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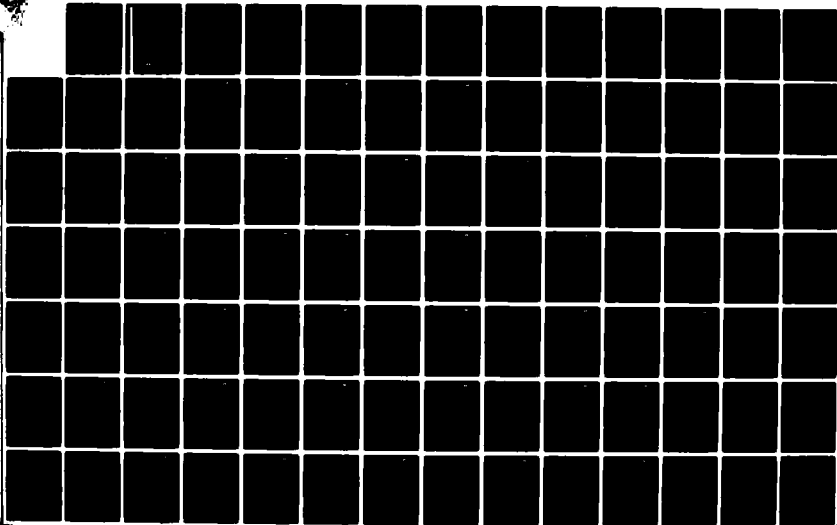
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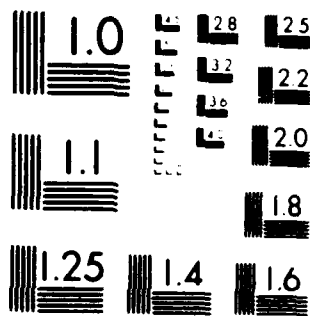
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VOLUME II

CAD/CAM HANDBOOK FOR POLYMER
COMPOSITE RELIABILITY

FINAL REPORT FOR THE PERIOD
November 1, 1980 through October 31, 1982

CONTRACT NO. DAAG29-80-C-0137

Prepared for

U.S. Army Research Office
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MARCH 1983

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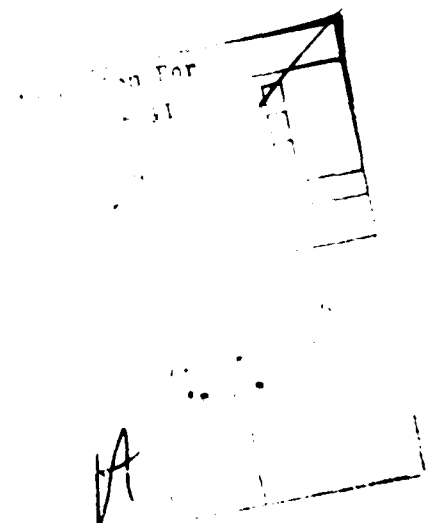
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**CAD/CAM HANDBOOK FOR POLYMER
COMPOSITE RELIABILITY**

**VOLUME II
FIGURES AND TABLES**





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Table 1-1

THE DEACON'S MASTERPIECE:
Or the Wonderful "One-Hoss-Shay."*
A Logical Story

Have you heard of the wonderful one-hoss-shay,
That was built in such a logical way
It ran a hundred years to a day,
And the, of a sudden - ah, but stay,
I'll tell you what happened without delay,

At age one hundred years to the day
There are traces of age in a one-hoss-shay
A general flavor of mild decay
But nothing local, as one may say.
There couldn't be, - for the Deacon's art
Had made it so like in very part
That there wasn't a chance for one to start.
And yet, as a whole, it is past a doubt
In another hour it will be worn out!

This morning the parson takes a drive.
All at once the horse stood still,
Close by the meet'n'-house on the hill.
-First a shiver, and then a thrill,
Then something decidedly like a spill,-
And the parson was sitting upon a rock,

-What do you think the parson found,
When he got up and stared around?
The poor old chaise in a heap or mound,
You see, of course, if you're not a dunce,
How it went to pieces at once,-
All at once, and nothing first,-
Just as bubbles do when they burst.

*Exerpts from a poem by Oliver Wendell Holmes, in "The Autocrat of the Breakfast Table," pp. 252-256, The Riverside Press, Cambridge, Mass. (1895) relating to "Structural design for reliability."

Table 1-2

Interaction Matrix Between Molecular Property and Mechanical Requirement;
 3 = Strong Interaction, 2 = Medium, 1 = Negligible, - = Unknown,
 Σ - Sum of Interactions

Molecular Property	Mechanical Requirement					
	T_g	E_e	τ_0	n	E_g	Σ
Volume Fraction Plasticizer	3	3	3	1	1	11
Volume Fraction Filler	2	3	2	3	1	11
Degree of Crystallinity	1	3	3	3	1	11
Molecular Weight	3	3	1	1	1	9
Crosslink Density	1	3	1	2	1	8
Chain Stiffness	3	1	0	2	1	7
Monomeric Friction Coefficient	3	1	3	0	0	7
Heterogeneity Index	2	1	2	1	1	7
Entanglement Molecular Wt	1	3	1	1	1	7
Solubility Parameter	3	1	0	0	2	6
Σ	22	22	16	14	10	

* T_g = glass temp; Modulus (E) vs time (t) = $E(t) = E_e + [E_g - E_e] [1 + t/\tau_0]^{-n}$
 where E_e = elastomeric modulus, E_g = glass modulus, τ_0 = glass to rubber relaxation time, n = exponent.



Table 1-3
Nomenclature for Polymer Reliability Relations

Symbol	Meaning
T_g	Reference glass transition defined by monomer composition.
ΣU_c	Summation of molecular molar cohesion.
Σh	Summation of molecular degrees of freedom.
$C(t)$	Time scale correction factor $C(t) = 25^\circ\text{C}$.
T_g	Nominal T_g as affected by mechanical (tensile) stress σ , moisture concentration C_{H_2O} , and U.V. radiation effects on polymer reciprocal molecular weight (M^{-1} , number average).
a_T	Time shift factor for rheological response.
T	Test temperature.
M_t	Time dependent modulus.
M_0	Glass (solid) state modulus.
M_r	Rubbery state modulus.
t, n	Test time and exponent.
τ_1	Relaxation time for glass to rubber transition.
τ_2	Terminal time for rubber to flow transition.
R_t	Reliability ($\equiv$ survival probability).
R_∞	Residual reliability at infinite time.
τ_0	Relaxation time for Weibull failure process.
σ_0	Stress (tensile) for Weibull failure process.
ϵ_0	Strain (tensile) for Weibull failure process.
$m(t), m(\sigma), m(\epsilon)$	Weibull distribution shape factors for time (t), stress (σ), and strain (ϵ) dominated failure.

Table 1-4
Weibull Strength Distributions

Composite Polymer		Test	Strength Distribution $R = \exp -(\sigma/\sigma_0)^m$	
EPON 828/CTBN % CTBN	T(°C)	Tensile	σ_0 (Kg/cm ²)	m(σ)
0	-150	N = 15	812	7.64
17	-150	14	679	9.78
50	-150	14	1274	15.5
0	100	15	95.6	6.82
17	100	15	42.1	8.33
50	100	15	26.6	5.44
<u>Uniaxial Graphite/Epoxy</u>		Interlaminar		
Herc. AS/3501-5		Shear	σ_0 (Kg/cm ²)	m(σ)
23°C air + 232°C spike		N = 18	1054	7.60
100°C water + 232°C spike		16	601	2.20
<u>Metal-Adhesive Joint</u>		Single Lap Shear		
AT2024T3-HT424 Epoxy SET (hr)	BET (hr)		σ_0 (Kg/cm ²)	m(σ)
0	0	N = 12	232	14.5
0	165, 449	12	184	15.4
0	808, 1023	12	165	10.0
21	0	12	208	15.0
20	669, 983	12	160	18.1
Ti-6Al-4V-HT424 Epoxy SET (hr)	BET (hr)		σ_0 (Kg/cm ²)	m(σ)
0	0	N = 12	270	7.65
0	(670, 1016)	12	182	6.22
21	0	12	272	7.65
21	(591, 997)	12	202	3.35

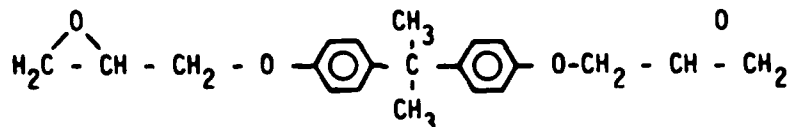
SET = surface exposure time

BET = bond exposure time at 54°C and 95% relative humidity.

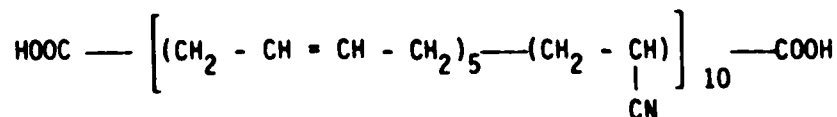


Table 1-5
Co-reactants for Three-Dimensional Epoxy-Nitrile
Rubber Block Copolymers

1. Epoxy: DGEBA (Epon 828, Shell Chemical Company), 100 pbw (parts by weight), $M_n = 380$ gm/mole.



2. Catalyst: Piperidine - 5 pbw
3. Carboxy terminated nitrile rubber (HYCAR CTBN, B.F. Goodrich Chemical Company) - 0, 17, 29, 39, 50% by weight based on 100 pbw Epoxy + 5 pbw piperidine.



$M_n = 3300 - 3500$ gm/mole

4. Mix items (1), (2), (3), above, degas, and cure for 16 hours at 120°C under dry N_2 .

Table 1-6
Chemical Characterization of Graphite-Epoxy Prepreg Materials

	This Study		Reference System
1) Epoxy Matrix	Hercules 3501-5	Fiberite 934	NARMCO 5208
2) Graphite Fiber	Hercules Type AS	U. Carbide T300	U. Carbide T300
3) % Total DDS Curative by IR Spectroscopy	29.2	27.8	22.1
4) % Free DDS Curative by Liquid Chromatography	18.1	14.5	17.8
5) Epoxide Equivalent	205	227	173
6) Wt% BF_3 Type Boron	0.047	0.022	0.0005
7) Relative Degree of Cure by Liquid Chromatography	22	27	6.9
8) Heat of Polymerization by DSC (cal/g polymer)	107	107	140



Table 1-7

Metal Joint Reliability Studies

1. Metal Adherends: Unclad 2024-T3 aluminum alloy surface treated by standard FPL sulfuric chromate etch and T8-6Al-4V titanium alloy treated by standard phosphate fluoride cleaning process. Coupon size 0.063 in. thick, 1 in. wide, and 4 in. long.
2. Adhesive: HT 424 epoxy-phenolic film adhesive (from American Cyanamid) with glass fiber carrier and standard weight 0.0135 ± 0.005 lb/sq. ft. Unfilled HT 424 primer with parts A and B used with adhesive.
3. Bonding Process: Treated metal coupons spray primed with 0.001 in. thickness HT 424 primer solution using clean dry argon carrier gas. Primer layers dried 30 min ambient 23°C and 60 min at 66°C . An adhesive film is placed in the 1.000 in. $\times$ 0.500 in. overlap between two metal adherends. Six such joints are aligned in a bonding jig with the glass carrier acting to provide constant glue line thickness 0.008 in. Cure cycles with 60 min temperature rise to 171°C and 60 min cure cycle at 171° followed by cooling to room temperature.
4. Tensile Lap Shear Testing: 1.5 in. $\times$ 1.0 in. $\times$ 0.063 in. aluminum alignment shims bonded to eliminate offset. Tests at 23°C using 0.01 in./min Instron crosshead rate and 4.5 in. jaw separation.



Table 2-1
Detailed Listing of Characterization Methods
(Sheet 1 of 4)

1. Chemical Quality Assurance

1. HPLC (high performance liquid chromatography)
2. GC/MS (gas chromatography/mass spectroscopy)
3. FTIR (Fourier transform infrared spectroscopy)
4. NMR (nuclear magnetic resonance spectroscopy)
5. Elemental Analysis
6. Surface Analysis

2. Processability Testing

1. DSC (differential scanning calorimetry)
2. TMA (thermal mechanical analysis)
3. DMA (dynamic mechanical analysis)
4. TGA (thermal gravimetric analysis)
5. SEA (surface energy analysis)

3. Cure Monitoring and Management

1. Temperature/Pressure/Vacuum
2. AC Dielectrometry
3. DC Conductivity
4. Acoustic Emission

4. Non-destructive Evaluation

1. US (ultrasonic) immersion C-scan reflector plate
2. US immersion C-scan through transmission
3. US contact through transmission
4. US contact pulse-echo
5. Fokker bond tester
6. 210 sonic bond tester
7. Sondicator
8. Harmonic bond tester
9. Neutron radiography
10. Low KV x-ray
11. Coin tap test
12. Acoustic emission
13. Thermography

5. Surface NDE

1. Ellipsometry
2. Surface Potential Difference (SPD)
3. Photoelectron Emission (PEE)
4. Surface Remission Photometry (SRP)

Table 2-1
(Sheet 2 of 4)

6. Performance and Proof Testing					
The following presents a listing of the properties of plastics reported in this book, the ASTM test numbers and the equivalent DIN test:					
ASTM-DIN Test Equivalents					
	Units of Measure		SI	Test	
	English	Metric		ASTM	DIN
<u>Processing</u>					
1. Processing Methods	°F	°C			
2. Comp'n Molding Temp	°F	°C			
3. Inject Stock Melt Temp	°F	°C			
4. Extrusion Temp	°F	°C			
5. Bulk Factor				D1895	D[53466]
6. Linear Mold Shrinkage	in./in.			D955	D[53464]
7. Melt Flow		g/10 min		D1238	D[53735]
8. Melting Point	°F	°C			
9. Density	lb/ft ³	g/cm ³	Mg/m ³	D792	D[53479]
10. Specific Volume	in. ³ /lb	cm ³ /g	m ³ /Mg	D792	D[53479]
<u>Mechanical Properties</u>					
11. Tensile Str. yield	10 ³ lb/in. ²	10 ² kg/cm ²	MPa	D638	
12. Tensile Str. Break	10 ³ lb/in. ²	10 ² kg/cm ²	MPa	D638	D[53455]
13. Tensile Str. low temp	10 ³ lb/in. ²	10 ² kg/cm ²	MPa	D638	D[53455]
14. Tensile Str. high temp	10 ³ lb/in. ²	10 ² kg/cm ²	MPa	D638	D[53455]
15. Elongation %, yield				D638	D[53455]
16. Elongation %, break				D638	D[53455]
17. Tensile Modulus	10 ⁵ lb/in. ²	10 ⁴ kg/cm ²	GPa	D638	D[53457]
18. Flexural Str. yield	10 ³ lb/in. ²	10 ² kg/cm ²	MPa	D790	D[53452]
19. Flexural Modulus	10 ⁵ lb/in. ²	10 ⁴ kg/cm ²	GPa	D790	D[53457]
20. Stiffness in Flex.	10 ⁵ lb/in. ²	10 ⁴ kg/cm ²	GPa	D747	
21. Compressive Str.	10 ³ lb/in. ²	10 ² kg/cm ²	MPa	D695	D[53454]
22. Izod. notched R.T.	ft lb/in.	Kg cm/cm	kJ/m	D256	
23. Izod. low temp	ft lb/in.	Kg cm/cm	kJ/m	D256	
24. Hardness	(test)				



Table 2-1
ASTM-DIN Test Equivalents
(Sheet 3 of 4)

	Units of Measure		SI	Test	
	English	Metric		ASTM	DIN
<u>Thermal Properties</u>					
25. Thermal Conductivity	BTU in./hr ft ² °F	10 ⁻⁴ cal/sec cm ² °C/cm	W/Km	C177	D[52612]
26. Specific Heat	BTU in./hr ft ²	cal/g°C	kJ/kg K	C351	
27. Linear Therm. Expan	10 ⁶ in./in.°F	10 ⁻⁵ mm/mm		D696	D[52328]
28. Vicat Soft Point	°F	°C		D1525	D[53460]
29. Brittle Temp	°F	°C		D746	
30. Continuous Svc Temp	°F	°C			
31. Defl Temp 264 lb/in. ² ,	18.5 kg/cm ²	1.81 MPa		D648	D[53461]
	°F	°C			
32. Defl Temp 66 lb/in. ² ,	4.6 kg/cm ²	0.45 MPa		D648	D[53461]
	°F	°C			
33. U.L. Temp Index		°C/mm			
<u>Electrical Properties</u>					
34. Volume Resistivity		Ohm cm		D257	D[53482]
35. Surface Resistivity		Ohm		D257	D[53482]
36. Insulation Resistance		Ohm		D257	D[53482]
37. Dielectric Strength	V/10 ⁻³ in.	kV/mm	MV/m	D149	D[53481]
38. Dielectric Constant	50-100 Hz			D150	D[53483]
39. Dielectric Constant	10 ² Hz			D150	D[53483]
40. Dielectric Constant	10 ⁴ Hz			D150	D[53483]
41. Dissipation Factor	50-100 Hz			D150	D[53483]
42. Dissipation Factor	10 ³ Hz			D150	D[53483]
43. Dissipation Factor	10 ⁴ Hz			D150	D[53483]
<u>Optical Properties</u>					
44. Refractive Index, Sodium D				D542	D[53491]
45. Clarity					
<u>Environmental Properties</u>					
46. Water Absorp. %, 24 hr				D570	D[53473]
47. Equil. Water Content %				D570	D[53473]

Table 2-1
(Sheet 4 of 4)

7. Durability Analysis and Service Life Prediction
(Some Current Programs)

1. U.S. Army Composite Materials Research Program (AMMRC).
2. AFML, "Processing Science of Epoxy Resin Composites, Contract No. F33615-80-C-5021.
3. AFML/ARPA, "Quantitative NDE, Contract No. F33615-74-C-5180.
4. AFML, "Integrated Methodology for Adhesive Bonded Joint Life Predictions," Contract No. F-33615-79-C-5088.



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Table 2-2

Standard Units and Conversion Factors

ASTM TEST DESCRIPTIONS AND UNITS
To Convert To Convert

To Convert To Convert

Metric Units	Metric Units	SI Units	English Units	Property	SI Units	English Units	Metric Units
kg/cm ²	1.0	kg/m ²	0.016	Density	kg/m ³	lb/ft ³	0.016
kgf/cm ²	10.196	kg/m ² or MPa	0.0069	Tensile Strength	MPa	lb/in ²	0.0703
kgf/cm ²	10.196	kg/m ² or MPa	0.0069	Tensile Modulus	MPa	lb/in ²	0.0703
kgf/cm ²	10.196	kg/m ² or MPa	0.0069	Flexural Strength	MPa	lb/in ²	0.0703
kgf/cm ²	10.196	kg/m ² or MPa	0.0069	Flexural Modulus	MPa	lb/in ²	0.0703
kgf/cm ²	10.196	kg/m ² or MPa	0.0069	Compressive Strength	MPa	lb/in ²	0.0703
kgf/cm ²	10.196	kg/m ² or MPa	0.0069	Impact	kJ/m ²	ft lb/in ²	5.44
kgf/cm ²	10.196	kg/m ² or MPa	0.0069	Charpy Impact	kJ/m ²	ft lb/in ²	2.181
kgf/cm ²	10.196	kg/m ² or MPa	0.0069	Thermal Conductivity	W/m	BTU in/hr ft ² F	3.45x10 ⁻⁶
cal/sec cm C	23.89	W/m	0.144	Specific Heat	kJ/kg	BTU/lb F	1.0
cal/g C	0.239	kJ/kg	4.187	Linear Expansion	m/m K	in/in F	1.8
cm/cm C	1.0	m/m K	1.8	Dielectric Strength	MPa	V/10 ⁻³ in	0.0394
W/m	1.0	W/m	0.0394				

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Temperature Conversion
 $^{\circ}\text{C} = (^{\circ}\text{F} - 32) \times 1.8$
 $^{\circ}\text{F} = (^{\circ}\text{C} \times 1.8) + 32$

$^{\circ}\text{C} = ^{\circ}\text{F} - 32$
 $^{\circ}\text{F} = ^{\circ}\text{C} + 32$

Special names and symbols for a few typical SI units are listed below:
The following table lists SI units prefixes for decimal multiplication and submultiples

Quantity	Name	Symbol	Factor	Prefix	Symbol
frequency	Hertz	Hz	10 ¹⁸	exa	E
power	Watt	W	10 ¹⁵	peta	P
electrical/resistance	Ohm	Ω	10 ¹²	tera	T
electrical/potential	Volt	V	10 ⁹	giga	G
force	Newton	N	10 ⁶	mega	M
pressure	Pascal	Pa	10 ³	kilo	k
energy, work	Joule	J	10 ²	hecto	h
length	meter	m	10 ¹	deka	da
mass	kilogram	kg	10 ¹	deci	d
time	second	s	10 ⁻²	centi	c
thermodynamic/temperature	Kelvin	K	10 ⁻³	milli	m
			10 ⁻⁶	micro	μ
			10 ⁻⁹	nano	n
			10 ⁻¹²	pico	p
			10 ⁻¹⁵	femto	f
			10 ⁻¹⁸	atto	a

Table 2-3
Detailed Listing of Characterized Properties

1. Chemical Quality Assurance
 1. Chemical composition
 2. Degree of cure
 3. Molecular weight distribution
 4. Number average molecular weight
 5. Weight average molecular weight
 6. Entanglement molecular weight
2. Processability
 1. Gel point
 2. Gel fraction
 3. Crosslink molecular weight
 4. Glass temperature
 5. Melt (flow) temperature
 6. Dynamic storage modulus
 7. Dynamic loss modulus
3. Cure Monitoring
 1. Temperature/pressure/vacuum
 2. Dynamic dielectric constant
 3. Dielectric loss factor
 4. DC conductivity
4. Nondestructive Evaluation
 1. Internal stress distributions
 2. Damage zone size
 3. Crack growth rate
5. Performance and Proof Testing
 1. Stress and environment dependent T_g
 2. Stress and environment dependent T_m
 3. Isothermal stress-strain-time-response
 4. Strength distribution
 5. Extensibility distribution
 6. Fracture energy distribution
6. Combined Bonding and Failure Testing
 1. Surface energy
 2. Surface chemistry
 3. Surface morphology
 4. Surface roughness



Table 2-4

Classification of Chromatographic Methods

- | |
|---|
| I. Gas Chromatography (GC)
Gas liquid (GLC)
Gas solid (GSC) |
| II. High Performance Liquid Chromatography (HPLC)
A. Planar Chromatography
Thin layer (TLC)
Paper (PC)
B. Column Chromatography
Exclusion (EC)
Gel Permeation (GPC)
Gel filtration (GFC)
Liquid-solid or adsorption (LSC)
Liquid-liquid or partition (LLC)
Bonded phase (BPC)
Ion exchange (IEC) |

From: H.M. McNair, American Laboratory, May 1980, pp. 33-44.

