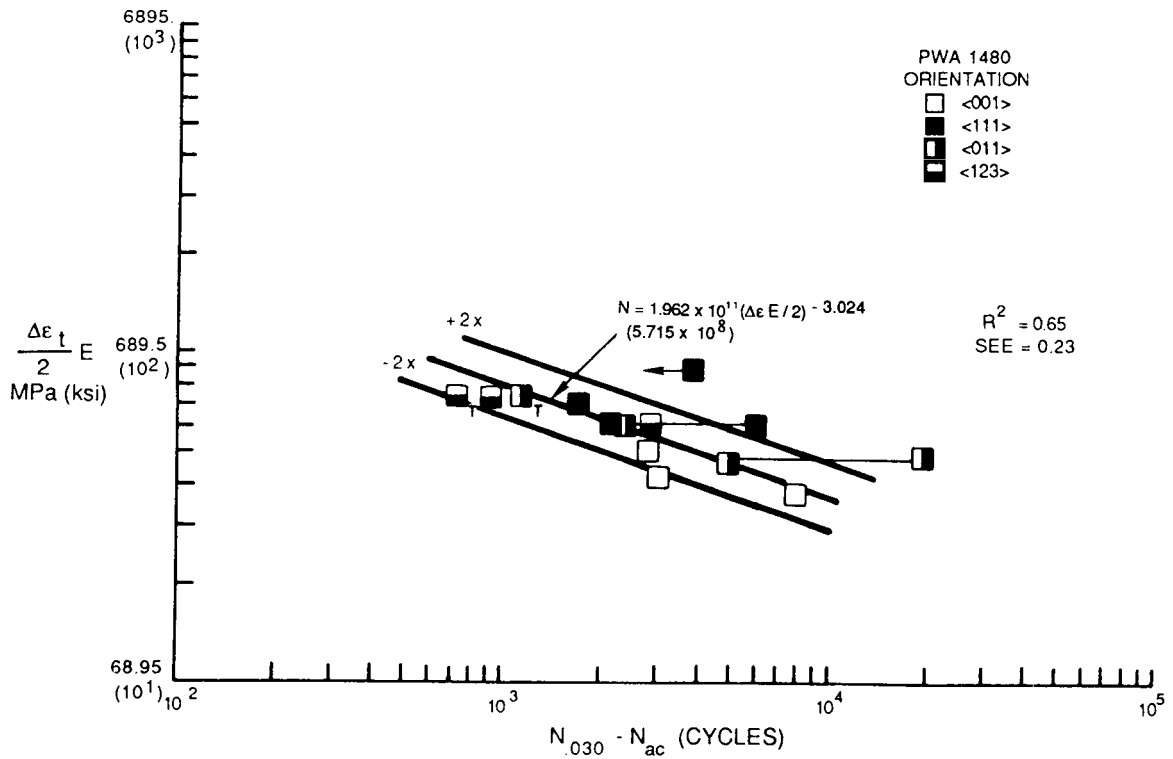


Figure 5 Modified Strain Range Model Correlation of PWA 273 Coated PWA 1480 Cracking Lives at 971C (1700F).