Table 2-5

Decision Matrix of Surface Characterization Methods for
Reinforcing Fiber Coatings (35 to 70 nm thickness)

4 = Excellent 3 = Acceptable 2 = Marginal 1 = Unacceptable 0 = No Information	Coating Durability	Molecular Orientations	Surface Concentration of Components	Surface Coating Uniformity	Fiber Curvatures	Adhesion Strength	Thickness Uniformity	Average Coating Thickness	Row Ave.
	3	4	3	4	4	2	1	1	2.75
	4	1	1	4	4	1	4	1	2.5
	4	4	4	1	1	1	1	1	2.13
	4	1	1	1	1	4	1	1	1.75
Surface Energy Analysis	3	4	3	4	4	2	1	1	2.75
Scanning Elect. Mic. + EDAX	4	1	1	4	4	1	4	1	2.5
Electron Spect. for Chem. Anal.	4	4	4	1	1	1	1	1	2.13
ASTM Adhesion Test	4	1	1	1	1	4	1	1	1.75
Fourier Transform IR	2	2	3	1	1	1	1	1	1.50
Optical Microscopy	1	1	1	1	1	1	1	1	1.0
Secondary Ion Mass Spec.	1	1	1	1	1	1	1	1	1.0
Laser Microprobe Mass Analyser	1	1	1	1	1	1	1	1	1.0
Raman Microspectroscopy	1	1	1	1	1	1	1	1	1.0
Col Ave.	2.33	1.78	1.78	1.67	1.67	1.44	1.33	1.00	



Table 2-6
Decision Matrix Between Nondestructive Evaluation (NDE)
Built-In Defects in Laminate Panels

Built-In Defects in Laminate Panels	Nondestructive Test (NDE) Method												Row Ave.
	(a) Reflector Plate	(b) 210 Sonic Bond	(c) Through Transmission	(d) Forker Bond Tester	(e) Contact Through Transmission	(f) Contact Pulse-Echo	(g) Immersion C-Scan	(h) Pulse-Echo	(i) Sonicator	(j) Harmonic Bond Tester	(k) Neutron Radiography	(l) Coin Tap Test	(m) Low KV X-Ray
(1) Void	2	2	2	2	2	2	2	2	2	2	2	1	0
(2) Void (C-10 repair)	2	2	2	2	2	2	2	2	2	2	2	1	0
(3) Void (9309 repair)	2	2	2	2	2	2	2	2	2	2	2	1	0
(4) Corroded Bond	2	2	2	2	2	2	2	2	2	2	2	1	0
(5) Lack of Bond (skin to adhesive)	2	2	2	2	2	2	2	2	2	2	2	1	0
(6) Porous Adhesive	2	2	2	2	2	2	2	2	2	2	2	1	0
(7) Manufacturer's Separator Sheet	2	2	2	2	2	2	2	2	2	2	2	1	0
(8) Burned Adhesive	2	2	2	2	2	2	2	2	2	2	2	1	0
(9) Thick Adhesive (1, 2, 3 ply)	2	2	2	2	2	2	2	2	2	2	2	1	0
Col. Ave.	2.00	1.89	1.89	1.78	1.67	1.56	1.56	1.56	1.77	1.77	1.77	0.56	0.44

Direction of Decreasing
Correlation:
0 = Defect Not Detected;
1 = Partial Detection;
2 = Detected

Table 2-7
Decision Matrix Between Nondestructive Evaluation (NDE)
Defects in Honeycomb Structures

Direction of Decreasing Correlation: 0 = Defect Not Detected; 1 = Partially Detected; 2 = Detected	Nondestructive Test (NDT) Method											Row Ave.
	(a) Neutron Radiography	(b) Coin Tap Test	(c) Contact Through Transmission	(d) Transmission C-Scan Pulse-Echo	(e) Transmission C-Scan Through Transmission	(f) Forker Bond Tester	(g) Low KV X-Ray	(h) Harmonic Bond Tester	(i) 210 Sonic Indicator	(j) Contact Pulse-Echo	(k) Contact Shear Wave	
(1) Void (Foam to Closure)	2	2	2	2	2	2	2	2	2	2	0	1.83
(2) Void (Adhesive to Skin)	2	2	2	2	2	2	2	2	2	2	0	1.67
(3) Inadequate Tie-In of Foam to Core	2	2	2	2	2	2	2	2	2	0	0	1.50
(4) Void (Adhesive to Core)	2	2	2	2	2	0	2	2	0	0	0	1.33
(5) Separator Sheet (Skin to Adhesive)	2	2	2	2	2	0	0	1	0	1	0	0.92
(6) Water Intrusion	2	2	2	0	2	0	2	0	0	0	0	0.83
(7) Crushed Core (After Bonding)	1	2	1	1	1	1	2	1	0	0	0	0.83
(8) Inadequate Foam Depth At Closure	2	1	0	0	0	2	2	0	1	2	0	0.83
(9) Separator Sheet (Adhesive to Core)	2	2	0	2	1	0	0	0	0	0	2	0.75
(10) Chem-Mill Step Void	2	0	0	0	0	0	0	0	0	0	0	0.17
Col. Ave.	1.90	1.60	1.30	1.30	1.20	1.10	1.00	1.00	0.9	0.8	0.7	0



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Table 3-1
Properties of the Elements
(Sheet 1 of 2)

Code No.	Z	SY	W G/Mole	D 10 ⁵ J/Mole	X	R 10 ⁻¹⁰ m	V	MV	S
1	1	H	1.008	4.35	2.20	0.32	1	1	3.13
2	3	LI	6.941	1.11	0.98	1.23	1	1	0.81
3	3	BE	9.012	(2.28)	1.57	0.90	2	2	2.22
4	5	B	10.81	(2.53)	2.04	0.82	3	3	3.66
5	6	C	12.01	3.48	2.55	0.77	4	4	5.19
6	7	N	14.01	1.61	3.04	0.75	3	5	6.67
7	8	O	16.00	1.39	3.44	0.73	2	2	2.74
8	9	F	19.00	1.53	3.98	0.72	1	1	1.39
9	11	NA	22.99	0.753	0.93	1.54	1	1	0.65
10	12	MG	24.31	(0.971)	1.31	1.36	2	2	1.47
11	13	AL	26.98	(2.06)	1.61	1.18	3	3	2.54
12	14	SI	28.09	1.77	1.90	1.11	4	4	3.60
13	15	P	30.97	2.15	2.19	1.06	5	5	4.72
14	16	S	32.06	2.13	2.58	1.02	6	6	5.88
15	17	CL	35.45	2.43	3.16	0.99	1	7	7.07
16	19	K	39.09	0.552	0.82	2.03	1	1	0.49
17	20	CA	40.08	(1.15)	1.00	1.74	2	2	1.15
18	21	SC	44.96	(2.58)	1.36	1.44	3	3	2.08
19	22	TI	47.90	(2.64)	1.54	1.32	4	4	3.03
20	23	V	50.94	(3.36)	1.63	1.22	5	5	4.10
21	24	CR	52.00	(2.38)	1.66	1.18	3	6	5.08
22	25	MN	54.94	(1.43)	1.55	1.17	2	7	5.98
23	26	FE	55.85	(2.03)	1.83	1.17	3	3	2.56
24	27	CO	58.93	(2.20)	1.88	1.16	2	3	2.59
25	28	NI	58.70	(2.12)	1.91	1.15	2	3	2.61
26	29	CU	63.55	(1.72)	1.90	1.17	2	2	1.71
27	30	ZN	65.38	(0.653)	1.65	1.25	2	2	1.60
28	31	GA	69.72	(1.36)	1.81	1.26	3	3	2.38
29	32	GE	72.59	1.57	2.01	1.22	4	4	3.28
30	33	AS	74.92	1.34	2.18	1.20	3	5	4.17
31	34	SE	78.96	1.84	2.55	1.16	4	6	5.17
32	35	BR	79.90	1.93	2.96	1.14	1	7	6.14
33	37	RB	85.47	0.519	0.82	2.16	1	1	0.46
34	38	SR	87.62	(1.05)	0.95	1.91	2	2	1.05
35	39	Y	88.91	(2.74)	1.22	1.62	3	3	1.85
36	40	ZR	91.22	(3.45)	1.33	1.45	4	4	2.76
37	41	NB	92.91	(4.85)	1.60	1.34	5	5	3.73

Table 3-1
Properties of the Elements
(Sheet 2 of 2)

Code No.	Z	SY	W G/Mole	D 10 ⁵ J/Mole	X	R 10 ⁻¹⁰ m	V	MV	S
38	42	MO	95.94	(4.30)	2.16	1.30	6	6	4.62
39	43	TC	98.0	(3.35)	1.90	1.27	7	7	5.51
40	44	RU	101.07	(3.35)	2.20	1.25	3	8	6.40
41	45	RH	102.91	(3.24)	2.28	1.25	3	4	3.20
42	46	PD	106.4	(1.93)	2.20	1.28	2	4	3.13
43	47	AG	107.87	(1.44)	1.93	1.34	1	1	0.75
44	48	CD	112.41	(0.552)	1.69	1.48	2	2	1.35
45	49	IN	114.82	(1.18)	1.78	1.44	3	3	2.08
46	50	SN	118.69	1.43	1.96	1.41	4	4	2.84
47	51	SB	121.75	1.26	2.05	1.40	3	5	3.57
48	52	TE	127.60	1.38	2.10	1.36	4	6	4.41
49	53	I	126.90	1.51	2.66	1.33	1	7	5.26
50	55	CS	132.91	0.448	0.79	2.35	1	1	0.43
51	56	BA	137.33	(1.12)	0.89	1.98	2	2	1.01
52	57	LA	138.91	(2.48)	1.10	1.69	3	3	1.78
53	72	HF	178.49	(4.72)	1.30	1.44	4	4	2.78
54	73	TA	180.95	(5.56)	1.50	1.34	5	5	3.73
55	74	W	183.85	(5.61)	2.36	1.30	6	6	4.62
56	75	RE	186.21	(3.97)	1.90	1.28	7	7	5.47
57	76	OS	190.2	(3.64)	2.20	1.26	4	8	6.35
58	77	IR	192.22	(3.48)	2.20	1.27	4	6	4.72
59	78	PT	195.09	(2.79)	2.28	1.30	4	4	3.08
60	79	AU	196.97	(1.86)	2.54	1.34	3	3	2.24
61	80	HG	200.59	(0.301)	2.00	1.49	2	2	1.34
62	81	TL	204.37	(0.866)	2.04	1.48	1	3	2.03
63	82	PB	207.2	(0.992)	2.33	1.47	2	4	2.72
64	83	BI	209.0	(1.03)	2.02	1.46	3	5	3.42
65	90	TH	232.04	(3.42)	1.30	1.65	4	4	2.42
66	92	U	238.03	(3.56)	1.38	1.42	6	6	4.22
67	94	PU	244.0	(2.29)	1.28	1.21	4	6	4.96
68	7	(N2)/2	14.01	4.73	3.04	0.55	3	5	6.67
69	8	(O2)/2	16.00	2.01	3.44	0.62	2	2	2.74



Table 3-2
Comparison of Single Bond Energies

Element	Group	Single Bond Energy (kcal/mol)		
		Ref. 2	Eq. (2) (C.N.=12)	Ratio
Lithium	IA	25.6	6.3	4.06
Sodium	IA	18	4.3	4.19
Potassium	IA	13.2	3.3	4.00
Rubidium	IA	12.4	3.4	3.65
Cesium	IA	10.7	3.0	<u>3.57</u>
				3.89 ± 0.27
Boron	IIIB	25.0	15.1	1.66
Germanium	IVB	37.6	13.2	2.85
Arsenic	VB	32.1	9.5	3.38
Tin	IVB	34.2	11.4	3.00
Antimony	VB	30.2	10.6	<u>2.85</u>
				2.75 ± 0.65

Table 3-3
Lattice Types and Packing Factors

Lattice Type	Coordination Number	Packing Factor (C)
Face centered cubic	12	1.414
Body centered cubic	8	1.299
Simple cubic	6	1.000
Tetrahedral	4	0.650

Table 3-4

Calculation of Heat of Formation for BeO, TiO₂, and Al₂O₃

Z, SY, W, D/1E5, X, R/1E-10, V, PH =

4 BE 9.012 2.28 1.57 0.9 2 7

8 0 16 1.39 3.44 0.73 2 2

To continue press ENTER

?

Chemical Analysis:

Bonding Elements	Bond Energy (J/mole)	% Ionic Energy	Bond Length (M*1E-10)	Moles
A B				
BE BE	228000	0	1.8	-1
(O2)/2(O2)/2	201000	0	1.24	-1
BE O	520951	64.776	1.4617	2
Total	612902			0

To continue press ENTER

Z, SY, W, D/1E5, X, R/1E-10, V, PH =

22 TI 47.0 2.64 1.54 1.32 4 7

8 0 16 1.39 3.44 0.73 2 2

To continue press ENTER

?

Chemical Analysis:

Bonding Elements	Bond Energy (J/mole)	% Ionic Energy	Bond Length (M*1E-10)	Moles
A B				
TI TI	264000	0	2.64	-2
(O2)/2(O2)/2	201000	0	1.24	-2
TI O	549865	63.3547	1.879	4
Total	1.26946E+06			0

To continue press ENTER

Z, SY, W, D/1E5, X, R/1E-10, V, PH =

13 AL 26.98 2.06 1.61 1.18 3 7

8 0 16 1.39 3.44 0.73 2 2

To continue press ENTER

?

Chemical Analysis:

Bonding Elements	Bond Energy (J/mole)	% Ionic Energy	Bond Length (M*1E-10)	Moles
A B				
AL AL	206000	0	2.36	-3
(O2)/2(O2)/2	201000	0	1.24	-3
AL O	495669	65.1986	1.7453	6
Total	1.75301E+06			0

To continue press ENTER

? -



Table 3-5
Comparison of Calculated and Experimental Heats of
Formation for Oxides

Compound	$-\Delta H_f(\text{calc.})$ (10^5 J/mole)	$-\Delta H_f$ (Ref. 7) (10^5 J/mole)	Difference (10^5 J/mole)
Al_2O_3	17.5	16.3	1.20
Fe_2O_3	13.1	11.2	1.90
TiO_2	12.7	9.11	3.59
MgO	8.13	5.20	2.93
SiO_2	7.91	8.56	-0.65
BeO	6.13	6.10	0.03
MoO_2	5.08	5.43	-0.35
WO_2	3.26	5.70	-2.44
Au_2O_3	2.83	-0.80	3.63
SeO_2	1.82	2.29	-0.47
Sum:			0.94
Std. Dev:			± 2.04

Table 3-6
Comparison of Calculated and Experimental Heats of
Formation for Chlorides

Compound	$-\Delta H_f(\text{calc.})$	$-\Delta H_f(\text{Ref. 7})$ (10^5 J/mole)	Difference
AlCl_3	6.95	6.95	0.0
FeCl_3	5.12	4.05	1.07
TiCl_4	10.1	7.50	2.60
MgCl	3.30	6.41	-3.11
SiCl_4	6.12	6.10	0.02
BeCl_2	4.87	5.11	-0.24
MoCl_4	3.86	3.30	0.56
AuCl_3	1.11	1.18	<u>-0.07</u>
Sum:			0.10
Std. Dev:			± 1.60



Table 3-7
Calculation of the Oxidation Dilation Factor ϕ for Metals

Oxide	Calculated (for Z = 12)			Exper. (7,8)	
	V(Me) (CC)	V(MeO _x) (CC) ^x	ϕ	V(MeO _x) (CC) ^x	ϕ
K ₂ O	57.02	20.55	0.36	40.6	0.45
BaO	26.45	13.00	0.49	26.8	0.67
MgO	8.57	6.34	0.74	11.3	0.81
Al ₂ O ₃	11.19	11.32	1.01	25.7	1.28
TiO ₂	7.84	8.48	1.08	18.7	1.78
Fe ₂ O ₃	10.92	11.52	1.05	30.5	2.14
Ta ₂ O ₅	16.40	20.31	1.24	53.9	2.50
Nb ₂ O ₅	16.40	20.60	1.26	59.5	2.68
MoO ₃	7.49	11.96	1.60	30.7	3.30
WO ₃	7.49	12.30	1.64	32.4	3.35

$$\phi = \frac{\text{molecular volume of metal compound MeX}_x}{\text{atomic volume of equal moles of metal Me}}$$

Table 3-8
Correlation Between Metal Oxidation State
and IEPS

Oxide	IEPS Range (pH Units)	Acid-Base Character
M ₂ O	pH > 11.5	strong base
MO	8.5 < pH < 12.5	intermediate base
M ₂ O ₃	6.5 < pH < 10.4	weak base
MO ₂	0 < pH < 7.5	intermediate acid
M ₂ O ₅ , MO ₃	pH < 0.5	strong acid

Table 3-9
Coulomb Bond Energies Between Water and Various Oxides

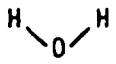
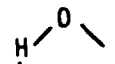
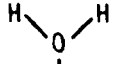
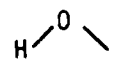
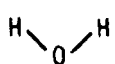
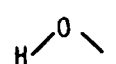
												
(Ag ₂ O)	Ag	O	Ag	O	Ag	O	Ag	O	Ag	O	Ag	O
												
(CuO)	O	Cu	O	Cu	O	Cu	O	Cu	O	Cu	O	Cu
												
(Fe ₂ O ₃)	O	Fe	O	Fe	O	Fe	O	Fe	O	Fe	O	Fe
												
(SiO ₂)	O	Si	O	Si	O	Si	O	Si	O	Si	O	Si
												
(CrO ₃)	O	Cr	O	Cr	O	Cr	O	Cr	O	Cr	O	Cr
												
Adsorbate: H ₂ O Substrate Oxide					Monobasic			Diacid				
					U _M (kJ/mole)							
					U _N			U _M				
								U _N				
Ag ₂ O					11.8			46.5				
CuO					25.7			46.5				
Fe ₂ O ₃					38.5			46.5				
SiO ₂					53.0			46.5				
CrO ₃					76.6			46.5				



Table 3-10

Coulomb Bond Energies Between Ammonia and Various Oxides

(Ag ₂ O)														
	0	Ag	0	Ag	0	Ag	0	Ag	0	Ag	0	Ag	0	Ag
(CuO)														
	0	Cu	0	Cu	0	Cu	0	Cu	0	Cu	0	Cu	0	Cu
(Fe ₂ O ₃)														
	0	Fe	0	Fe	0	Fe	0	Fe	0	Fe	0	Fe	0	Fe
(SiO ₂)														
	0	Si	0	Si	0	Si	0	Si	0	Si	0	Si	0	Si
(CrO ₃)														
	0	Cr	0	Cr	0	Cr	0	Cr	0	Cr	0	Cr	0	Cr
Adsorbate: NH ₃				Monobasic				Diacid						
Substrate Oxide				U _M (kJ/mole)		U _N		U _M		U _N				
Ag ₂ O				17.5		2.0		46.5		9.6				
CuO				38.1		4.3		46.5		9.5				
Fe ₂ O ₃				57.2		6.4		46.5		9.3				
SiO ₂				78.7		8.8		46.5		9.3				
CrO ₃				113.8		13.4		46.5		9.2				

Table 3-11
Coulomb Bond Energies Between Chromium Trioxide and Various Oxides

$\begin{array}{c} \text{O} \\ \parallel \\ \text{O}=\text{Cr}=\text{O} \\ \parallel \\ \text{O} \end{array}$		$\begin{array}{c} \text{O} \\ \parallel \\ \text{O}=\text{Cr}=\text{O} \\ \parallel \\ \text{O} \end{array}$	
(Ag ₂ O)	0 Ag 0 Ag 0 Ag 0 Ag 0 Ag 0 Ag 0 Ag 0 Ag 0	$\begin{array}{c} \text{O} \\ \parallel \\ \text{O}=\text{Cr}=\text{O} \\ \parallel \\ \text{O} \end{array}$	
$\begin{array}{c} \text{O} \\ \parallel \\ \text{O}=\text{Cr}=\text{O} \\ \parallel \\ \text{O} \end{array}$		$\begin{array}{c} \text{O} \\ \parallel \\ \text{O}=\text{Cr}=\text{O} \\ \parallel \\ \text{O} \end{array}$	
(CuO)	0 Cu 0 Cu 0 Cu 0 Cu 0 Cu 0 Cu 0 Cu 0 Cu 0 Cu 0 Cu	$\begin{array}{c} \text{O} \\ \parallel \\ \text{O}=\text{Cr}=\text{O} \\ \parallel \\ \text{O} \end{array}$	
$\begin{array}{c} \text{O} \\ \parallel \\ \text{O}=\text{Cr}=\text{O} \\ \parallel \\ \text{O} \end{array}$		$\begin{array}{c} \text{O} \\ \parallel \\ \text{O}=\text{Cr}=\text{O} \\ \parallel \\ \text{O} \end{array}$	
(Fe ₂ O ₃)	0 Fe 0 Fe 0 Fe 0 Fe 0 Fe 0 Fe 0 Fe 0 Fe 0 Fe 0 Fe 0 Fe	$\begin{array}{c} \text{O} \\ \parallel \\ \text{O}=\text{Cr}=\text{O} \\ \parallel \\ \text{O} \end{array}$	
$\begin{array}{c} \text{O} \\ \parallel \\ \text{O}=\text{Cr}=\text{O} \\ \parallel \\ \text{O} \end{array}$		$\begin{array}{c} \text{O} \\ \parallel \\ \text{O}=\text{Cr}=\text{O} \\ \parallel \\ \text{O} \end{array}$	
(SiO ₂)	0 Si 0 Si 0 Si 0 Si 0 Si 0 Si 0 Si 0 Si 0 Fe 0 Fe 0 Fe	$\begin{array}{c} \text{O} \\ \parallel \\ \text{O}=\text{Cr}=\text{O} \\ \parallel \\ \text{O} \end{array}$	
$\begin{array}{c} \text{O} \\ \parallel \\ \text{O}=\text{Cr}=\text{O} \\ \parallel \\ \text{O} \end{array}$		$\begin{array}{c} \text{O} \\ \parallel \\ \text{O}=\text{Cr}=\text{O} \\ \parallel \\ \text{O} \end{array}$	
(CrO ₃)	0 Cr 0 Cr 0 Cr 0 Cr 0 Cr 0 Cr 0 Cr 0 Cr 0 Cr 0 Cr 0 Cr 0 Cr	$\begin{array}{c} \text{O} \\ \parallel \\ \text{O}=\text{Cr}=\text{O} \\ \parallel \\ \text{O} \end{array}$	
Adsorbate:CrO ₃		Dibasic	
Substrate Oxide		U _M (kJ/mole)	U _N
Ag ₂ O		24.9	8.8
CuO		40.9	14.2
Fe ₂ O ₃		81.7	28.0
SiO ₂		112.8	38.6
CrO ₃		162.7	58.5
		Monoacid	
		U _M	U _N
Ag ₂ O		76.6	27.1
CuO		76.6	26.7
Fe ₂ O ₃		76.6	26.2
SiO ₂		76.6	26.2
CrO ₃		76.6	27.6



Table 3-12

Coulomb Bond Energies Between R-CH₂ Si(OH)₃ and Various Oxides

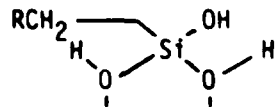
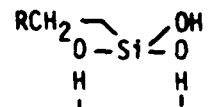
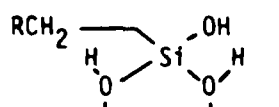
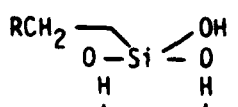
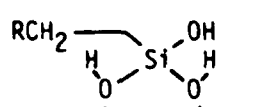
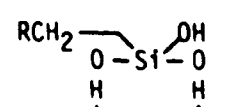
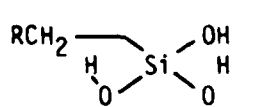
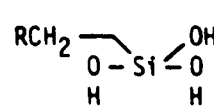
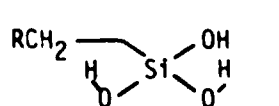
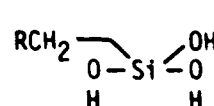
					
(Ag ₂ O) 0 Ag 0 Ag 0 Ag 0 Ag 0 Ag 0 Ag 0 Ag 0	Ag 0 Ag 0 Ag 0				
					
(CuO) 0 Cu 0 Cu 0 Cu 0 Cu 0 Cu 0 Cu 0 Cu 0	Cu 0 Cu 0 Cu 0				
					
(Fe ₂ O ₃) 0 Fe 0 Fe 0 Fe 0 Fe 0 Fe 0 Fe 0 Fe 0	Fe 0 Fe 0 Fe 0				
					
(SiO ₂) 0 Si 0 Si 0 Si 0 Si 0 Si 0 Si 0 Si 0	Si 0 Si 0 Si 0				
					
(CrO ₃) 0 Cr 0 Cr 0 Cr 0 Cr 0 Cr 0 Cr 0 Cr 0	Cr 0 Cr 0 Cr 0				
Adsorbate: R ₃ Si(OH) ₂		Dibasic		Diacid	
Substrate Oxide		U _M (kJ/mole)	U _N	U _M	U _N
Ag ₂ O		23.6	6.63	45.6	16.4
CuO		51.4	14.6	45.6	16.1
Fe ₂ O ₃		77.0	21.8	45.6	15.9
SiO ₂		106.0	30.0	45.6	15.9
CrO ₃		153.2	45.6	45.6	16.7

Table 3-13
Bond Properties for Adsorbates and Substrate Oxides

Bond + - -	D _{AB} (kJ/mole)	%I	L _{AB}	μ (debye)	R _A	R _B
H - O	435	34.1	0.94	1.54	0.32	0.73
H - N	366	18.6	0.99	0.88	0.32	0.75
Cr = O	1051	58.2	1.64	4.58	1.18	0.62
Ag - O	362	60.9	1.93	5.64	1.34	0.73
Cu - O	384	59.5	1.76	5.03	1.17	0.73
Fe - O	421	59.4	1.76	4.56	1.17	0.73
Si - O	387	59.1	1.70	4.82	1.11	0.73
Cr - O	494	61.9	1.75	5.20	1.18	0.73
Si - C	303	13.4	1.82	1.17	1.11	0.77



Table 3-14
Comparison of Revised (Ref. 1 = X) and Pauling (Ref. 2 = X_p)
Values of Elemental Electronegativity

AT. No.	SY	X	X_p	$X - X_p$	AT. No.	SY	X	X_p	$X - X_p$
1	H	2.20	2.1	0.10	37	RB	0.82	0.8	0.02
3	LI	0.98	1.0	-0.02	38	SR	0.95	1.0	-0.05
4	BE	1.57	1.5	0.07	38	Y	1.22	1.2	0.02
5	B	2.04	2.0	0.04	40	ZR	1.33	1.4	-0.07
6	C	2.55	2.5	0.05	41	NB	1.60	1.6	0.0
7	N	3.04	3.0	0.04	42	MO	2.16	1.8	0.36
8	O	3.44	3.5	-0.06	43	TC	1.90	1.9	0.0
9	F	3.98	4.0	-0.02	44	RU	2.20	2.2	0.0
					45	RH	2.28	2.2	0.08
					46	PD	2.20	2.2	0.0
11	NA	0.93	0.9	0.03	47	AG	1.93	1.9	0.03
12	MG	1.31	1.2	0.11	48	CD	1.63	1.7	-0.01
13	AL	1.61	1.5	0.11	49	IN	1.78	1.7	0.08
14	SI	1.90	1.8	0.10	50	SN	1.96	1.8	0.16
15	P	2.19	2.1	0.19	51	SB	2.05	1.9	0.15
16	S	2.58	2.5	0.08	52	TE	2.10	2.1	0.0
17	CL	3.16	3.0	0.16	53	I	2.66	2.5	0.16
19	K	0.82	0.8	0.02	55	CS	0.79	0.7	0.09
20	CA	1.00	1.0	0.0	56	BA	0.89	0.9	-0.01
21	SC	1.36	1.3	0.06	57	LA	1.10	1.1	0.0
22	TI	1.54	1.5	0.04	72	HF	1.30	1.3	0.0
23	V	1.63	1.6	0.03	73	TA	1.50	1.5	0.0
24	CR	1.66	1.6	0.06	74	W	2.36	1.7	0.66
25	MN	1.55	1.5	0.05	75	RE	1.90	1.9	0.0
26	FE	1.83	1.8	0.03	76	OS	2.20	2.2	0.0
27	CO	1.88	1.8	0.08	77	IR	2.20	2.2	0.0
28	NI	1.91	1.8	0.11	78	PT	2.28	2.2	0.08
29	CU	1.90	1.9	0.0	79	AU	2.54	2.4	0.14
30	ZN	1.65	1.6	0.05	80	HG	2.00	1.9	0.10
31	GA	1.81	1.6	0.21	81	TL	2.04	1.8	0.24
32	GE	2.01	1.8	0.21	82	PB	2.33	1.8	0.53
33	AS	2.18	2.0	0.18	83	BI	2.02	1.9	0.12
34	SE	2.55	2.4	0.15					
35	BR	2.96	2.8	0.16	90	TH	1.30	1.3	0.0
					92	U	1.38	1.7	-0.32
					94	PU	1.28	-	-



Table 4-1
Functional Group Properties for Polymers

Unit No.	(R = 0.314 J/K ² mole) Structure Group	U (J/mole)	N	V (m ³ /mole)	M (kg/mole)	Polymer Unit
1	-CH ₂ -	4.14E3	8	2.22E-5	1.4E-2	ethylene
2	-CH(CH ₃)-	1.28E4	11	4.44E-5	2.8E-2	propylene
3	-C((CH ₃) ₂)-	1.19E4	14	6.64E-5	4.2E-2	isobutylene
4	-CH(C ₆ H ₅)-	3.01E4	15	1.11E-4	9.0E-2	styrene
5	-P-C ₆ H ₄ -	2.38E4	5	8.86E-5	7.6E-2	terephthalate
6	-H-C ₆ H ₄ -	2.58E4	10	8.86E-5	7.6E-2	isophthalate
7	-C(CH ₃)CH-	1.15E4	11	5.92E-5	4.0E-2	isoprene
8	-CHCH-	7.49E3	8	3.70E-5	2.6E-2	1,4-butadiene
9	-CH(CHCH ₂)-	1.29E4	11	5.90E-5	4.0E-2	1,2-butadiene
10	-CH(C ₆ H ₁₁)-	2.56E4	21	1.48E-4	9.6E-2	vinyl cyclohexane
11	-CH(C(O)OCH ₃)-	2.81E4	23	7.57E-5	7.2E-2	methacrylate
12	-C(CH ₃)(C(O)OCH ₃)-	4.60E4	26	9.79E-5	8.6E-2	methylmethacrylate
13	-CH(CH ₃)O-	1.39E4	17	5.54E-5	4.4E-2	propylene oxide
14	-C(O)O-	1.41E4	12	3.32E-5	4.4E-2	ethylene adipate
15	-CH(OC(O)CH ₃)-	3.17E4	23	7.57E-5	7.2E-2	vinyl acetate
16	-C(O)-	7.32E3	6	2.22E-5	2.8E-2	ketone
17	-CH(C(O)OH)-	3.51E4	20	5.64E-5	5.8E-2	acrylic acid
18	-CH(OH)-	2.66E4	14	4.90E-5	3.0E-2	vinyl alcohol
19	-CH(OCN(O))-	2.86E4	20	5.54E-5	5.8E-2	vinyl formate
20	-O-	6.82E3	6	1.06E-5	1.6E-2	ether
21	-NHCO-	4.44E4	13	3.79E-5	4.3E-2	amide
22	-NHCO(O)-	2.63E4	19	4.89E-5	5.9E-2	urethane
23	-CH(CN)-	2.41E4	8	4.89E-5	3.9E-2	acrylonitrile
24	-CH(CL)-	1.75E4	8	4.07E-5	4.85E-2	vinyl chloride
25	-C(CL)CH-	1.26E4	8	5.55E-5	6.05E-2	neoprene
26	-C((CL) ₂)-	1.13E4	8	5.92E-5	8.30E-2	vinylidene chloride
27	-CF ₂ -	4.81E3	8	3.48E-5	5.0E-2	tetrafluoroethylene
28	-CH ₂ CF ₂ -	1.48E4	16	5.70E-5	6.4E-2	vinylidene fluoride
29	-CF(CF ₃)-	1.84E4	13	6.96E-5	1.0E-1	perfluoropropylene
30	-Si((CH ₃) ₂)O-	1.72E4	30	8.62E-5	7.4E-2	dimethylsiloxane
31	-N((C(O)) ₂)C ₆ H ₂ ((C(O)) ₂)N-	1.10E5	62	2.01E-4	2.14E-1	imide
32	-S-	8.26E3	8	2.56E-5	3.2E-2	sulfide
33	-S((O) ₂)	4.54E4	23	4.04E-5	6.40E-2	sulfone

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Table 4-2
Sample Computations for Methacrylates (Upper Case) and
Butadiene-Styrene Copolymers (Lower Case)

Unit No.	Moles	Structure Unit	Polymer Reference
I. Main Chain Units			
1	1	-CH ₂ -	ethylene
12	1	-C(CH ₃)(C(O))CH ₃ -	methyl methacrylate
II. Side Chain Units			
1	11	-CH ₂ -	ethylene
Glass Spec. Vol. (M ³ M/kg) = 9.89634E-04 (CC/G) = 0.989634			
Glass C.E.D. (J/M ³ M) = 3.7802E+08 (CAL/CC) = 90.3904			
Glass Temp (K) = 214.007 (C) = -59.1928			
Entang. M _w (kg/mole) = 88.7177 (g/mole) = 88717.7			
I. Main Chain Units			
1	0.87	-CH ₂ -	ethylene
8	0.87	-CHCH-	1,4-butadiene
1	0.87	-CH ₂ -	ethylene
1	0.13	-CH ₂ -	ethylene
4	0.13	-CH(C ₆ H ₅)-	styrene
Glass Spec. Vol. (M ³ M/kg) = 1.00516E-03 (CC/G) = 1.00516			
Glass C.E.D. (J/M ³ M) = 2.96893E + 8 (CAL/CC) = 70.9575			
Glass Temp (K) = 208.462 (C) = -64.7382			
Entang. M _w (kg/mole) = 2.58618 (g/mole) = 2586.18			



Table 4-3
Comparison of Calculated and Experimental T_g (Ref 2,4)

Methacrylates		V_p (g/cc)	δ^2 (cal/cc)	T_g (C)	M_e (kg/mole)	T_g (exp) (C)
methyl		0.829	144	107	18.2	105
ethyl		0.861	131	63	23.1	61
propyl		0.886	122	33	28.4	31
butyl		0.907	115	12	34.0	12
hexyl		0.938	105	-17	46.1	-19
octyl		0.989	90	-36	59.3	-38
dodecyl		0.989	90	-59	88.7	-62
Butadiene-Styrene Copolymers						
Mole (B)	Mole (S)					
0	1	0.883	88	110	20.2	100
0.2	0.8	0.902	86	69	12.8	-
0.4	0.6	0.923	82	28	8.2	-
0.61	0.39	0.954	77	-14	5.0	-12
0.64	0.36	0.959	77	-20	4.7	-13
0.72	0.28	0.973	75	-35	3.9	-34
0.77	0.23	0.983	74	-45	3.4	-37
0.87	0.13	1.01	71	-64	2.6	-51, -60
0.95	0.05	1.03	68	-80	2.0	-71, -76
0.99	0.01	1.04	67	-88	1.8	-74
1.00	0	1.04	67	-90	1.7	-79, -87

Table 4-4
Calculated and Experimental Values of M_e

Polymer	M_e (kg/mole)	M_e (exp) (kg/mole)
poly-n-octylmethacrylate	59.3	87
poly-n-hexylmethacrylate	46.1	33.9
polymethylmethacrylate	18.2	4.7-10.0
polystyrene	20.2	17.3-18.1
styrene-butadiene copolymer (0.87 mole St, 0.13 mole Bd)	2.6	3.0
poly-1,4-polybutadiene	1.7	1.7-2.9



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Table 4-5
Relation of Stress-Strain Curve Number to Test Temperature

Curve No.	Temp (K)	Curve No.	Temp (K)	Curve No.	Temp (K)
1	180	8	285	15	390
2	195	9	300	16	405
3	210	10	315	17	420
4	225	11	330	18	435
5	240	12	345	19	450
6	255	13	360	20	465
7	270	14	375	21	480

Table 4-6
Functional Group Properties for Polymers

Structure Group	U (J/mole)	H	N	V (m ³ /mole)	M (kg/mole)	Reference Polymer
-M-C6H4-	2.58E4	10	3	8.86E-5	7.6E-2	isophthalate
-P-C6H4-	2.38E4	5	4	8.86E-5	7.6E-2	terephthalate
-O-	6.82E3	6	1	1.06E-5	1.6E-2	ether
-CHCH-	7.49E3	8	2	3.70E-5	2.6E-2	1, 4-butadiene
-S((O)2)-	4.54E4	23	1	4.04E-5	6.4E-2	sulfone



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Table 4-7
Computed Estimates of ATS Physical Properties from Chemical Structure

Unit No.	Moles	Structures Unit	Polymer Reference
6	2	-M-C6H4	Isophthalate
5	2	-P-C6H4	Terephthalate
20	2	-O-	Ether
8	2	-CHCH-	1-4-Butadiene
33	1	-S((O)2)-	Sulfone

Glass Spec. Vol (M³/KG) = 7.48009E-04 (CC/G) = .748009

Glass C.E.O. (J/M³) = 5.09055E+08 (CAL/CC) = 121.664

Glass Temp. (K) 540.383 (C) = 267.183

Entang. M_w (KG/Mole) = 3.39525 (G/MOLE) = 3395.25

U,R,V,M,N 173220 81 4.9E-04 452 21 (Summed Values)

Table 4-8
Relation of Stress-Strain Curve Number to Test Temperature at
Constant Time $t = 1.0$ s

Curve No.	Temperature		Curve No.	Temperature	
	°C	K		°C	K
1	-50	223	11	200	473
2	-25	248	12	225	498
3	0	273	13	250	523
4	25	248	14	275	548
5	50	323	15	300	573
6	75	348	16	325	598
7	100	373	17	350	623
8	125	398	18	375	648
9	150	423	19	400	673
10	175	448			



Table 5-1
Properties of Commercial Reinforcing Fibers
(from Ref. 5, p. 47)

Fiber	Spec. Vol. (cc/g)	Tensile Properties			
		E (GPa)	S _D (GPa)	ε _D (%)	W _D (MPa)
Graphite (UHM-S)	0.510	500	1.86	0.37	3.44
(HM-S)	0.523	360	2.34	0.65	7.60
(HT-S)	0.565	244	2.82	1.16	16.36
(A-S)	0.571	208	2.82	1.36	19.18
Boron (W-core)	0.377	386	3.41	0.88	15.00
Aramid-49	0.690	138	2.76	2.00	27.60
E-glass	0.394	72.5	3.44	4.74	81.53

Table 5-2
Estimated Elemental Properties of Carbon

HOW MANY ELEMENTS? 1
ELEMENT CODE NO.=? 5
MOLES OF ELEMENT=? 2
NUMBER OF CHEMICAL BOND TYPES=? 1
FOR A-B BOND, ELEMENT A CODE NO.=? 5
ELEMENT B CODE NO.=? 5
MOLES OF A-B BONDS=? 4

ELEMENTARY PROPERTIES
Z, SY, W, D/1E5, X, R/1E-10, V, PH =
5 0 12.01 3.48 2.55 77 4 5
TO CONTINUE PRESS ENTER

CHEMICAL ANALYSIS

BONDING ELEMENTS	BOND ENERGY (J/MOLE)	% IONIC ENERGY	BOND LENGTH ($\text{\AA} \times 10^{-10}$)	MOLES
A B				
C C	348030	0	1.54	4
TOTAL	1.392E+06			4

TO CONTINUE PRESS ENTER

PHYSICAL ANALYSIS

ELEMENTS	MOLES	MOLECULAR WT. (KG/MOLE)	SPECIF. VOLUME (CM^3/G)
C	2		
		24.02	
(Z=12)	(Z=8)	(Z=6)	(Z=4)
129547	140348	18313	292413

TO CONTINUE T RUN AND PRESS ENTER
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Table 5-3

Estimated Intramolecular Properties of Silica

HOW MANY ELEMENTS? 2
ELEMENT CODE NO.=? 12
MOLES OF ELEMENT=? 1
ELEMENT CODE NO.=? 7
MOLES OF ELEMENT=? 2
NUMBER OF CHEMICAL BOND TYPES=? 1
FOR A-B BOND, ELEMENT A CODE NO.=? 12
ELEMENT B CODE NO.=? 7
MOLES OF A-B BONDS=? 4

ELEMENTARY PROPERTIES

Z, SY, M, D/IES, X, R/1E-10, V, PH =

14 SI 28 89 : 1.77 1 9 1 11 4 7

8 9 16 1.39 3.44 73 2 2

TO CONTINUE PRESS ENTER

?

CHEMICAL ANALYSIS

BONDING ELEMENTS	BOND ENERGY (J/MOLE)	% IONIC ENERGY	BOND LENGTH (M*1E-10)	MOLES
A B				
SI 0	386960	59.1583	1.7814	4
TOTAL	1.54744E+06			4

TO CONTINUE PRESS ENTER

?