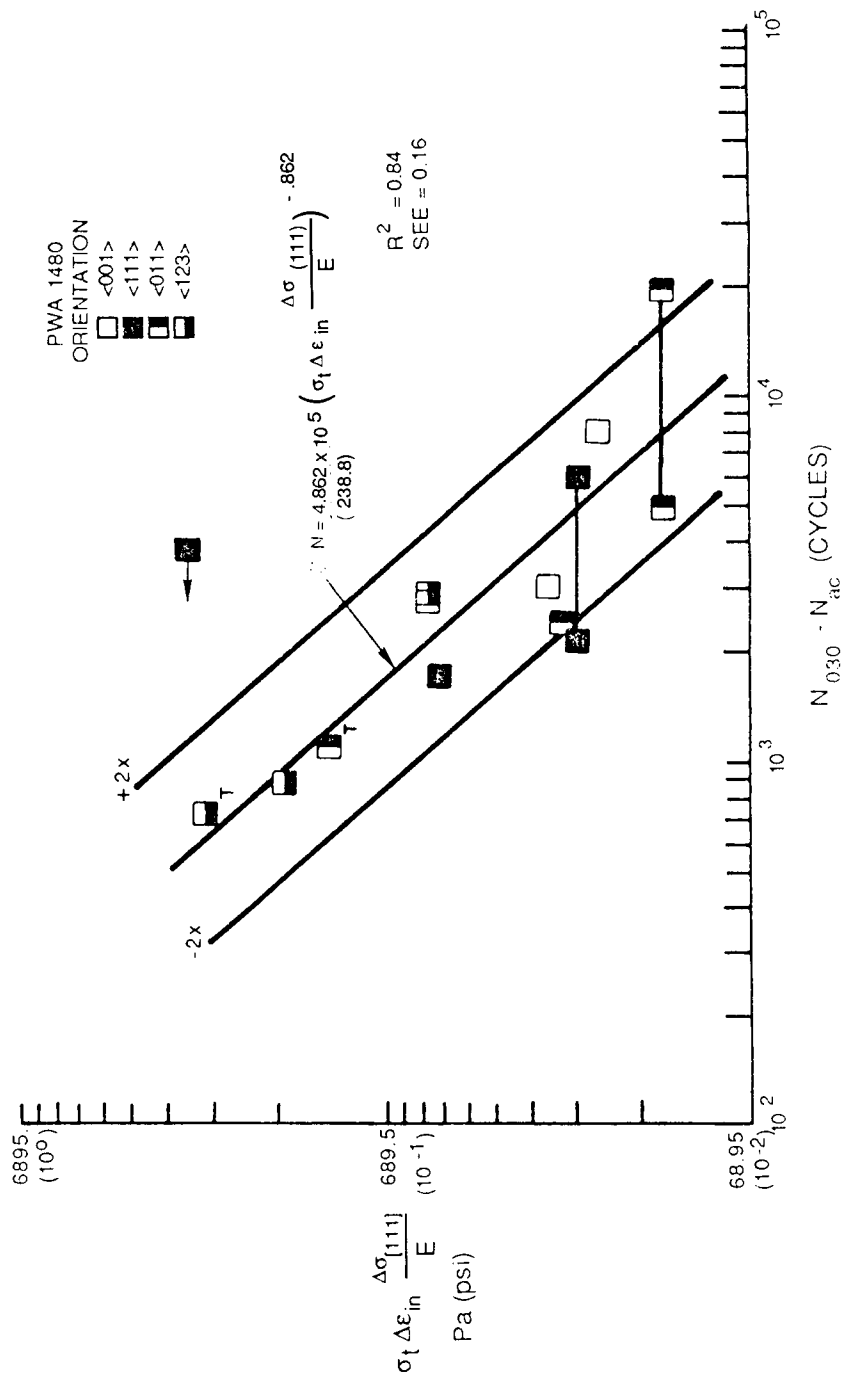


Figure 6 Modified Hysteretic Energy Model Correlation of PWA 273 Coated PWA 1480 Cracking Lives at 971C (1700F).

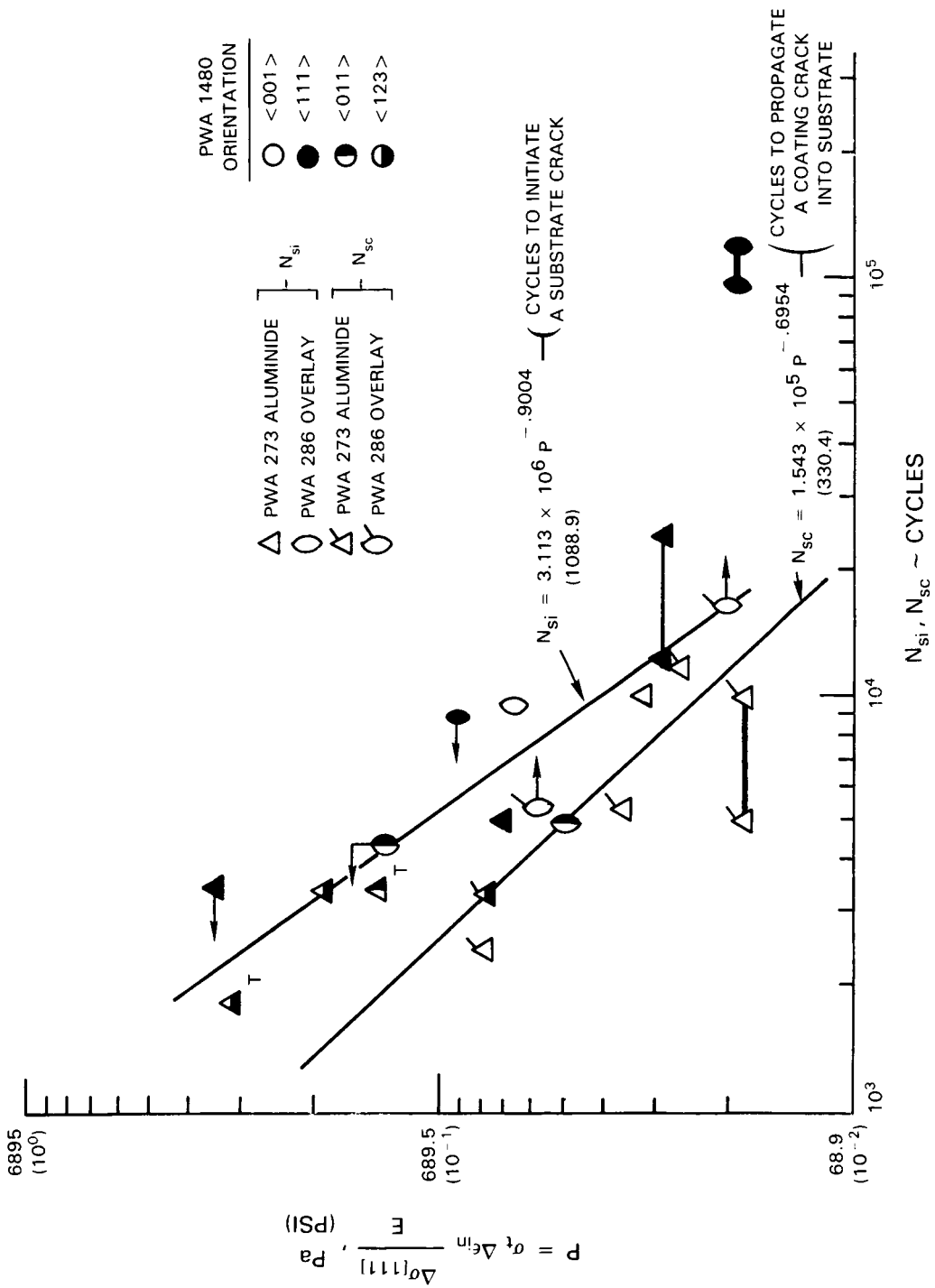


Figure 7 Modified Hysteretic Energy Approach Correlation of PWA 1480 Lives at 972C (1700F). Both N_{sc} and N_{si} Crack Initiation Modes are Shown.