PHYSICAL ANALYSIS

ELEMENTS MOLES

SI 1

O 2

MOLECULAR WT. (KG/MOLE)= .06809

(G/MOLE)= 68.09

SPECIFIC VOLUME (CC/G) :

(Z=12)

(Z=8)

(Z=6)

(Z=4)

104749

113965

148114

228352

TO CONTINUE TYPE RUN AND PRESS ENTER

READY

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Table 5-4
Estimated Intramolecular Properties of Aramid

HOW MANY ELEMENTS=? 4
ELEMENT CODE NO.=? 1
MOLES OF ELEMENT=? 5
ELEMENT CODE NO.=? 5
MOLES OF ELEMENT=? 7
ELEMENT CODE NO.=? 6
MOLES OF ELEMENT=? 1
ELEMENT CODE NO.=? 7
MOLES OF ELEMENT=? 1
NUMBER OF CHEMICAL BOND TYPES=? 2
FOR A-B BOND, ELEMENT A CODE NO.=? 5
ELEMENT B CODE NO.=? 5
MOLES OF A-B BONDS=? 10
FOR A-B BOND, ELEMENT A CODE NO.=? 6
ELEMENT B CODE NO.=? 5
MOLES OF A-B BONDS=? 2

1 H 1.000 4.35 2.2 .32 1 7
6 C 12.01 3.48 2.55 .77 4 5
7 N 14.01 1.61 3.04 .75 3 2
8 O 16 1.39 3.44 .73 2 2

TO CONTINUE PRESS ENTER

?

CHEMICAL ANALYSIS:

BONDING ELEMENTS	BOND ENERGY (J/MOLE)	% IONIC ENERGY	BOND LENGTH (M*1E-10)	MOLES
A B	348000	0	1.54	10
C C	277670	8.34433	1.4759	2
N C				12
TOTAL	4.83534E+06			

TO CONTINUE PRESS ENTER

?

PHYSICAL ANALYSIS:

ELEMENTS MOLES

H 5
C 7
N 1
O 1

MOLECULAR WT. (KG/MOLE)= 119.12
(G/MOLE)= 119.12

SPECIFIC VOLUME (CC/G)

(Z=12) (Z=3) (Z=6) (Z=4)
179209 134979 253402 398675

TO CONTINUE TYPE RUN AND PRESS ENTER

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Table 5-5
Calculated Specific Bond Energy for Fibers
(Chemical energy/unit mass)

Fibers	Molar Composition	Molar of Bonds	Total Bond Energy (J/mol)	Mol. Wt. (g/mol)	Spec. Bond Energy (J/g)
<u>Commercial</u>					
Carbon	(C ₂)	4	1.39E6	24.02	5.79E4
Boron	(B ₂)	3	7.59E6	21.62	3.51E4
Aramid-49		12	4.04E6	119.1	3.39E4
Alumina	(Al ₂ O ₃)	6	2.97E6	102.0	2.91E4
Silica	(SiO ₂)	4	1.55E6	60.1	2.58E4
Aluminum	(Al ₂)	3	6.18E5	53.96	1.15E4
Titanium	(Ti) ₂	4	1.06E6	95.8	1.11E4
Iron	(Fe ₂)	3	6.09E5	111.7	5.45E3
<u>Candidates</u>					
Boron Nitride	(B ₁₂ N ₅)	3	9.11E5	24.82	3.67E4
Silicon Carbide	(SiC)	4	1.21E6	40.1	3.02E4
Polyethylene	(-CH ₂ -)	1	3.48E5	14.0	2.48E4
<u>Carbon Precursor</u>					
PAN	[CH ₂ -CH(CN)]	2	6.96E5	51.1	1.36E4

Table 5-6

Estimated Physical Properties of Equimolar TGMDA and DDS
Linear Polymer (see Fig. 5-3)

MONOMER-POLYMER PREDICTION PART-1, D. H. KAEUBLE MAY 1961
HOW MANY MAIN CHAIN UNITS?? 6
STRUCTURE UNIT NO =? 5
MOLES OF STRUCTURE UNIT=? 4
STRUCTURE UNIT NO =? 33
MOLES OF STRUCTURE UNIT=? 1
STRUCTURE UNIT NO =? 1
MOLES OF STRUCTURE UNIT=? 5
STRUCTURE UNIT NO =? 18
MOLES OF STRUCTURE UNIT=? 2
STRUCTURE UNIT NO =? 21
MOLES OF STRUCTURE UNIT=? 4
STRUCTURE UNIT NO =? 16
MOLES OF STRUCTURE UNIT=? -4
HOW MANY SIDE GROUPS? (NONE=0) 3
STRUCTURE UNIT NO =? 1
MOLES OF STRUCTURE UNIT=? 2
STRUCTURE UNIT NO =? 8
MOLES OF STRUCTURE UNIT=? 2
STRUCTURE UNIT NO =? 23
MOLES OF STRUCTURE UNIT=? 2

1. MAIN CHAIN UNITS
UNIT NO. MOLES STRUCTURE
UNIT

5	4	-P-C6H4-
33	1	-S((O)2)-
1	5	-CH2-
18	2	-CH(OH)-
21	4	-NHC(O)-
16	-4	-C(O)-

POLYMER
REFERENCE
TEREPHTHALATE
SULFONE
ETHYLENE
VINYL ALCOHOL
AMIDE
KETONE

11 SIDE CHAIN UNITS

1	2	-CH2-
8	2	-CHCH-
20	2	-O-

ETHYLENE
1-4-BUTADIENE
ETHER

GLASS SPEC. VOL (CM³/KG) = 0.30266E-04 (CC/G) = 0.30266

GLASS C.E.D. (J/CM²) = 7.13963E+09 (CAL/CC) = 170.637

GLASS TEMP. (K) = 351.407 (C) = 273.207

ENTANG. MW. (KG/MOLE) = 4.33352 (G/MOLE) = 4033.52

U.W.V.M.N 399720 103 0.052E-04 67 20

TO CONTINUE TYPE RUN AND PRESS ENTER

READY
>



Table 5-7

Estimated Physical Properties of 2 Moles of TGMDA and
1 Mole of DDS Linear Polymer (see Fig. 5-4)

MONOMER-POLYMER PREDICTION PART-1, D. H. KAEHLER MAY, 81
HOW MANY MAIN CHAIN UNITS?? 6
STRUCTURE UNIT NO. ?? 5
MOLES OF STRUCTURE UNIT=? 6
STRUCTURE UNIT NO.=? 33
MOLES OF STRUCTURE UNIT=? 1
STRUCTURE UNIT NO.=? 1
MOLES OF STRUCTURE UNIT=? 10
STRUCTURE UNIT NO.=? 19
MOLES OF STRUCTURE UNIT=? 4
STRUCTURE UNIT NO.=? 21
MOLES OF STRUCTURE UNIT=? 6
STRUCTURE UNIT NO.=? 16
MOLES OF STRUCTURE UNIT=? -6
HOW MANY SIDE GROUPS? (NONE=0)? 3
STRUCTURE UNIT NO.=? 1
MOLES OF STRUCTURE UNIT=? 4
STRUCTURE UNIT NO.=? 8
MOLES OF STRUCTURE UNIT=? 4
STRUCTURE UNIT NO.=? 20
MOLES OF STRUCTURE UNIT=? 4

I. MAIN CHAIN UNITS
UNIT NO. MOLES STRUCTURE
UNIT

5	6	-P-C6H4-
33	1	-S(O)2-
1	10	-CH2-
19	4	-CH(OH)-
21	6	-NHCO-
16	-6	-C(O)-

POLYMER
REFERENCE
TEREPHTHALATE
SULFONE
ETHYLENE
VINYL ALCOHOL
AMIDE
KETONE

II. SIDE CHAIN UNITS:

1	4	-CH2-
8	4	-CHCH-
20	4	-O-

ETHYLENE
1-4-BUTADIENE
ETHER

GLASS SPEC. VOL. (CM³/KG) = 0.59914E-04 (CC/G) = .859914
GLASS C.E.D. (J/CM³) = 6.67803E+08 (CAL/CC) = 159 605
GLASS TEMP. (K) = 502.673 (C) = 229.479
ENTANG. NO. (KG/MOLE) = 5.15813 (G/MOLE) = 5168 13
U.H.V.M. 632200 319 1.3634E-03 1.094 45
TO CONTINUE TYPE RUN AND PRESS ENTER
READY
>

Table 5-8

Estimated Physical Properties of TGMDA Linear
Homopolymer (see Fig. 5-5)

MONOMER-POLYMER PREDICTION PART-1 D H KAELE MA' 31
HOW MANY MAIN CHAIN UNITS?? 5
STRUCTURE UNIT NO =? 5
MOLES OF STRUCTURE UNIT=? 2
STRUCTURE UNIT NO.=? 1
MOLES OF STRUCTURE UNIT=? 5
STRUCTURE UNIT NO =? 8
MOLES OF STRUCTURE UNIT=? 1
STRUCTURE UNIT NO.=? 21
MOLES OF STRUCTURE UNIT=? 2
STRUCTURE UNIT NO.=? 16
MOLES OF STRUCTURE UNIT=? -2
HOW MANY SIDE GROUPS? (NONE=0): 3
STRUCTURE UNIT NO =? 20
MOLES OF STRUCTURE UNIT=? 4
STRUCTURE UNIT NO =? 1
MOLES OF STRUCTURE UNIT=? 2
STRUCTURE UNIT NO.=? 8
MOLES OF STRUCTURE UNIT=? 2.

I. MAIN CHAIN UNITS
UNIT NO. MOLES STRUCTURE
UNIT

5 2 -P-C6H4-
1 5 -CH2-
8 1 -CHCH-
21 2 -NHCO-
16 -2 -CO-

POLYMER
REFERENCE
TEREPHTHALATE
ETHYLENE
1-4-BUTADIENE
AMIDE
KETONE

II. SIDE CHAIN UNITS:

20 4 -O-
1 2 -CH2-
8 2 -CHCH-

ETHER
ETHYLENE
1-4-BUTADIENE

GLASS SPEC. VOL. (MM³/KG)= 0.45986E-04 (CC/G)= .945986

GLASS C.E.D. (J/MM³)= 5.57993E+08 (CAL/CC)= 133.36

GLASS TEMP. (K)= 402.405 (C)= 129.295

ENTANG. MW. (KG/MOLE)= 5.30042 (G/MOLE)= 5300.42

J.H.V.M.H 200490 120 5.174E-04 .422 17

TO CONTINUE TYPE RUN AND PRESS ENTER

READY

>



Table 5-9

First Estimate of the Physical Properties of Equimolar
Isoamyl-Neopentyl Acrylate Copolymer

MONOMER-POLYMER PREDICTION PART-1, D. H. KHELBLE MAY, 81

HOW MANY MAIN CHAIN UNITS?? 1

STRUCTURE UNIT NO.=? 1

MOLES OF STRUCTURE UNIT=? 4

HOW MANY SIDE GROUPS? (NONE=0)? 4

STRUCTURE UNIT NO.=? 14

MOLES OF STRUCTURE UNIT=? 2

STRUCTURE UNIT NO.=? 1

MOLES OF STRUCTURE UNIT=? 5

STRUCTURE UNIT NO.=? 2

MOLES OF STRUCTURE UNIT=? 1

STRUCTURE UNIT NO.=? 3

MOLES OF STRUCTURE UNIT=? 1

UNIT NO. MOLES STRUCTURE
UNIT

1 4 -CH2-

II. SIDE CHAIN UNITS:

14 2 -C(O)O-

1 5 -CH2-

2 1 -CH(CH3)-

3 1 -C(CH3)2-

POLYMER
REFERENCE
ETHYLENE

ETHYLENE ADIPATE

ETHYLENE

PROPYLENE

ISOBUTYLENE

GLASS SPEC. VOL. (M*1000/KG)= 9.16437E-04 (CC/G)= .916437

GLASS C.E.D. (J/M*1000)= 3.44195E+08 (CAL/CC)= 82.2626

GLASS TEMP. (K)= 204.575 (C)=-68.6251

ENTANG. MU. (KG/MOLE)= 34.185 (G/MOLE)= 34185

U.H.V.M.N 90160 121 3.772E-04 284 4

TO CONTINUE TYPE RUN AND PRESS ENTER

READY

>

Table 5-10

Second Estimate of the Physical Properties of Equimolar
Isoamyl-Neopentyl Acrylate Copolymer

MONOMER-POLYMER PREDICTION PART-1, D H KHELBLE MAY, 81
 HOW MANY MAIN CHAIN UNITS?? 2
 STRUCTURE UNIT NO =? 1
 MOLES OF STRUCTURE UNIT=? 2
 STRUCTURE UNIT NO =? 2
 MOLES OF STRUCTURE UNIT=? 2
 HOW MANY SIDE GROUPS? (NONE=0)? 4
 STRUCTURE UNIT NO =? 14
 MOLES OF STRUCTURE UNIT=? 2
 STRUCTURE UNIT NO =? 1
 MOLES OF STRUCTURE UNIT=? 3
 STRUCTURE UNIT NO =? 2
 MOLES OF STRUCTURE UNIT=? 1
 STRUCTURE UNIT NO =? 3
 MOLES OF STRUCTURE UNIT=? 1

I. MAIN CHAIN UNITS:

UNIT NO. MOLES STRUCTURE

UNIT NO.	MOLES	STRUCTURE UNIT
1	2	-CH ₂ -
2	2	-CH(CH ₃)-

POLYMER
 REFERENCE
 ETHYLENE
 PROPYLENE

II. SIDE CHAIN UNITS:

UNIT NO.	MOLES	STRUCTURE UNIT
14	2	-C(O)O-
1	3	-CH ₂ -
2	1	-CH(CH ₃)-
3	1	-C(CH ₃) ₂ -

ETHYLENE ADIPATE
 ETHYLENE
 PROPYLENE
 ISOBUTYLENE

GLASS SPEC. VOL. (M³/KG)= 9.16437E-04 (CC/G)= 916437GLASS C.E.D. (J/M³M)= 3.78706E+08 (CAL/CC)= 93.5109

GLASS TEMP. (K)= 240.30 (C)= -32.8198

ENTANG. MW. (KG/MOLE)= 34.185 (G/MOLE)= 34185

U.H.V.M.N 99200 111 3.772E-04 284 4

TO CONTINUE TYPE RUN AND PRESS ENTER

READY

>



Table 5-11

Relations Between Polymer Chemistry and Physical Properties

Polymer Number	Polymer	Calc.				Exp. (18)
		V_s ($\frac{cc}{g}$)	δ^2 ($\frac{cal}{cc}$)	T_g (K)	M_e ($\frac{kg}{mol}$)	M_e ($\frac{kg}{mol}$)
1	p-dimethyl siloxane	0.81	68.7	163	10.6	12.2
2	p-isobutylene	1.09	62.1	201	8.2	8.0
3	p-cis-isoprene	1.05	65.7	201	3.1	3.8
4	p-cis-transbutadiene	1.04	66.7	183	1.7	2.2
5	p-cisbutadiene	1.04	66.7	183	1.7	3.0
6	p-ethylene	1.09	64.2	150	2.1	2.5
7	p-propylene	1.09	87.5	240	4.9	3.5
8	p-styrene	0.88	88.5	384	20.2	17.5
9	p- α -methyl styrene	0.91	90.3	434	25.2	20.4
10	p-ethyleneoxide	0.86	94.5	190	1.5	3.0
11	p-propyleneoxide	0.92	105.9	254	3.5	3.9
12	p-tetramethylene oxide	0.95	81.0	173	1.8	1.3
13	p-methylacrylate	0.79	113.3	276	13.6	12.1
14	p-methylmethacrylate	0.83	143.7	380	18.1	15.8
15	p-n-butylmethacrylate	0.91	115.3	285	34.0	30.2
16	p-n-hexylmethacrylate	0.94	105.4	256	46.1	45.9
17	p-n-octylmethacrylate	0.96	98.8	237	59.3	57.0
18	p-2 ethylbutylmethacrylate	0.94	112.2	288	46.1	21.4
19	p-vinylacetate	0.79	125.9	304	13.6	12.3
20	p-vinylalcohol	1.12	148.6	362	5.4	3.8
21	p-vinylchloride	0.69	118.4	351	6.9	3.2
22	p-decamethyleneadipate	0.92	78.6	177	2.1	2.2
23	p-decamethylenesebecate	0.95	75.8	172	2.1	2.4
24	p-decamethylenesuccinate	0.90	80.5	181	2.1	2.3
25	p-ethyleneterephthalate	0.72	104.0	348	2.4	1.7
26	p-ethyleneisophthalate	0.72	104.0	348	2.4	1.7
27	p-bisphenol-A-carbonate	0.70	96.4	400	3.5	2.5
28	p-bisphenol-A-diphenyl-sulfone	0.75	118.4	533	3.6	3.6
29	p-2-methyl-6 phenyl-1,4-phenylene oxide	0.80	96.0	613	10.3	1.7
30	p-2, 6-dimethyl-1, 4-phenylene oxide	0.83	93.2	501	4.8	1.7
31	p-caprolactam	0.91	150.5	321	2.2	2.5
32	p-propylene sulfide	0.87	93.1	250	5.4	10.0
33	p-acrylic acid	0.75	171.8	363	9.6	2.4
34	p-acrylonitrile	0.93	136.7	450	6.5	0.65
35	p-tetrafluoroethylene	0.48	47.6	169	12.0	6.6
36	p-acrylamide	0.80	220.3	463	9.8	4.6
37	p-phenyleneterephthalamide	0.73	185.5	938	2.7	0.6
38	p-benzamide	0.73	185.5	938	2.7	0.4
39	p-n-hexylisocyanate	0.93	139.2	299	28.8	3.7
40	p-n-butylisocyanate	0.88	165.5	351	18.6	0.35

Table 5-12
Summed Properties of Functional Groups

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Polymer Number	U ($\frac{\text{J}}{\text{mol}}$)	H	V ($\frac{\text{cc}}{\text{mol}}$)	M ($\frac{\text{g}}{\text{mol}}$)	N	$-\left(\frac{\partial \sigma_{12}}{\partial T}\right)_g$ ($\frac{\text{bar}}{\text{deg}}$)	Shear Yield σ_{12} (at 293K) bar
1	17200	30	86.2	74	2	9.9	0
2	16040	22	88.8	56	2	7.0	0
3	19780	27	103.6	68	4	7.4	0
4	15770	24	81.4	54	4	8.3	0
5	15770	24	81.4	54	4	8.3	0
6	4140	8	22.2	14	1	10.2	0
7	16940	19	66.6	42	2	8.0	0
8	34240	23	133.0	104	2	4.9	446
9	40740	24	155.0	118	2	5.7	804
10	15100	22	55.0	44	3	11.3	0
11	23760	25	77.2	53	3	9.1	0
12	23380	30	99.4	72	5	11.1	0
13	32240	31	97.9	86	2	8.9	0
14	50140	34	120.1	100	2	8.0	696
15	62560	58	186.7	142	2	8.8	0
16	70840	74	231.1	170	2	9.1	0
17	79120	90	275.5	198	2	9.2	0
18	75360	60	231.1	170	2	8.4	0
19	35840	31	97.9	86	2	8.9	98
20	30740	22	71.2	44	2	8.7	600
21	21640	16	62.9	62.5	2	7.2	418
22	86160	136	377.2	284	18	10.2	0
23	102720	168	466.0	340	22	10.2	0
24	77280	120	332.8	256	16	10.2	0
25	60280	45	199.4	192	10	6.4	352
26	62280	50	199.4	192	9	7.1	227
27	80980	52	287.2	254	12	5.1	546
28	166660	79	482.6	442	20	4.6	1104
29	58560	24	210.0	182	5	3.3	947
30	43420	22	143.6	120	5	5.3	1102
31	65100	53	148.9	113	7	10.1	283
32	25200	27	93.1	74	3	8.2	0
33	39240	28	78.6	72	2	9.7	679
34	28240	16	71.1	53	2	6.4	1005
35	4810	8	34.8	50	1	9.9	0
36	52680	29	82.3	71	2	6.5	1105
37	68200	18	126.5	119	6	4.03	2599
38	68200	18	126.5	119	6	4.03	2599
39	69240	61	171.1	127	2	10.1	61
40	60960	45	126.7	99	2	8.5	493



Table 5-13

Polymerized Silane Chemistry and Surface Properties^{19,20}

Test Liquid				H ₂ O	Glycerol	Eth. Glycol	PG E-200	PG 15-200	PB 1200
γ_{LV} (dyn/cm)				7.28	64.0	48.3	43.5	36.6	31.3
$2\alpha_L$ (dyn/cm) ^{1/2}				9.34	12.16	10.70	10.62	10.20	9.90
β_L/α_L				1.54	0.94	0.81	0.74	0.64	0.53
R-Structure	Source	γ_{SV}^d dyn/cm	γ_{SV}^p dyn/cm	$M_{SL}/2\alpha_L$ (dyn/cm) ^{1/2}					
H ₂ N(CH ₂) ₂ NH(CH ₂) ₃ -	DC Z-6020	30.0	4.6		7.54	7.21	6.99	6.92	
$\begin{array}{c} \text{CH}_3\text{O} \\ \\ \text{CH}_2=\text{C}-\text{C}-\text{O}-(\text{CH}_2)_3- \end{array}$	DC Z-6030	8.4	41.7		9.08	8.03	7.41	7.42	6.21
$\begin{array}{c} \text{A} \\ \\ \text{CH}_2-\text{CH}-\text{CH}_2\text{O}(\text{CH}_2)_3- \\ \text{(catalyzed)} \end{array}$	DC Z-6040	10.2	43.6	13.23	9.69	8.57	8.13	7.12	
$\begin{array}{c} \text{A} \\ \\ \text{CH}_2-\text{CH}-\text{CH}_2\text{O}-(\text{CH}_2)_3- \\ \text{(noncatalyzed)} \end{array}$	DC Z-6040	17.6	25.4	11.94	9.01	8.29	7.87		
Cl-(CH ₂) ₃ -	DC XZ-B-0999	36.5	3.8	9.09	7.80	7.21	7.90		
NH ₂ -(CH ₂) ₃	UC A-1100	17.9	19.8	11.35	7.63	7.76	7.41	7.63	
HS-(CH ₂) ₃	DC XZ-B-0951	67.4	0.0		8.06	8.33	8.02		
CH ₂ =CH-		28.5	2.1	7.72	6.25	6.35	6.56	6.81	5.90

Analysis of vapor-liquid-solid interactions for polymerized coatings of reactive silane coupling agents with structure R-Si(OCH₃)₃.

Table 5-14
Reactive Silane Monomers^{19,20}

SC5291.7FR

Number	Reactive Silane
41	(dimethyl)(dimethoxy)silane - model compound
42	tetraethoxy silane
43	(vinyl)(triethoxy)silane
44	(γ -chloropropyl)(trimethoxy)silane
45	(γ -mercaptopropyl)(trimethoxy)silane
46	(methacryloxypropyl)(trimethoxy)silane
47	(γ -glycidoxypropyl)(trimethoxy)silane
48	(β -3, 4-epoxycyclohexylethyl)(trimethoxy)silane
49	(γ -aminopropyl)(trimethoxy)silane
50	(γ -aminopropyl)(trimethoxy)silane
51	N- β -aminoethyl- γ -aminopropyl(trimethoxy)silane
52	(4-styryl-methylene- β -aminoethyl- γ -aminopropyl)(trimethoxy)silane



Table 5-15

Linear Hydroxy Polymers of Reactive Silane Primers

Number	Linear Polymer
41	(dimethyl)siloxane
42	(dihydroxy)siloxane
43	(vinyl)(hydroxy)siloxane
44	(γ -chloropropyl)(hydroxy)siloxane
45	(γ -mercaptopropyl)(hydroxy)siloxane
46	(methacryloxypropyl)(hydroxy)siloxane
47	(γ -glycidoxypropyl)(hydroxy)siloxane
48	(β -3, 4-epoxycyclohexylethyl)(hydroxy)siloxane
49	(γ -aminopropyl)(hydroxy)siloxane
50	(γ -aminopropyl)(hydroxy)siloxane
51	N- β -aminoethyl- γ -aminopropyl(hydroxy)siloxane
52	(4-styryl-methylene- β -aminoethyl- γ -aminopropyl)(hydroxy)siloxane

Table 5-16

Summed Values of Monomer Group Properties for Lienenar
Hydroxy Polymers of Reactive Silane Primers

Number	U J/mole	H	V (cc/mole)	M	N
41	17200	30	86.2	74	2
42	44800	36	95.4	78	2
43	34350	33	105.6	88	2
44	52640	49	153.7	138.5	2
45	47540	57	161.7	136	2
46	66280	72	227.4	188	2
47	64550	77	215.6	176	2
48	62630	52	242	186	2
49	76360	56	151	119	2
50	76360	56	151	119	2
51	121720	79	211	162	2
52	157150	100	359	278	2



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Table 5-17

Calculated Properties of Linear Hydroxy Polymers
of Reactive Silanes at T_g

Number	V_s (cc/g)	δ^2 (cal/cc)	T_g (K)	M_e (kg/mole)
41	0.80	69	163	10.6
42	0.84	162	325	12.1
43	0.83	112	276	14.6
44	0.77	118	284	29.4
45	0.82	101	226	29.8
46	0.83	100	246	50.5
47	0.85	103	227	45.8
48	0.90	89	315	51.8
49	0.87	174	354	25.0
50	0.87	174	354	25.0
51	0.90	198	396	41.7
52	0.89	151	404	96.3

Table 5-18

Correlation Between Crosslink Density (ρ/M_c) and Maximum Network Extensibility $\lambda_b(\max) = K(\rho/M_c)^{1/2}$

Polymer	T_g (°C)	$(M_c/\rho)^{1/2}$ (cc/mole) ^{1/2}	$\lambda_b(\max)$	K	Ref.
Silicone elastomer	-123	153	6.85	0.045	28
SBR elastomer	-61	113	7.20	0.064	28
Polybutadiene	-86	112	5.09	0.045	28
EPR elastomer	-55	105	6.85	0.065	28
Butyl elastomer	-70	104	6.17	0.059	28
Viton - b elastomer		93	5.19	0.056	28
Butyl elastomer	-70	92	7.20	0.078	28
Epoxy thermosett	115	31	1.59	0.051	28
Epoxy thermosett	72	23.2	1.27	0.055	29
Epoxy - polyamide	45	34.6	1.46	0.042	29
Epoxy - polyamide	20	56.4	1.95	0.035	29
Epoxy - polyamide	6	72	2.50	0.035	29
Viton - B elastomer		466	19.10	0.041	30
Viton - B elastomer		245	15.5	0.063	30
Viton - B elastomer		187	12.6	0.067	30
Viton - B elastomer		143	8.9	0.062	30
Viton - B elastomer		128	7.9	0.062	30
Viton - B elastomer		92	5.7	0.062	30
Epoxy - CTBN (50%)	-50	52.4	2.78	0.053	31
Epoxy - CTBN (39%)		47.0	2.41	0.051	31
Epoxy - CTBN (29%)		34.6	1.56	0.045	31
Epoxy - CTBN (17%)		30.6	1.32	0.044	31
Epoxy	100	29.2	1.35	0.046	31
Ave. =				0.0515	
Std. dev. =				±0.0150	



Table 5-19

Correlation Between Entanglement Crosslink Density (ρ/M_e) and Maximum
Craze Extensibility $\lambda_c = K_c \cdot (M_e/\rho)^{1/2}$

Polymer	M_e (gm/mole)	$(M_e/\rho)^{1/2}$	λ_c	K_c
p-tert.-butylstyrene	4.3E4	203	7.2	0.035
p-para vinyltoluene	2.5E4	151	4.5	0.030
p-styrene	1.9E4	129	3.8	0.029
p-styrene-maleicanhydride (9 wt%)	1.9E4	128	4.2	0.033
p-styrene-acrylonitrile (24 wt%)	1.2E4	103	2.7	0.026
p-methylmethacrylate	9.2E3	87	2.0	0.023
p-styrene-methylmethacrylate (65 wt%)	9.0E3	87	2.0	0.023
p-styrene-acrylonitrile (66 wt%)	6.4E3	76	2.0	0.026
p-2,6 dimethyl-1,4-phenylene oxide (-E)	4.3E3	60	2.6	0.043
p-2,6 dimethyl-1,4-phenylene oxide (-M)	7.4E3	78	2.6	0.033
p-bisphenol-A carbonate	2.5E3	42	2.0	0.048
			Ave. =	0.032
			Std. Dev. =	± 0.008

Note: M_e and λ_c data generated by experiments of Donald and Kramer (Ref. 7)
and ρ is calculated from molecular structure.

Table 5-20
Correlation of Polymer Cohesive Energy δ_p^2 Density and Maximum
Tensile Strength $(\sigma_{11})_b$ at 80 to 130K

Chemical Composition		Calc. δ_p^2 (bar)	Meas. $(\sigma_{11})_b$ (bar)	$(\sigma_{11})_b/\delta_p^2$
1)	Fluorocopolymer (C ₂ F ₄) _{1.0} (C ₃ F ₆) _{0.136}	1667	980	0.59
2)	C ₂ F ₄ Homopolymer	1735	794	0.46
3)	Fluorocopolymer (CF ₂ CFCI) _{1.0} (CF ₂ CH ₂) _{0.031}	2608	1147	0.44
4)	Bisphenol-A Carbonate (OC ₆ H ₄ C(CH ₃) ₂ C ₆ H ₄ OC(O))	4088	1333	0.33
5	Polyethylene Terephthalate	5225	2108	0.40
6	Polyimide (N(CO) ₂ C ₆ H ₂ (CO ₂)NC ₆ H ₄ OC ₆ H ₄)	6186	2157	<u>0.35</u>
Average				0.43
Standard dev. $\pm$				0.09



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Table 5-21

Estimated Cure Path Properties of Equimolar
TGMDA and DDS (see Table 5-6)

A AND B COREACTION-MOL. WT. DIST -THERMAL TRANS -D H. KHELBLE-OCT
27.1982
IF NONSTOICHIOMETRIC REACTION HAVE MOLES OF B IN EXCESS
MOLES OF TYPE A (MOLE)=? 1
TYPE A FUNCTIONALITY(=2)=? 4
MOL. WT. OF TYPE A (G/MOLE)=? 248
MOLES OF TYPE B (MOLE)=? 1
TYPE B FUNCTIONALITY (=2)=? 4
MOL. WT. OF TYPE B (G/MOLE)=? 422
FRACTION OF MOLECULES OF FUNCTIONALITY >2=? 1
NUMBER OF A AND B MAIN CHAIN ATOMS (A1 A2)=? 11 17
MOL. WT. BETWEEN ENTANGLEMENTS (G/MOLE)=? 4833
GLASS COORDINATION NUMBER (8<2<18)=? 10
MONOMER AND LINEAR POLYMER GLASS TEMPERATURES (T1,T2) IN DEG K=
? 269.551

GEL POINT (% A REACTED)= 33.3333

GEL POINT (% B REACTED)= 33.3333

INITIAL NUM. AVE. DEG. OF POLYMERIZATION= 2.23368

TO ANALYSE POLYMERIZATION PRESS ENTER?

% A REACTED	BRANCH COEF	NUM. AVE. MW(G/MOL)	WT. AVE. MW(G/MOL)	GLASS TEMP(K)	FLOW TEMP(K)
0	0	335	335	260	267.829
3 32667	0332667	358 877	384 519	269 469	277 773
6 65334	0665334	386 42	446 388	279 653	289 48
9 98001	0998001	418 541	525 082	290 638	300 049
13 3057	133057	455 486	631 787	302 52	312 539
16 6333	166333	501 998	779 984	315 416	326 28
19 96	1996	557 59	1031 66	329 46	341 283
23 2857	232857	627 029	1370 31	344 313	357 83
26 6134	266134	716 221	2103 95	361 567	376 516
29 94	2994	934 995	4276 06	380 253	398 276
33 2657	332657	1001	823324	400 353	491 121

TO ANALYSE CROSSLINKING PRESS ENTER?

%A REACTED	BRANCH COEF	WT. FR. GEL	NUM. AVE. MW(G/MOL)	X-LINK MW (G/MOL)	GLASS TEMP(K)
33 4169	334169	0100001	1010.07	2 67126E+07	401 837
34 2996	342996	109	1066.85	212041	407 83
35 2344	352344	208	1139.02	54751 8	415 019
36 4317	364317	307	1234.5	23473 1	423 796
37 7555	377555	406	1367.97	12439 1	434 764
39 3337	393337	505	1570 37	7370 28	443 917
41 2786	412786	604	1920 57	4653 78	468 049
43 7981	437981	703	2700 79	3035 76	495 843
47 3477	473477	802	6315.3	1387 04	541 671
53 317	53317	901	3.25E+00	1243 37	590 897
98 087	98087	1	3.35E+00	344 897	727 705

% B REACTED= 98.087

READY

TO CONTINUE TYPE RUN AND PRESS ENTER

Table 5-22

SC5291.7FR

Estimated Cure Path Properties of 2 Moles of TGMDA
and 1 Mole of DDS (see Table 5-7)

A AND B COREACTION MOL. WT. DIST. -THERMAL TRANS -D.H KHELBLE-OCT
27.1982
IF NONSTOICHIOMETRIC REACTION HAVE MOLES OF B IN EXCESS
MOLES OF TYPE A (MOLE)=? 1
TYPE A FUNCTIONALITY(=2)=? 4
MOL. WT. OF TYPE A (G/MOLE)=? 248
MOLES OF TYPE B (MOLE)=? 2
TYPE B FUNCTIONALITY(=2)=? 4
MOL. WT. OF TYPE B (G/MOLE)=? 422
FRACTION OF MOLECULES OF FUNCTIONALITY >2=? 1
NUMBER OF A AND B MAIN CHAIN ATOMS (A1,A2)=? 11,17
MOL. WT. BETWEEN ENTANGLEMENTS (G/MOLE)=? 5169
GLASS COORDINATION NUMBER (3<Z<10)=? 10
MONOMER AND LINEAR POLYMER GLASS TEMPERATURES (T₁,T₂) IN DEG K=
? 269,593
GEL POINT (% A REACTED)= 66.6657
GEL POINT (% B REACTED)= 33.3333

INITIAL NUM. AVE. DEG. OF POLYMERIZATION= 2.6749
TO ANALYSE POLYMERIZATION PRESS ENTER?

% A REACTED	BRANCH COEF.	NUM. AVE. MW(G/MOL)	WT. AVE. MW(G/MOL)	GLASS TEMP(K)	FLOW TEMP(K)
0	0	364	364	260	263.066
6.65334	.0332667	389.944	417.886	268.635	277.179
13.3067	.0665334	419.871	485.93	277.962	286.934
19.96	.0998001	454.773	571.437	287.747	297.407
26.6134	.133067	496.003	686.479	298.36	308.694
33.2667	.166133	545.455	847.337	309.796	320.912
39.92	.1996	605.059	1089.37	322.123	334.215
46.5734	.232867	681.309	1488.93	335.492	348.829
53.2267	.266134	778.222	2296.08	349.939	365.143
59.8801	.2994	907.279	4645.22	365.327	384.175
66.5334	.332667	1097.51	242657	393.135	475.197

TO ANALYSE CROSSLINKING PRESS ENTER?

% A REACTED	BRANCH COEF.	WT. FR. GEL	NUM. AVE. MW(G/MOL)	X-LINK MW (G/MOL)	GLASS TEMP(K)
66.6339	.334169	.0100001	1097.51	2.90251E+07	383.978
68.8993	.342996	.109	1159.21	230396	388.993
70.5838	.352944	.208	1237.62	59491.5	395.02
72.0634	.364317	.307	1341.36	25511.6	402.332
75.5111	.377555	.486	1486.39	13515.9	411.572
78.6674	.393337	.585	1726.31	8008.31	423.393
82.5573	.412786	.684	2086.83	5856.65	439.291
87.5962	.437981	.793	2934.59	3298.56	462.172
94.6954	.473477	.882	6861.99	2159.05	499.291
99.9268	.499632	.95348	435168	1789.73	530.892

% B REACTED= 49.9632 TO CONTINUE TYPE RUN AND PRESS ENTER
READY
)



Table 5-23

SC5291.7FR

Estimated Cure Path for TGMDA Homopolymer
(see Table 5-8)

A AND B COREACTION-MOL. WT. DIST -THERMAL TRANS -D H. KHELBLE-OCT
27, 1982

IF NONSTOICHIOMETRIC REACTION HAVE MOLES OF B IN EXCESS

MOLES OF TYPE A (MOLE)=? 1

TYPE A FUNCTIONALITY(=2)=? 4

MOL. WT. OF TYPE A (G/MOLE)=? 422

MOLES OF TYPE B (MOLE)=? 1

TYPE B FUNCTIONALITY (=2)=? 4

MOL. WT. OF TYPE B (G/MOLE)=? 422

FRACTION OF MOLECULES OF FUNCTIONALITY >2=? 1

NUMBER OF A AND B MAIN CHAIN ATOMS (A1,A2)=? 17,17

MOL. WT. BETWEEN ENTANGLEMENTS (G/MOLE)=? 5300

GLASS COORDINATION NUMBER (8<2<10)=? 10

MONOMER AND LINEAR POLYMER GLASS TEMPERATURES (T1,T2) IN DEG. K=
? 260,482

GEL POINT (% A REACTED)= 33.3333

GEL POINT (% B REACTED)= 33.3333

INITIAL NUM. AVE. DEG. OF POLYMERIZATION= 4.52747

TO ANALYSE POLYMERIZATION PRESS ENTER?

% A REACTED	BRANCH COEF.	NUM. AVE. MW(G/MOL)	WT. AVE. MW(G/MOL)	GLASS TEMP(K)	FLOW TEMP(K)
0	0	422	422	260	268.5
3.32667	.0332667	452.878	484.38	266.258	275.243
6.65334	.0665334	486.773	562.315	272.824	292.344
9.98001	.0998001	527.237	662.455	279.722	289.84
13.3067	.133067	575.837	795.863	286.978	297.73
16.6333	.166333	632.368	982.422	294.621	306.226
19.95	.1995	702.397	1261.79	302.681	315.259
23.2867	.232867	789.888	1726.18	311.196	325.057
26.6134	.266134	902.824	2550.35	320.203	335.992
29.94	.2994	1051.85	5306.56	329.747	348.693
33.2667	.332667	1260.96	281322	339.877	437.852

TO ANALYSE CROSSLINKING PRESS ENTER? -

% A REACTED	BRANCH COEF.	WT. FR. GEL	NUM. AVE. MW(G/MOL)	X-LINK MW (G/MOL)	GLASS TEMP(K)
33.4169	.334169	.0100001	1272.38	3.365E+07	340.351
34.2996	.342996	.109	1343.92	267108	343.267
35.2944	.352944	.208	1434.83	68970.9	346.821
36.4317	.364317	.307	1555.1	29576.7	351.202
37.7555	.377555	.406	1723.23	15669.5	356.595
39.3337	.393337	.505	1978.19	9284.36	363.753
41.8736	.418736	.604	2419.35	5862.38	373.166
43.7981	.437981	.703	3402.19	3824.16	386.481
47.3477	.473477	.802	7955.39	2583.87	407.368
93.317	.93317	.901	4.22E+08	1562.5	431.108
98.087	.98087	.901	4.22E+08	434.467	530.321

% B REACTED= 98.087 TO CONTINUE TYPE RUN AND PRESS ENTER
READY

Table 5-24

SC5291.7FR

Estimated Polymerization Path for Equimolar Isoamyl-Neopentyl
Acrylate Copolymer (see Table 5-9)

A AND B COREACTION-MOL. WT. DIST -THERMAL TRANS.-D H.KAELBLE-OCT
27,1982
IF NONSTOICHIOMETRIC REACTION HAVE MOLES OF B IN EXCESS
MOLES OF TYPE A (MOLE)=? 1
TYPE A FUNCTIONALITY(=>2)=? 2
MOL. WT. OF TYPE A (G/MOLE)=? 142
MOLES OF TYPE B (MOLE)=? 1
TYPE B FUNCTIONALITY(=>2)=? 2
MOL. WT. OF TYPE B (G/MOLE)=? 142
FRACTION OF MOLECULES OF FUNCTIONALITY >2=? 0
NUMBER OF A AND B MAIN CHAIN ATOMS (A1,A2)=? 2,2
MOL. WT. BETWEEN ENTANGLEMENTS (G/MOLE)=? 34185
GLASS COORDINATION NUMBER (8<Z<16)=? 10
MONOMER AND LINEAR POLYMER GLASS TEMPERATURES (T1,T2) IN DEG. K=
? 69,240
GEL POINT (% A REACTED)= 100
GEL POINT (% B REACTED)= 103
INITIAL NUM. AVE. DEG. OF POLYMERIZATION= 1.03977
TO ANALYSE POLYMERIZATION PRESS ENTER? -

% A REACTED	BRANCH COEF.	NUM. AVE MW(G/MOL)	WT. AVE MW(G/MOL)	GLASS TEMP.(K)	FLOW TEMP.(K)
0	0	142	142	69	70.8494
9.98001	9.96006E-03	143.429	144.857	69.4932	71.3977
19.96	.0399402	147.892	153.784	71.0159	73.0966
29.94	.0896405	155.982	169.955	73.7076	76.0596
39.92	.159361	168.919	195.833	77.9391	80.591
49.9	.249001	189.002	236.163	83.8818	87.1751
59.8801	.359562	221.379	300.755	92.6766	96.6839
69.8601	.488043	277.367	412.734	105.785	119.755
79.8401	.537444	391.663	641.327	126.415	132.784
89.8201	.806765	734.855	1327.71	162.294	171.113
99.8001	.996206	35552.9	70963.8	237.548	264.913

% B REACTED= 99.8001 TO CONTINUE TYPE RUN AND PRESS ENTER
READY
>



Table 5-25

Estimated Polymerization Path for Polystyrene

A AND B COREACTION-MOL. WT. DIST.-THERMAL TRANS.-D. H. KAELEBLE-OCT
27, 1982

IF NONSTOICHIOMETRIC REACTION HAVE MOLES OF B IN EXCESS

MOLES OF TYPE A (MOLE)=? 1

TYPE A FUNCTIONALITY(=2)=? 2

MOL. WT. OF TYPE A (G/MOLE)=? 104

MOLES OF TYPE B (MOLE)=? 1

TYPE B FUNCTIONALITY(=2)=? 2

MOL. WT. OF TYPE B (G/MOLE)=? 104

FRACTION OF MOLECULES OF FUNCTIONALITY >2=? 0

NUMBER OF A AND B MAIN CHAIN ATOMS (A1,A2)=? 2,2

MOL. WT. BETWEEN ENTANGLEMENTS (G/MOLE)=? 20200

GLASS COORDINATION NUMBER (8<Z<10)=? 10

MONOMER AND LINEAR POLYMER GLASS TEMPERATURES (T1,T2) IN DEG. F=

? 110,384

GEL POINT (% A REACTED)= 100

GEL POINT (% B REACTED)= 100

INITIAL NUM. AVE. DEG. OF POLYMERIZATION= 1.00365

TO ANALYSE POLYMERIZATION PRESS ENTER? _

% A REACTED	BRANCH COEF.	NUM. AVE MW(G/MOL)	WT. AVE MW(G/MOL)	GLASS TEMP(K)	FLOW TEMP(K)
0	0	104	104	110	111.849
9.98001	9.96006E-03	105.046	106.093	110.787	112.692
19.96	.0398402	108.315	112.631	113.219	115.239
29.94	.0896425	114.241	124.481	117.517	119.863
39.92	.159361	123.715	143.431	124.113	126.866
49.9	.249001	138.492	172.965	133.767	137.06
59.8801	.359562	162.136	220.271	147.919	151.827
69.8601	.480043	203.142	302.284	158.774	173.744
79.8401	.637444	286.852	469.704	201.777	208.145
89.8201	.886765	538.204	972.408	259.226	268.861
99.8001	.996006	26030.7	51973.5	380.217	407.779

% B REACTED= 99.8001 TO CONTINUE TYPE RUN AND PRESS ENTER
READY



Table 6-1

Chemical Structure and Thermal Transitions of
Six Film Forming Polymers

No.	Repeat Unit Structure	Thermal Transition (K)		
		T _y	T _g	T _c
1	$\left[\text{CF}_2 - \text{CF}_2 \right]_x \left[\text{CF}_2 - \overset{\text{CF}_3}{\underset{\text{CF}}{\text{C}}} \right]_{0.14x}$	177	358	555
2	$-\text{CF}_2 - \text{CF}_2 -$	177	400	600
3	$\left[\text{CF}_s - \overset{\text{Cl}}{\underset{\text{CF}}{\text{C}}} \right]_x \left[\text{CF}_2 - \text{CH}_2 \right]_{0.03x}$	273	323	493
4	$\left[\text{C} \begin{array}{c} \text{O} \\ \\ \text{O} \end{array} - \text{C}_6\text{H}_4 - \overset{\text{CH}_3}{\underset{\text{CH}_3}{\text{C}}} - \text{C}_6\text{H}_4 - \text{C} \right]$	176	423	538
5	$\left[\text{O} - \text{CH}_2 - \text{CH}_2 - \text{O} - \overset{\text{O}}{\underset{ }{\text{C}}} - \text{C}_6\text{H}_4 - \overset{\text{O}}{\underset{ }{\text{C}}} \right]$	243	350	536
6	$\left[\text{N} \begin{array}{c} \text{O} \\ \\ \text{C} \\ \\ \text{O} \end{array} \text{C}_6\text{H}_2 \text{C} \begin{array}{c} \text{O} \\ \\ \text{C} \\ \\ \text{O} \end{array} \text{N} - \text{C}_6\text{H}_4 - \text{O} - \text{C}_6\text{H}_4 \right]$	180	530	-

T_A is an amorphous transition below T_g involving local motion of 2-4 atoms.

T_g is the amorphous glass transition involving cooperative motion of 20-40 atoms in chain segments.

T_c is the crystalline phase melting temperature involving cooperative motion of the entire polymer molecule.

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Table 6-2
Input Format for Chemical-Mechanical Property Program
(Upper symbols found in Ref. 1 and lower symbols in Table 6-3)

		Polymer or Experiment Name				
Polymer Properties	R1	AOS				
	R2	M_p (g/mol) AA	X_p (mole) AB	Σh_p AC	ρ_p (g/cc) AD	$(T_{gAR})_p$ (K) AE
		Z_{gp} AF	V_{gp}^0 (cc/mol) AG	Q_{LP} AH	δ_p (cal/cc) ^{1/2} AI	AR_p (S ⁻¹) AJ
	R4	M_D (g/mol) AK	M_C (g/mol) AL	M_e (g/mol) AM	τ_g (S) AN	ϕ AP
		M_D (g/mol) AQ	X_D (mol) AR	Σh_D AS	ρ_D (g/cc) AT	$(T_{gAR})_D$ (K) AU
	R6	Z_{gD} AV	V_{GD}^0 (cc/mol) AW	Q_{LD} AX	δ_D (cal/cc) ^{1/2} AY	AR_D (S ⁻¹) AZ
		A (S ⁻¹) BA	t_I (S) BB	T (K) BC	ΔT (K) BD	NT BE
	R7					
		C1	C2	C3	C4	C5
Diluent Properties						
Use Condition						



Table 6-3

Input Nomenclature for Chemical-Mechanical Program

Row	Symbol	Meaning
2	AA	Polymer molecular weight (number ave.)
	AB	Moles polymer
	AC	Polymer repeat unit rotational degrees of freedom
	AD	Polymer density
	AE	Polymer glass temperature at reference strain rate AJ
3	AF	Total adjacent lattice (Z) sites for glass (nominally = 10)
	AG	Polymer glass repeat unit molar volume
	AH	Intermolecular lattice sites in polymer liquid (nominally = 9)
	AI	Polymer solubility parameter
	AJ	Strain (or thermal scan) rate for reference polymer glass temperature (nominally = 1.0)
4	AK	Polymer repeat unit molecular weight
	AL	Molecular weight between crosslinks (number ave.)
	AM	Molecular weight between entanglements (number ave.)
	AN	Relaxation time at T_g (nominally = 1.0)
	AP	Polymer-diluent interaction parameters (nominally = 1.0)
5	AQ	Diluent molecular weight
	AR	Moles diluent
	AS	Diluent molecular rotational degrees of freedom
	AT	Diluent density
	AU	Diluent glass temperature at reference rate AZ
6	AV	Total adjacent lattice (Z) sites of diluent glass (nominally = 10)
	AW	Diluent glass molar volume
	AX	Intermolecular lattice (q) sites of diluent liquid (nominally = 9)
	AY	Diluent solubility parameter
	AZ	Strain (or thermal scan) rate for diluent reference glass temperature (nominally = 1.0)
7	BA	Mechanical (or thermal scan) strain rate (nominally = 1.0)
	BB	Constant time for isochronal stress-strain response (nominally = 1.0)
	BC	Starting temperature for family of stress-strain curves
	BD	Temperature increment
	BE	Number of temperatures

Table 6-4
Nomenclature for Intermediate Results in
Chemical-Mechanical Program

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Line No.	Symbol	Meaning
1	BF	Wood constant in T_g calculation
	BG	Rate ratio in polymer T_g calculation
	BH	Log BG
	BI	Polymer T_g at rate BA (K)
	BJ	Polymer T_g change with shear stress (K/bar)
2	BK	Rate ratio in diluent T_g calculation
	BL	Log BK
	BM	Diluent T_g at rate BA (K)
	BN	Diluent T_g change with shear stress (K/bar)
3	TG	T_g of polymer-diluent at zero stress (K)
	UR	Polymer-diluent T_g change with shear stress (K/bar)
4	BO	Volume fraction polymer
	BQ	Volume fraction diluent
	BR	Cohesive energy of polymer-diluent solution (cal/cc)
5	BS	Fraction of effective crosslinked segments
	BT	Fraction of effective entangled segments
6	BU	Glass state shear modulus (bar)
	BV	Rubber state shear modulus at τ_g (bar)
	BX	Rubber state shear modulus at τ_l (bar)
	BY	Rubber state shear modulus at τ_m (bar)
	BZ	Crosslink network shear modulus ^m (bar)
7	SB	Brittle shear strength (bar)
	TL	$\log_{10} (\tau_m/\tau_g)$
	TM	Melt (or flow) temperature (K)
	NH	Fraction Neohookian versus Hookian tensile response
8	T	Current temperature (K)
	SM	Flow shear strength (bar)
	SS	Current shear strength (bar)



Table 6-5
Estimated Mechanical Properties of an Acrylate Copolymer

POLYMER-DILUENT-EQUIMOLAR ISOAMYL-NEOPENTYL ACRYLATE
POLYMER PROPERTIES:

AA,AB,AC,AD,AE= 1 03E+06 1 121 1.09 230

AF,AG,AH,AI,AJ= 10 260 9 9.07 1

AK,AL,AM,AN,AP= 284 1 03E+06 34200 1 1

DILUENT PROPERTIES:

AQ,AR,AS,AT,AU= 284 0 121 1.09 59

AV,AW,AX,AY,AZ= 10 260 9 9.07 1

TEST CONDITIONS:

BA,BB,BC,BD,BE= 1 1 100 25 15

FRACTION NEOHOOKIAN TENSILE RESPONSE= 0

PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:

BF,BG,BH,BI,BJ= 1 1 0 230 114881

BK,BL,BM,BN= 1 0 59 114391

TG,UR= 230 114391

EO,BQ,BR= 1 0 82.2649

SS,BT= 0 933592

SU,SV,SW,SY,SZ= 27547.9 27547.9 609377 157335 0

SB,TL,TM,NH= 960.491 12.1372 349.002 0

T,SM,SS= 100 2157.48 860.491

SHEAR AND TENSION ANALYSIS:

INPUT NUMBER OF STRESS INCREMENTS? 12

INPUT NUMBER OF STRESS INCREMENTS? 12

SHEAR MODULUS (BAR)	SHEAR STRESS (BAR)	SHEAR STRAIN	TENSILE STRESS (BAR)	TENSILE STRAIN
0	0	0	0	0
27547.9	71.7076	2.60361E-03	143.415	1.73534E-03
27547.9	143.415	5.20503E-03	286.83	3.47069E-03
27547.9	215.123	7.80904E-03	430.245	5.20603E-03
27547.9	286.83	.0104121	573.661	6.94137E-03
27547.9	358.538	.0130151	717.276	8.67672E-03
27547.9	430.245	.0156181	860.491	.0104121
27547.9	501.953	.0182211	1003.91	.0121474
27547.9	573.661	.0208241	1147.32	.0138827
27547.9	645.368	.0234271	1290.74	.0156181
27547.9	717.076	.0260301	1434.15	.0173534
27547.9	788.783	.0286332	1577.57	.0190888
27547.9	860.491	.0312362		

SHEAR FAILURE PROPERTIES:

STRESS(BAR)= 860.491 STRAIN= .0312362 ENERGY/VOL(BAR)= 11.2927

E-MODULUS(BAR)= 23147.9

E-WORK(BAR)= 11.2927

E-STRAIN= .0312362

P-WORK(BAR)= 0

TENSILE FAILURE PROPERTIES:

STRESS(BAR)= 1636.56 STRAIN= .0204074 ENERGY/VOL(BAR)= 17.2091

E-MODULUS(BAR)= 82543.7

E-WORK(BAR)= 17.2091

E-STRAIN= .0204074

P-WORK(BAR)= 0

PRESS ENTER TO CONTINUE

Table 6-6
Calculated Effects of Isochronal Loading Time t Upon the
Shear and Tensile Failure Properties of Equimolar Isoamyl-Neopentyl
Acrylate Linear Polymer ($M_n = 1.06 \text{ E6}$) at $T = 296\text{K}$ with
Hookian Response

t (s)	Shear			Tension		
	σ_b (bar)	γ_b	W_s (bar)	S_b (bar)	ϵ_b	W_T (bar)
2E2	9.6	55	243	2.82	5.8	8.19
1E2	52.4	334	8.3E3	7.37	13.2	48.7
1E1	224	1200	1.35E5	19.3	22.2	215
1	461	2156	5.2E5	34.5	25.8	444
1E-2	860	2310	1.13E6	107	15.1	806
1E-4	860	582	3.08E5	278	5.2	814
1E-5	860	186	9.88E4	441	3.2	791
1E-6	860	58	3.1E4	582	1.96	726
1E-8	860	5.9	3.1E3	1010	0.70	491
1E-10	860	0.58	312	1449	0.18	196
1E-12	860	0.067	32	1664	0.033	35.9
1E-14	860	0.034	13.5	1686	0.020	17.2



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Table 6-7
Estimated Effects of Low Moisture (0 - 2 Wt%) on
Cured Epoxy Thermoset

POLYMER-DILUENT=TCMDA/DD8 EPOXY+0% H2O

POLYMER PROPERTIES:

AA,AB,AC,AD,AE= 495000 1 319 1.16 483

AF,AG,AH,AI,AJ= 10 943 9 12.6 1

AK,AL,AM,AN,AP= 1094 1709 5168 1 32

DILUENT PROPERTIES:

AQ,AR,AS,AT,AU= 18 0 20 1 137

AV,AW,AX,AY,AZ= 10 18 11 23.2 1

TEST CONDITIONS:

BA,BB,BC,BD,BE= 1 1 300 25 15

FRACTION NEOHOOKIAN TENSILE RESPONSE= 0

PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:

BF,BG,BH,BI,BJ= 3.81052 1 0 483 158045

BK,BL,BM,BN= 1 0 137 0393688

TG,UR= 483 158045

BO,BQ,BR= 1 0 158.76

BS,ET= 993095 979119

BU,BV,BX,BY,BZ= 53163.7 53163.7 9.8124 1.38231 35.8285

SB,TL,TM,NH= 1660.63 11.5743 585.517 0

T,SM,SS= 300 1806.56 1660.63

SHEAR AND TENSION ANALYSIS:

INPUT NUMBER OF STRESS INCREMENTS? -

POLYMER-DILUENT=TCMDA/DD8 EPOXY+2% H2O

POLYMER PROPERTIES:

AA,AB,AC,AD,AE= 495000 1 319 1.16 483

AF,AG,AH,AI,AJ= 10 943 9 12.6 1

AK,AL,AM,AN,AP= 1094 1709 5168 1 32

DILUENT PROPERTIES:

AQ,AR,AS,AT,AU= 18 550 20 1 137

AV,AW,AX,AY,AZ= 10 18 11 23.2 1

TEST CONDITIONS:

BA,BB,BC,BD,BE= 1 1 300 25 15

FRACTION NEOHOOKIAN TENSILE RESPONSE= 0

PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:

BF,BG,BH,BI,BJ= 3.81052 1 0 483 158045

BK,BL,BM,BN= 1 0 137 0393688

TG,UR= 458.498 149641

BO,BQ,BR= 977326 1022674 156.065

BS,ET= 993095 978635

BU,BV,BX,BY,BZ= 52261.1 51958.2 8.36124 1.22215 33.2358

SB,TL,TM,NH= 1632.44 11.5956 561.582 0

T,SM,SS= 300 1748.06 1632.44

SHEAR AND TENSION ANALYSIS:

INPUT NUMBER OF STRESS INCREMENTS? -

Table 6-8

Estimated Effects of Medium Moisture (4 - 6 Wt%) on
Cured Epoxy Thermoset

POLYMER-DILUENT=TCMDA/DDS EPOXY+4% H2O

POLYMER PROPERTIES:

AA,AB,AC,AD,AE= 495000 1 319 1 16 483

AF,AG,AH,AI,AJ= 10 943 9 12 6 1

AK,AL,AM,AN,AP= 1094 1709 5168 1 32

DILUENT PROPERTIES:

AQ,AR,AS,AT,AU= 18 1100 20 1 137

AV,AW,AX,AY,AZ= 10 13 11 23 2 1

TEST CONDITIONS:

BA,BB,BC,BD,BE= 1 1 303 25 15

FRACTION NEOHOOKIAN TENSILE RESPONSE= 0

PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:

BF,BG,BH,BI,BJ= 3.81052 1 0 483 158045

BK,BL,BM,BN= 1 0 137 0393668

TG,UR= 437.238 142349

BO,BQ,BR= 955658 0443425 153.977

BS,BT= 993095 97815

BU,BV,BX,BY,BZ= 51562 6 50806 3 7.79674 1 15249 30 9882

SB,TL,TM,NH= 1610.62 11.6135 543 799 0

T,SM,SS= 300 1691.61 1610.62

SHEAR AND TENSION ANALYSIS:

INPUT NUMBER OF STRESS INCREMENTS? -

POLYMER-DILUENT=TCMDA/DDS EPOXY+6% H2O

POLYMER PROPERTIES:

AA,AB,AC,AD,AE= 495000 1 319 1 16 483

AF,AG,AH,AI,AJ= 10 943 9 12 6 1

AK,AL,AM,AN,AP= 1094 1709 5168 1 32

DILUENT PROPERTIES:

AQ,AR,AS,AT,AU= 18 1650 20 1 137

AV,AW,AX,AY,AZ= 10 12 11 23 2 1

TEST CONDITIONS:

BA,BB,BC,BD,BE= 1 1 300 25 15

FRACTION NEOHOOKIAN TENSILE RESPONSE= 0

PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:

BF,BG,BH,BI,BJ= 3.81052 1 0 483 158045

BK,BL,BM,BN= 1 0 137 0393668

TG,UR= 418.614 125961

BO,BQ,BR= 934929 0650711 152.432

BS,BT= 993095 977666

BU,BV,BX,BY,BZ= 51044.5 49704.3 7.30274 1.09137 29.0213

SB,TL,TM,NH= 1594.43 11.6204 522 577 0

T,SM,SS= 300 1637.07 1594.43

SHEAR AND TENSION ANALYSIS:

INPUT NUMBER OF STRESS INCREMENTS? -



Table 6-9

Estimated Effects of High Moisture (8 - 10 Wt%) on
Cured Epoxy Thermoset

POLYMER-DILUENT=TMDA/DDS EPOXY+8% H2O

POLYMER PROPERTIES:

AA,AB,AC,AD,AE= 495000 1 .319 1.16 483

AF,AG,AH,AI,AJ= 10 943 9 12.5 1

AK,AL,AM,AN,AP= 1094 1709 5168 1 .32

DILUENT PROPERTIES:

AQ,AR,AS,AT,AU= 18 2200 20 1 137

AV,AW,AX,AY,AZ= 10 18 11 23.2 1

TEST CONDITIONS:

BA,BB,BC,BD,BE= 1 1 300 25 15

FRACTION NEOHOOKIAN TENSILE RESPONSE= 0

PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:

BF,BG,BH,BI,BJ= 3.81052 1 0 483 .158045

BK,BL,BM,BN= 1 0 137 .0393688

TG,UR= 402.166 .130319

BO,BQ,BR= .915001 .0849195 151.361

BS,BT= .993095 .977122

BU,BV,BX,BY,BZ= 50685 .48649 6.86686 1.0373 27.2858

SB,TL,TM,NH= 1583.23 11.6409 506.465 0

T,SM,SS= 300 1584 3 1583 23

SHEAR AND TENSION ANALYSIS:

INPUT NUMBER OF STRESS INCREMENTS? _

POLYMER-DILUENT=TCMDA/DDS EPOXY+10% H2O

POLYMER PROPERTIES:

AA,AB,AC,AD,AE= 495000 1 .319 1.16 483

AF,AG,AH,AI,AJ= 10 943 9 12.5 1

AK,AL,AM,AN,AP= 1094 1709 5168 1 .32

DILUENT PROPERTIES:

AQ,AR,AS,AT,AU= 18 2750 20 1 137

AV,AW,AX,AY,AZ= 10 18 11 23.2 1

TEST CONDITIONS:

BA,BB,BC,BD,BE= 1 1 300 25 15

FRACTION NEOHOOKIAN TENSILE RESPONSE= 0

PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:

BF,BG,BH,BI,BJ= 3.81052 1 0 483 .158045

BK,BL,BM,BN= 1 0 137 .0393688

TG,UR= 307.534 .125301

BO,BQ,BR= .896057 .103943 150.711

BS,BT= .993095 .976697

BU,BV,BX,BY,BZ= 50468.4 47637.7 6.47946 .989109 25.7433

SB,TL,TM,NH= 1576.44 11.6512 492.112 0

T,SM,SS= 300 1533.21 1633.21

SHEAR AND TENSION ANALYSIS:

INPUT NUMBER OF STRESS INCREMENTS? _

Table 6-10

Second Estimated Effects of Low Moisture (0 - 2 Wt%)
on Cured Epoxy Thermoset

POLYMER-DILUENT=TGMDA/DDS EPOXY+0% H2O

POLYMER PROPERTIES:

AA,AB,AC,AD,AE= 495000 1 319 1.16 483

AF,AG,AH,AI,AJ= 10 943 9 12.6 1

AK,AL,AM,AN,AP= 1094 1709 5168 1 .32

DILUENT PROPERTIES:

AQ,AR,AS,AT,AU= 10 0 20 1 137

AV,AW,AX,AY,AZ= 10 10 11 23.2 1

TEST CONDITIONS:

BA,BB,BC,BD,BE= 1 1 220 40 15

FRACTION NEOHOOKIAN TENSILE RESPONSE= 0

PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:

BF,BG,BH,BI,BJ= 5.33473 1 0 483 158045

BK,BL,BM,BN= 1 0 137 .0281206

TG,UR= 483 158045

BO,BQ,BR= 1 0 158.76

BS,BT= .993095 .979119

BU,BV,BX,BY,BZ= 53163 7 53163 7 9.0124 1.30231 35.8285

SB,TL,TM,NH= 1660.63 11.5743 585.517 0

T,SM,SS= 220 2312 74 1660.63

SHEAR AND TENSION ANALYSIS:

INPUT NUMBER OF STRESS INCREMENTS? -

POLYMER-DILUENT=TGMDA/DDS EPOXY+2% H2O

POLYMER PROPERTIES:

AA,AB,AC,AD,AE= 495000 1 319 1.16 483

AF,AG,AH,AI,AJ= 10 943 9 12.6 1

AK,AL,AM,AN,AP= 1094 1709 5168 1 .32

DILUENT PROPERTIES:

AQ,AR,AS,AT,AU= 10 550 20 1 137

AV,AW,AX,AY,AZ= 10 10 11 23.2 1

TEST CONDITIONS:

BA,BB,BC,BD,BE= 1 1 220 40 15

FRACTION NEOHOOKIAN TENSILE RESPONSE= 0

PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:

BF,BG,BH,BI,BJ= 5.33473 1 0 483 158045

BK,BL,BM,BN= 1 0 137 .0281206

TG,UR= 449.543 145519

BO,BQ,BR= .977326 .022674 156.065

BS,BT= .993095 .978635

BU,BV,BX,BY,BZ= 52261.1 51959.2 8.19975 1.19854 32.5939

SB,TL,TM,NH= 1632.44 11.6126 553.179 0

T,SM,SS= 220 2209.59 1632.44

SHEAR AND TENSION ANALYSIS:

INPUT NUMBER OF STRESS INCREMENTS? -



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Table 6-11

Second Estimated Effects of Medium Moisture (4 - 6 Wt%)
on Cured Epoxy Thermoset

POLYMER-DILUENT=TCMDA/DDS EPOXY+4% H2O

POLYMER PROPERTIES:

AA,AB,AC,AD,AE= 495000 1 319 1.16 483

AF,AG,AH,AI,AJ= 10 943 9 12.6 1

AK,AL,AM,AN,AP= 1094 1709 5168 1 .32

DILUENT PROPERTIES:

AQ,AR,AS,AT,AU= 18 1100 28 1 137

AV,AW,AX,AY,AZ= 10 10 11 23.2 1

TEST CONDITIONS:

BA,BB,BC,BD,BE= 1 1 220 40 15

FRACTION NEOHOOKIAN TENSILE RESPONSE= 0

PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:

BF,BG,BH,BI,BJ= 5.33473 1 0 483 158045

BK,BL,BM,BN= 1 0 137 .0201206

TG,UR= 422.152 .135196

BO,BQ,BR= .955658 .0443425 153.979

BS,BT= 993095 .97815

BU,BV,BX,BY,BZ= 51562.6 50806 3 7.52773 1.11272 29 919

SB,TL,TM,NH= 1610.62 11.644 526 535 0

T,SM,SS= 220 2267 33 1610 62

SHEAR AND TENSION ANALYSIS:

INPUT NUMBER OF STRESS INCREMENTS? _

POLYMER-DILUENT=TCMDA/DDS EPOXY+6% H2O

POLYMER PROPERTIES:

AA,AB,AC,AD,AE= 495000 1 319 1.16 483

AF,AG,AH,AI,AJ= 10 943 9 12.6 1

AK,AL,AM,AN,AP= 1094 1709 5168 1 .32

DILUENT PROPERTIES:

AQ,AR,AS,AT,AU= 18 1650 28 1 137

AV,AW,AX,AY,AZ= 10 10 11 23.2 1

TEST CONDITIONS:

BA,BB,BC,BD,BE= 1 1 220 40 15

FRACTION NEOHOOKIAN TENSILE RESPONSE= 0

PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:

BF,BG,BH,BI,BJ= 5.33473 1 0 483 158045

BK,BL,BM,BN= 1 0 137 .0201206

TG,UR= 399.185 .126542

BO,BQ,BR= .934929 .0650711 152.432

BS,BT= .993095 .977666

BU,BV,BX,BY,BZ= 51044.5 49704.3 6.9624 1.0405 27.6687

SB,TL,TM,NH= 1594.43 11.6699 504.193 0

T,SM,SS= 220 2245.04 1594.43

SHEAR AND TENSION ANALYSIS:

INPUT NUMBER OF STRESS INCREMENTS? _

Table 6-12

Second Estimated Effects of High Moisture (8 - 10 Wt%)
on Cured Epoxy Thermoset

POLYMER-DILUENT=TGMDA/DDS EPOXY+8% H2O

POLYMER PROPERTIES:

AA,AB,AC,AD,AE= 495000 1 319 1.16 483

AF,AG,AH,AI,AJ= 10 943 9 12.6 1

AK,AL,AM,AN,AP= 1094 1709 5168 1 .32

DILUENT PROPERTIES:

AQ,AR,AS,AT,AU= 10 2200 20 1 137

AV,AW,AX,AY,AZ= 10 10 11 23.2 1

TEST CONDITIONS:

BA,BB,BC,BD,BE= 1 1 220 40 15

FRACTION NEOHOOKIAN TENSILE RESPONSE= 0

INTERMEDIATE RESULTS:

BF,BC,BH,BI,BJ= 5.33473 1 0 483 158045

BK,BL,BM,BN= 1 0 137 .0201206

TG,UP= 379.504 .119182

BO,BQ,BR= .915001 .0049195 151.361

BS,BT= .993095 .977162

BU,BV,BX,BY,BZ= 50685 9 48649 6.47992 .978844 25.2482

SB,TL,TM,NH= 1583.23 11.6913 485.179 0

T,SM,SS= 220 2225 1583.23

SHEAR AND TENSION ANALYSIS:

INPUT NUMBER OF STRESS INCREMENTS? _

POLYMER-DILUENT=TGMDA/DDS EPOXY+10% H2O

POLYMER PROPERTIES:

AA,AB,AC,AD,AE= 495000 1 319 1.16 483

AF,AG,AH,AI,AJ= 10 943 9 12.6 1

AK,AL,AM,AN,AP= 1094 1709 5168 1 .32

DILUENT PROPERTIES:

AQ,AR,AS,AT,AU= 10 2750 20 1 137

AV,AW,AX,AY,AZ= 10 10 11 23.2 1

TEST CONDITIONS:

BA,BB,BC,BD,BE= 1 1 220 40 15

FRACTION NEOHOOKIAN TENSILE RESPONSE= 0

PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:

BF,BC,BH,BI,BJ= 5.33473 1 0 483 158045

BK,BL,BM,BN= 1 0 137 .0201206

TG,UR= 362.632 .112046

BO,BQ,BR= .896057 .103943 150.711

BS,BT= .993095 .976697

BU,BV,BX,BY,BZ= 50468.4 47637.7 6.0631 .925551 24.0891

SB,TL,TM,NH= 1576.44 11.7089 468.293 0

T,SM,SS= 220 2204.71 1576.44

SHEAR AND TENSION ANALYSIS:

INPUT NUMBER OF STRESS INCREMENTS? _



Table 6-13

Calculated Mechanical Response of Cured TGMDA/DDS
Epoxy (0 Wt% H₂O, T_g = 483K, t = 1 s)

Shear

T (K)	σ_b (bar)	γ_b	W_S (bar)	W_E (bar)	W_p (bar)	G_E (bar)	γ_E
220	1.66E3	2.24E-2	1.85E1	1.85E1	0	7.39E4	2.34E-2
260	1.66E3	2.24E-2	1.85E1	1.85E1	0	7.39E4	2.34E-2
300	1.66E3	3.22E-2	3.42E1	1.92E1	1.50E1	7.17E4	2.32E-2
340	1.55E3	1.31E-1	1.77E2	2.81E1	1.49E2	4.30E4	3.61E-2
380	1.30E3	2.30E-1	2.56E2	4.29E1	2.13E2	1.97E4	6.59E-2
420	1.05E3	3.61E-1	3.02E2	7.55E1	2.26E2	7.27E3	1.44E-1
460	7.94E2	5.94E-1	3.25E2	1.46E2	1.78E2	2.15E3	3.70E-1
500	5.41E2	9.27E-1	2.01E2	2.01E2	0	4.67E2	9.27E-1
540	2.88E2	1.08	7.80E1	7.80E1	0	1.35E2	1.08
580	3.49E1	4.84E-1	7.46	7.46	0	6.36E1	4.84E-1
585	0	0	0	0	0	0	0

Tension

T (K)	S_b (bar)	ϵ_b	W_T (bar)	W_E (bar)	W_p (bar)	E_E (bar)	ϵ_E
220	3.27E3	1.47E-2	2.40E1	2.40E1	0	2.22E5	1.47E-2
260	3.27E3	1.47E-2	2.40E1	2.40E1	0	2.22E5	1.47E-2
300	3.26E3	1.94E-2	3.89E1	2.44E1	1.45E1	2.18E5	1.49E-2
340	2.94E3	5.64E-2	1.40E2	2.56E1	1.14E2	1.69E5	1.74E-2
380	2.37E3	9.66E-2	2.01E2	2.80E1	1.73E2	1.00E5	2.36E-2
420	1.80E3	1.61E-1	2.48E2	4.24E1	2.05E2	3.85E4	4.70E-2
460	1.25E3	2.71E-1	2.55E2	8.29E1	1.73E2	9.42E3	1.33E-1
500	7.20E2	5.03E-1	1.64E2	1.64E2	0	1.30E3	5.03E-1
540	3.53E2	6.30E-1	6.39E1	6.39E1	0	3.22E2	6.30E-1
580	5.49E1	2.72E-1	6.76	6.76	0	1.83E2	2.71E-1
585	0	0	0	0	0	0	0

Table 6-14
Calculated Mechanical Response of 2 Wt% Moisture
in Cured Epoxy ($T_g = 449.6K$, $t = 1$ s)

Shear

T (K)	σ_b (bar)	γ_b	W_S (bar)	W_E (bar)	W_p (bar)	G_E (bar)	γ_E
220	1.63E3	2.23E-2	1.82E1	1.82E1	0	7.26E4	2.24E-2
260	1.63E3	2.23E-2	1.82E1	1.82E1	0	7.26E4	2.24E-2
300	1.63E3	8.79E-2	1.21E2	2.26E1	9.03E1	5.89E4	2.77E-2
340	1.46E3	1.85E-1	2.29E2	4.24E1	1.87E1	2.53E4	5.79E-2
380	1.19E3	3.43E-1	3.30E2	7.76E1	2.53E2	9.12E3	1.30E-1
420	9.15E2	3.36E-1	1.90E2	1.18E2	7.18E1	3.56E3	2.57E-1
460	6.40E2	8.26E-1	2.25E2	2.25E2	0	6.61E2	8.26E-1
500	3.65E2	1.18	9.28E1	9.28E1	0	1.34E2	1.18
540	9.05E1	8.49E-1	2.76E1	2.76E1	0	7.66E1	8.49E-1
553	0	0	0	0	0	0	0

Tension

T (K)	S_b (bar)	ϵ_b	W_T (bar)	W_E (bar)	W_p (bar)	E_E (bar)	ϵ_E
220	3.22E3	1.47E-2	2.36E1	2.36E1	0	2.18E5	1.47E-2
260	3.22E3	1.47E-2	2.36E1	2.36E1	0	2.18E5	1.47E-2
300	3.15E3	3.69E-2	9.16E1	2.46E1	6.70E1	2.02E5	1.56E-2
340	2.71E3	8.29E-2	1.91E2	3.36E1	1.58E2	1.10E5	2.47E-2
380	2.08E3	1.45E-1	2.54E2	4.71E1	2.08E2	4.59E4	4.53E-2
420	1.53E3	1.95E-1	2.04E2	9.44E1	1.10E2	1.24E4	1.23E-1
460	8.72E2	4.69E-1	2.12E2	1.96E2	1.61E1	1.94E3	4.50E-1
500	4.27E2	7.13E-1	8.40E1	8.40E1	0	3.30E2	7.13E-1
540	1.23E2	4.74E-1	2.30E1	2.30E1	0	2.05E2	4.74E-1
553	0	0	0	0	0	0	0



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Table 6-15
Calculated Mechanical Response of 4 Wt% Moisture
in Cured Epoxy ($T_g = 422K$, $t = 1$ s)

Shear

T (K)	σ_b (bar)	γ_b	W_S (bar)	W_E (bar)	W_p (bar)	G_E (bar)	γ_E
220	1.61E3	2.24E-2	1.80E1	1.80E1	0	7.17E4	2.24E-2
260	1.61E3	2.24E-2	1.80E1	1.80E1	0	7.17E4	2.24E-2
300	1.61E3	1.72E-1	2.36E2	4.08E1	1.95E2	3.18E4	5.06E-2
340	1.38E3	3.20E-1	3.65E2	7.75E1	2.87E2	1.23E4	1.12E-1
380	1.08E3	5.21E-1	4.24E2	1.40E2	2.84E2	4.19E3	2.59E-1
420	7.88E2	7.41E-1	3.06E2	2.78E2	2.75E1	1.12E3	7.06E-1
460	4.92E2	1.15	1.04E2	1.04E2	0	1.58E2	1.15
500	1.96E2	1.09	5.75E1	5.75E1	0	9.72E1	1.09
527	0	0	0	0	0	0	0

Tension

T (K)	S_b (bar)	ϵ_b	W_T (bar)	W_E (bar)	W_p (bar)	E_E (bar)	ϵ_E
220	3.17E3	1.47E-2	2.33E1	2.33E1	0	2.15E5	1.47E-2
260	3.17E3	1.47E-2	2.33E1	2.33E1	0	2.15E5	1.47E-2
300	2.99E3	7.61E-2	1.95E2	3.26E1	1.63E2	1.37E5	2.18E-2
340	2.43E3	1.35E-1	2.84E2	4.43E1	2.40E2	6.67E4	3.65E-2
380	1.78E3	2.20E-1	3.14E2	7.61E1	2.38E2	2.07E4	8.57E-2
420	1.13E3	3.96E-1	2.85E2	1.62E2	1.23E2	3.94E3	2.87E-1
460	5.77E2	7.04E-1	9.07E1	9.07E1	0	3.66E2	7.04E-1
500	2.39E2	6.39E-1	4.99E1	4.99E1	0	2.44E2	6.39E-1
527	0	0	0	0	0	0	0

Table 6-16
Calculated Mechanical Response of 6 Wt% Moisture
in Cured Epoxy ($T_g = 399K$, $t = 1$ s)

Shear

T (K)	σ_b (bar)	γ_b	W_S (bar)	W_E (bar)	W_p (bar)	G_E (bar)	γ_E
220	1.59E3	2.24E-2	1.78E1	1.78E1	0	7.09E4	2.24E-2
260	1.59E3	3.32E-2	3.28E1	1.85E1	1.44E1	6.88E4	2.32E-2
300	1.59E3	1.15E-1	1.34E2	4.85E1	8.57E1	2.62E4	6.08E-2
340	1.30E3	4.35E-1	4.45E2	1.20E2	3.25E2	7.04E3	1.84E-1
380	9.81E2	6.71E-1	4.33E2	2.26E2	2.06E2	2.13E3	4.61E-1
420	6.65E2	1.02	2.11E2	2.11E2	0	4.04E2	1.02
460	3.49E2	1.13	6.77E1	6.77E1	0	1.07E2	1.13
500	3.31E1	5.56E-1	7.89	7.89	0	5.11E1	5.56E-1
504	0	0	0	0	0	0	0

Tension

T (K)	S_b (bar)	ϵ_b	W_T (bar)	W_E (bar)	W_p (bar)	E_E (bar)	ϵ_E
220	3.14E3	1.47E-2	2.30E1	2.30E1	0	2.13E5	1.47E-2
260	3.13E3	1.94E-2	3.74E1	2.34E1	1.40E1	2.09E5	1.50E-2
300	2.98E3	7.17E-2	1.65E2	4.89E1	1.15E2	9.06E4	3.28E-2
340	2.20E3	1.81E-1	3.31E2	6.60E1	2.64E2	3.66E4	6.01E-2
380	1.50E3	3.06E-1	3.32E2	1.28E2	2.03E2	8.80E3	1.71E-1
420	8.29E2	6.05E-1	2.05E2	2.06E2	0	1.12E3	6.05E-1
460	4.03E2	7.35E-1	8.15E1	8.15E1	0	3.02E2	7.35E-1
500	5.06E1	3.09E-1	6.96	6.96	0	1.46E2	3.09E-1
504	0	0	0	0	0	0	0



Table 6-17
Calculated Mechanical Response of 8 Wt% Moisture
in Cured Epoxy ($T_g = 380K$, $t = 1$ s)

Shear

T (K)	σ_b (bar)	γ_b	W_S (bar)	W_E (bar)	W_p (bar)	G_E (bar)	γ_E
220	1.58E3	2.24E-2	1.77E1	1.77E1	0	7.04E4	2.24E-2
260	1.58E3	7.64E-2	9.99E1	2.11E1	7.88E1	5.94E4	2.66E-2
300	1.55E3	3.49E-1	4.42E2	1.01E2	3.41E2	1.20E4	1.30E-1
340	1.22E3	3.79E-1	3.21E2	1.40E2	1.81E2	5.32E3	2.29E-1
380	8.82E2	4.59E-1	1.56E2	1.56E2	0	1.48E3	4.59E-1
420	5.47E2	1.19	8.62E1	8.62E1	0	1.22E2	1.19
460	2.11E2	1.14	5.80E1	5.80E1	0	9.00E1	1.14
485	0	0	0	0	0	0	0

Tension

T (K)	S_b (bar)	ϵ_b	W_T (bar)	W_E (bar)	W_p (bar)	E_E (bar)	ϵ_E
220	3.12E3	1.47E-2	2.29E1	2.29E1	0	2.11E5	1.47E-2
260	3.06E3	3.42E-2	8.09E1	2.37E1	5.72E1	1.98E5	1.55E-2
300	2.71E3	1.45E-1	3.33E2	5.99E1	2.74E2	6.15E4	4.41E-2
340	2.05E3	1.88E-1	2.84E2	1.01E2	1.82E2	2.07E4	9.89E-2
380	1.38E3	2.81E-1	1.70E2	1.70E2	0	4.29E3	2.81E-1
420	6.14E2	7.81E-1	1.08E2	1.08E2	0	3.52E2	7.81E-1
460	2.52E2	6.76E-1	5.09E1	5.09E1	0	2.23E2	6.76E-1
485	0	0	0	0	0	0	0

Table 6-18
Calculated Mechanical Response of 10 Wt% Moisture
in Cured Epoxy ($T_g = 363K$, $t = 1$ s)

Shear

T (K)	σ_D (bar)	γ_D	W_S (bar)	W_E (bar)	W_P (bar)	G_E (bar)	γ_E
220	1.58E3	2.24E-2	1.76E1	1.76E1	0	7.01E4	2.24E-2
260	1.58E3	1.02E-1	1.33E2	2.85E1	1.05E2	4.37E4	3.61E-2
300	1.50E3	4.33E-1	5.11E2	1.37E2	3.74E2	8.16E3	1.83E-1
340	1.14E3	6.78E-1	5.14E2	2.60E2	2.54E2	2.51E3	4.55E-1
380	7.87E2	1.05	2.98E2	2.98E2	0	5.38E2	1.05
420	4.32E2	1.24	8.89E1	8.89E1	0	1.16E2	1.24
460	7.79E1	9.04E-1	2.41E1	2.41E1	0	5.89E1	9.04E-1
468	0	0	0	0	0	0	0

Tension

T (K)	S_D (bar)	ϵ_D	W_T (bar)	W_E (bar)	W_P (bar)	E_E (bar)	ϵ_E
220	3.11E3	1.47E-2	2.28E1	2.28E1	0	2.10E5	1.47E-2
260	3.05E3	4.92E-2	1.19E2	2.93E1	8.94E1	1.54E5	1.95E-2
300	2.54E3	1.79E-1	3.79E2	7.62E1	3.03E2	4.22E4	6.01E-2
340	1.74E3	3.15E-1	4.10E2	1.36E2	2.74E2	1.10E4	1.57E-1
380	9.93E2	5.85E-1	2.48E2	2.48E2	0	1.45E3	5.85E-1
420	4.87E2	7.74E-1	8.53E1	8.53E1	0	2.84E2	7.74E-1
460	1.03E2	5.08E-1	2.01E1	2.01E1	0	1.56E2	5.09E-1
468	0	0	0	0	0	0	0

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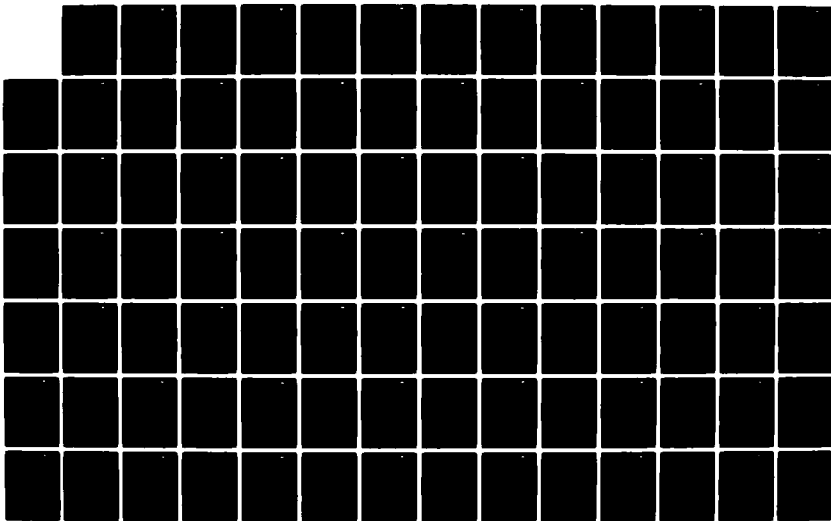
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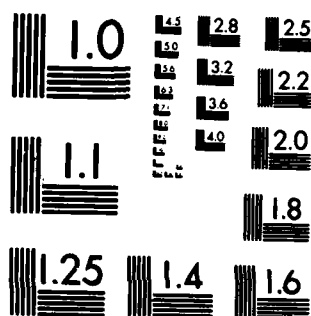
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Table 6-19
Relations Between English and SI Units in The Composite
Fracture Energy and Strength Model

Input Variable	English Units	SI Units
D, V	2E-4 in, 0.5	5.08E-6m, 0.5
E, S	1E7 psi, 4E5 psi	6.89E10 N/m ² , 2.76E9N/m ²
G, L	5E5 psi, 5E3 psi	3.44E9N/m ² , 3.44E7N/m ²
Y, YY	1E6 psi, 1E4 psi	6.89E9N/m ² , 6.89E7N/m ²
LB, LF	5E3 psi, 5E2 psi	3.44E7N/m ² , 3.44E6N/m ²
<u>Output (1)</u>		
Inter-fiber Spacing	(in.) = 1.7E-4	(m) = 4.30E-6
Shear Stress Conc.	(in.) ⁻¹ = 4360	(m) ⁻¹ = 1.71E5
Max. F-M Bond St.	(psi) = 8.7E5	(N/m ²) = 6.01E8
F-M Debond Length	(in.) = 3.7E-3	(m) = 9.61E-4
Inter. Shear St.	(psi) = 5000	(N/m ²) = 3.44E7
Comp. Tens. Mod.	(psi) = 5.5E6	(N/m ²) = 3.79E10
Comp. Tens. St.	(psi) = 1.04E5	(N/m ²) = 7.18E8
Crit. Crack Length	(in.) = 7.5E-3	(m) = 1.92E-3
<u>Output (2)</u>		
Unflawed St. (min)	(psi) = 6.11E4	(N/m ²) = 4.2E8
Unflawed St. (max)	(psi) = 1.76E4	(N/m ²) = 1.22E9
Crit. Stress Int (min)	(lb ² /in. ³) ^{1/2} = 9406	(N ² /m ³) ^{1/2} = 3.27E7
Crit. Stress Int (max)	(lb ² /in. ³) ^{1/2} = 2.7E4	(N ² /m ³) ^{1/2} = 9.47E7
<u>Output (3)</u>		
F-M Bond Stress	(psi) = 5000	(N/m ²) = 3.44E7
Fiber (W _{Fb} /A)	(lb/in.) = 1.67	(N/m) = 2.95E3
Matrix (W _{Sb} /A)	(lb/in.) = 14.4	(N/m) = 2.53E4
Frict. (W _{Fb} /A)	(lb/in.) = 118	(N/m) = 2.08E5
Tot. (W _b /A)	(lb/in.) = 134	(N/m) = 2.36E5
Crit. Length (L _c)	(in.) = 7.54E-3	(m) = 1.92E-3

Table 6-20

First Estimate of Composite Fracture Energy and Strength
(English Units, LB = 5000 psi, LF = 500 psi)

FIBER DIAMETER(D), VOLUME FRACTION(V)= 2E-04 .5
FIBER TENSILE MODULUS(E), STRENGTH(S)= 1E+07 400000
MATRIX SHEAR MODULUS(G), STRENGTH(L)= 500000 5000
MATRIX TENSILE(Y), STRENGTH(Y)= 1E+06 10000
F-M BOND STRENGTH(LB), FRICT. STRENGTH(LF)= 5000 500

INTER-FIBER SPACING(R1)= 1.69212E-04
SHEAR STRESS CONC.(A)= 4360.29
MAX. F-M BOND STRENGTH(LM)= 87205.7
F-M DEBOND LENGTH(BL)= .0377066
INTERLAM. SHEAR STRENGTH(IL)= 5000
COMPOSITE TENSILE MODULUS= 3.5E+06
COMPOSITE CONTINUUM TENSILE STRENGTH= 104055
CRITICAL CRACK LENGTH= .0754131
TO CONTINUE PRESS ENTER? -

FRACTURE MECHANICS ANALYSIS

UNFLAWED STRENGTH (MIN.)= 61114.4 (MAX.)= 176749
CRIT. STRESS INTENSITY (MIN.)= 29746.9 (MAX.)= 86031.3
FLAW SIZE CRACK LENGTH MIN. STRENGTH MAX. STRENGTH
.0753959 4.71332E-03 61121.3 176769
.0752844 9.42664E-03 61166.6 176900
.0745363 .0189531 61472.8 177786
.0709825 .0377065 62992.8 182182
.0754131 .0754131 61114.4 176749
.150801 .150826 43218 124991
.301652 .301652 30557.2 88374.6
.603304 .603304 21607.2 62490.3
1.20661 1.20661 15278.6 44187.3
2.41322 2.41322 10803.6 31245.2
TO CONTINUE PRESS ENTER? -

FRACTURE WORK PER UNIT CROSSSECTION AREA

F-M BOND STRESS	FIBER WORK	MATRIX WORK	FRICT. WORK	TOTAL WORK	CRIT. FIBER LENGTH
5000	16.7585	144.129	1184.82	1345.71	.0754131
PRESS ENTER TO CONTINUE?					
0	17.7778	0	1333.33	1351.11	.08
9689.53	13.0823	263.374	1053.5	1332.67	.0711111
19379.1	13.0272	460.905	806.584	1281.32	.0622222
29068.6	11.0519	592.593	592.593	1197.04	.0533333
38758.1	9.07694	658.436	411.523	1079.04	.0444444
48447.6	7.90124	658.436	263.375	929.712	.0355556
58137.2	5.92592	592.593	148.148	746.667	.0266667
67826.7	3.95062	460.905	65.8436	530.7	.0177778
77516.2	1.97531	263.374	16.4609	281.811	8.88889E-03
87205.7	0	0	0	0	0
PRESS ENTER TO CONTINUE? -					



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Table 6-21

Second Estimate of Composite Fracture Energy and Strength
(English Units, LB = 5000 psi, LF = 5000 psi)

FIBER DIAMETER(D), VOLUME FRACTION(V)= 2E-04 .5
FIBER TENSILE MODULUS(E), STRENGTH(S)= 1E+07 400000
MATRIX SHEAR MODULUS(G), STRENGTH(L)= 500000 5000
MATRIX TENSILE(Y), STRENGTH(Y)= 1E+06 10000
F-M BOND STRENGTH(LB), FRIC. STRENGTH(LF)= 5000 5000

INTER-FIBER SPACING(RI)= 1.69212E-04
SHEAR STRESS CONC.(A)= 4360.29
MAX. F-M BOND STRENGTH(LM)= 87205.7
F-M DEBOND LENGTH(BL)= 3.77066E-03
INTERLAM. SHEAR STRENGTH(IL)= 5000
COMPOSITE TENSILE MODULUS= 9.5E+06
COMPOSITE CONTINUUM TENSILE STRENGTH= 104055
CRITICAL CRACK LENGTH= 7.54131E-03
TO CONTINUE PRESS ENTER?

FRACTURE MECHANICS ANALYSIS

UNFLAWED STRENGTH (MIN.)= 61114.4 (MAX.)= 176749
CRIT. STRESS INTENSITY (MIN.)= 9406.81 (MAX.)= 27205.5
FLAW SIZE CRACK LENGTH MIN STRENGTH MAX STRENGTH
7.53959E-03 4.71332E-04 61121.4 176773
7.52844E-03 9.42664E-04 61166.6 176900
7.45363E-03 1.08533E-03 61472.8 177786
7.09825E-03 3.77065E-03 62992.8 182182
7.54131E-03 7.54131E-03 61114.4 176749
0.150801 0.150826 43219 124991
0.0301652 0.0301652 30557.2 88374.7
0.0603304 0.0603304 21607.2 62490.4
0.120661 0.120661 15278.6 44187.4
0.241322 0.241322 10803.6 31245.2
TO CONTINUE PRESS ENTER?

FRACTURE WORK PER UNIT CROSSSECTION AREA

F-M BOND STRESS	FIBER WORK	MATRIX WORK	FRIC. WORK	TOTAL WORK	CRIT. FIBER LENGTH
5000	1.67585	14.4129	118.482	134.571	7.54131E-03
0	1.77778	0	133.333	135.111	8E-03
9689.53	1.58025	26.3375	105.35	133.267	7.11111E-03
19379.1	1.38272	46.0905	80.6584	128.132	6.22222E-03
29068.6	1.18519	59.2593	59.2593	119.704	5.33333E-03
38758.1	.987654	68.8436	41.1523	107.984	4.44444E-03
48447.6	.790124	68.8436	26.3375	92.9712	3.55556E-03
58137.2	.592593	59.2592	14.8148	74.6667	2.66667E-03
67826.7	.395062	46.0905	6.58437	53.07	1.77778E-03
77516.2	.197531	26.3374	1.64609	28.1811	8.88889E-04
87205.7	0	0	0	0	0

PRESS ENTER TO CONTINUE?

Table 6-22
Relations Between English and SI Units in the Peel
Mechanics Model

Input Variable	English Units	SI Units
H, A	1E-3 in., 8E-3 in.	2.54E-5m, 2.03E-4m
B, E	1.0 in., 1E4 psi	2.54E-2m, 6.89E7 N/m ²
Y, SA	5E4 psi, 2E4 psi	3.45E8m, 1.38E8N/m ²
G, LA	1.67E4 psi, 6.67E3 psi	1.15E8N/m ² , 4.60E7 N/m ²
<u>Output (1)</u>		
Cleavage Stress Conc.	(in. ⁻¹) = 6.95E2	(m ⁻¹) = 2.74E4
Shear Stress Conc.	(in. ⁻¹) = 3.23E2	(m ⁻¹) = 1.27E4
180 Deg. Radius of Curv.	(in.) = 3.22E-4	(m) = 8.209E-6
0 Deg. Peel Force	(lb) = 20.6	(N) = 91.8
180 Deg. Peel Force	(lb) = 16.0	(N) = 71.2
<u>Output (2)</u>		
Peel Angle	(deg) = 177.9	(deg) = 177.9
Peel Work	(lb/in.) = 35.2	(N/m) = 6.16E3
Peel Force	(lb) = 14.8	(N) = 65.8
K	.963	.963
Tensile Stress	(psi) = 2E4	(N/m ²) = 1.38E8
Shear Stress	(psi) = -4.79E3	(N/m ²) = -3.30E7



Table 6-23
First Estimate of Laminate Peel and Shear Properties
(Flexible Adherend Tensile Modulus = $1E4$ psi, English Units)

RIBBON HALF THICKNESS(H), ADHESIVE THICKNESS(A)? .001, .008
BOND WIDTH(B), RIBBON TENSILE MODULUS(E)? $1E4$
ADHESIVE TENSILE MODULUS(Y), STRENGTH(SA)? $5E4, 2E4$
ADHESIVE SHEAR MODULUS(G), STRENGTH(LA)? $1.67E4, 6.67E3$
CLEAVAGE STRESS CONC.(BA)= 695.789
SHEAR STRESS CONC.(GA)= 323.071
180 DEG. RAD. OF CURV.(R)= $3.22749E-04$
0 DEG. PEEL FORCE(FS)= 20.6456
180 DEG. PEEL FORCE(PC)= 16
PEEL ANGLE PEEL WORK PEEL FORCE K TENSILE STRESS SHEAR STRESS

177.943	35.1768	14.8403	962536	20000	-4791.38
147.943	17.0924	8.31579	692002	20000	-2276.95
117.944	11.5577	7.02883	567962	20000	-1064.12
87.9443	8.67872	7.53096	476341	20000	87.2691
77.9462	8.06533	8.11386	447893	20000	547.412
67.9481	7.65196	9.00554	419243	20000	1092.33
57.95	7.53574	10.35	389619	20000	1774.4
47.9519	7.96186	12.424	358076	20000	2688.27
37.9538	9.59627	15.8136	323088	20000	4028.42
32.9542	11.4109	18.3874	304058	20000	4984.66
27.9546	14.6422	21.9796	283097	20000	6272.44
22.955	14.3437	22.4215	279083	16881.5	6670
17.9553	12.8328	21.7833	280759	12948.7	6670
12.9557	14.7599	21.1855	281979	9210.26	6670
7.9561	11.0648	20.8462	282874	5598.38	6670

Table 6-24

Second Estimate of Laminate Peel and Shear Properties
(Flexible Adherend Tensile Modulus = $5E4$ psi, English Units)

RIBBON HALF THICKNESS(H)= ADHESIVE THICKNESS(A)= .001, .008					
BOND WIDTH(B)= RIBBON TENSILE MODULUS(E)= $1.5E4$					
ADHESIVE TENSILE MODULUS(Y), STRENGTH(SA)= $5E4, 2E4$					
ADHESIVE SHEAR MODULUS(G), STRENGTH(LA)= $1.67E4, 6.57E3$					
CLEAVAGE STRESS CONC (BA)= 465.303					
SHEAR STRESS CONC (GA)= 144.402					
180 DEG. RAD. OF CURV (R)= $7.21688E-04$					
0 DEG. PEEL FORCE(PS)= 46.165					
180 DEG. PEEL FORCE(PC)= 16					
PEEL ANGLE	PEEL WORK	PEEL FORCE	K	TENSILE STRESS	SHEAR STRESS
177.943	31.5538	15.2039	.974606	20000	-219.22
147.943	18.7644	9.89172	.755712	20000	-121.22
117.944	13.3668	8.83588	.6368	20000	-598
87.9443	9.94176	9.81231	.543725	20000	50.85
77.9462	9.82195	10.6822	.513914	20000	322.30
67.9481	8.19742	11.9768	.483483	20000	649.68
57.95	7.49203	13.9851	.451604	20000	1065.11
47.9519	6.99257	16.8666	.417214	20000	1632.14
37.9538	6.94726	21.7879	.378777	20000	2473.07
32.9542	7.38912	25.3918	.357308	20000	3073.33
27.9546	8.22931	30.3457	.333734	20000	3893.35
22.955	10.307	38.1692	.307336	20000	5073.06
17.9553	14.1381	48.5277	.280809	19354.7	6670
12.9557	18.4262	47.3713	.282806	13769.4	6670
7.9561	11.3131	46.6142	.282796	8377	6670



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Table 6-25

Third Estimate of Laminate Peel and Shear Properties
(Flexible Adherend Tensile Modulus = $2.5E5$ psi, English Units)

RIBBON HALF THICKNESS(H), ADHESIVE THICKNESS(A)? 001.008					
BOND WIDTH(B), RIBBON TENSILE MODULUS(E)? $1.25E5$					
ADHESIVE TENSILE MODULUS(Y), STRENGTH(SA)? $5E4.2E4$					
ADHESIVE SHEAR MODULUS(G), STRENGTH(LA)? $1.67E4, 6.67E3$					
CLEAVAGE STRESS CONC.(BA)= 311.166					
SHEAR STRESS CONC.(GA)= 64.6142					
180 DEG. RAD. OF CURV (R)= $1.61374E-03$					
0 DEG. PEEL FORCE(PS)= 183.228					
180 DEG. PEEL FORCE(PC)= 16					
PEEL ANGLE	PEEL WORK	PEEL FORCE	K	TENSILE STRESS	SHEAR STRESS
177.943	31.1472	15.4591	.982733	20000	-998.235
147.943	21.2076	11.4085	.811585	20000	-624.753
117.944	15.9552	10.7849	.703537	20000	-326.554
87.9443	12.1653	12.4569	.612631	20000	28.8703
77.9462	11.0442	13.7214	.582451	20000	185.146
67.9481	9.96251	15.5635	.551143	20000	377.556
57.95	8.91483	18.2822	.517826	20000	626.859
47.9519	7.91789	22.4474	.481313	20000	971.426
37.9538	7.04729	29.2785	.439834	20000	1491.29
32.9542	6.73657	34.4802	.416371	20000	1869.45
27.9546	6.62322	41.7936	.390373	20000	2385.37
22.955	6.94244	52.6562	.360978	20000	3132.91
17.9553	8.34284	70.178	.326816	20000	4313.65
12.9557	13.8984	102.425	.285449	20000	6449.67
7.9561	11.8676	184.232	.282823	12523.8	6670



SC78-3047

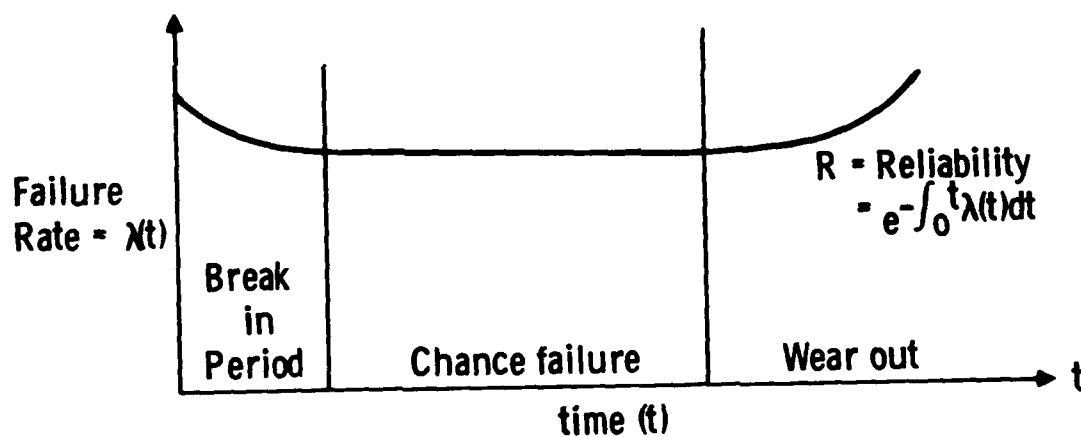


Fig. 1-1 Failure rate criteria for reliability.

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$\sigma(X)$ = Allowable Stress Dist.

$\sigma(x)$ = Applied Stress Dist.

R = Reliability

$$= \int_{-\infty}^{\infty} \sigma(x) \left[\int_x^{\infty} \sigma(X) dX \right] dx$$

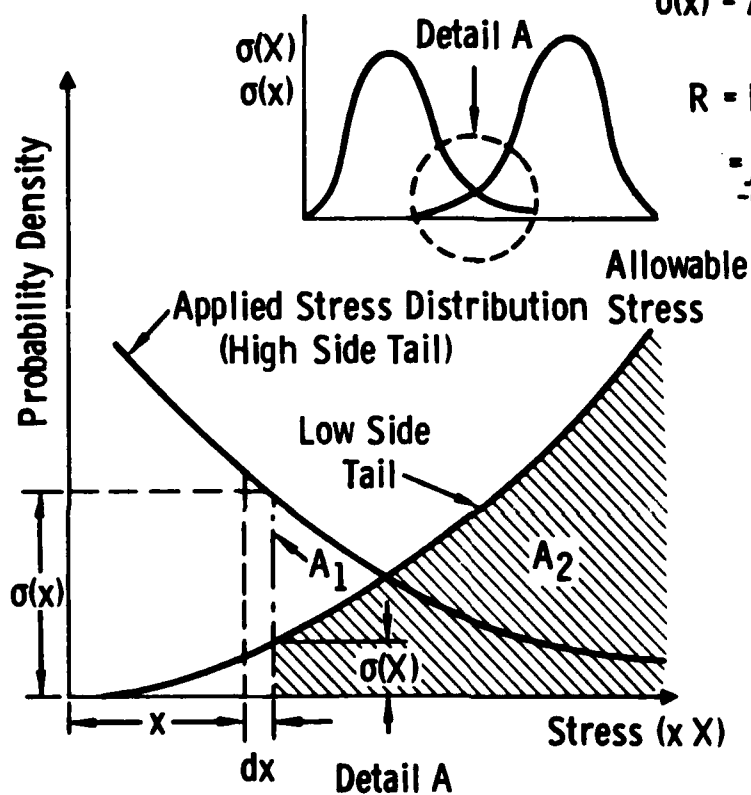


Fig. 1-2

Applied and allowable stress distribution analysis of reliability.



SC78-3049

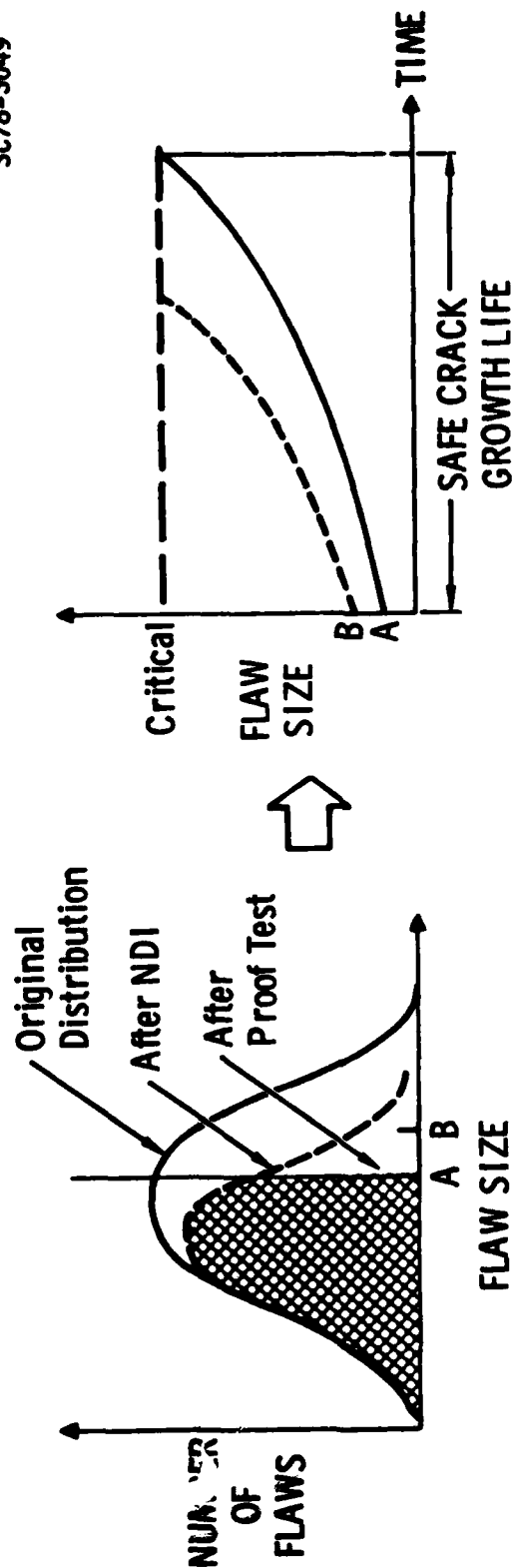


Fig. 1-3 Fracture mechanics criteria for structure reliability.

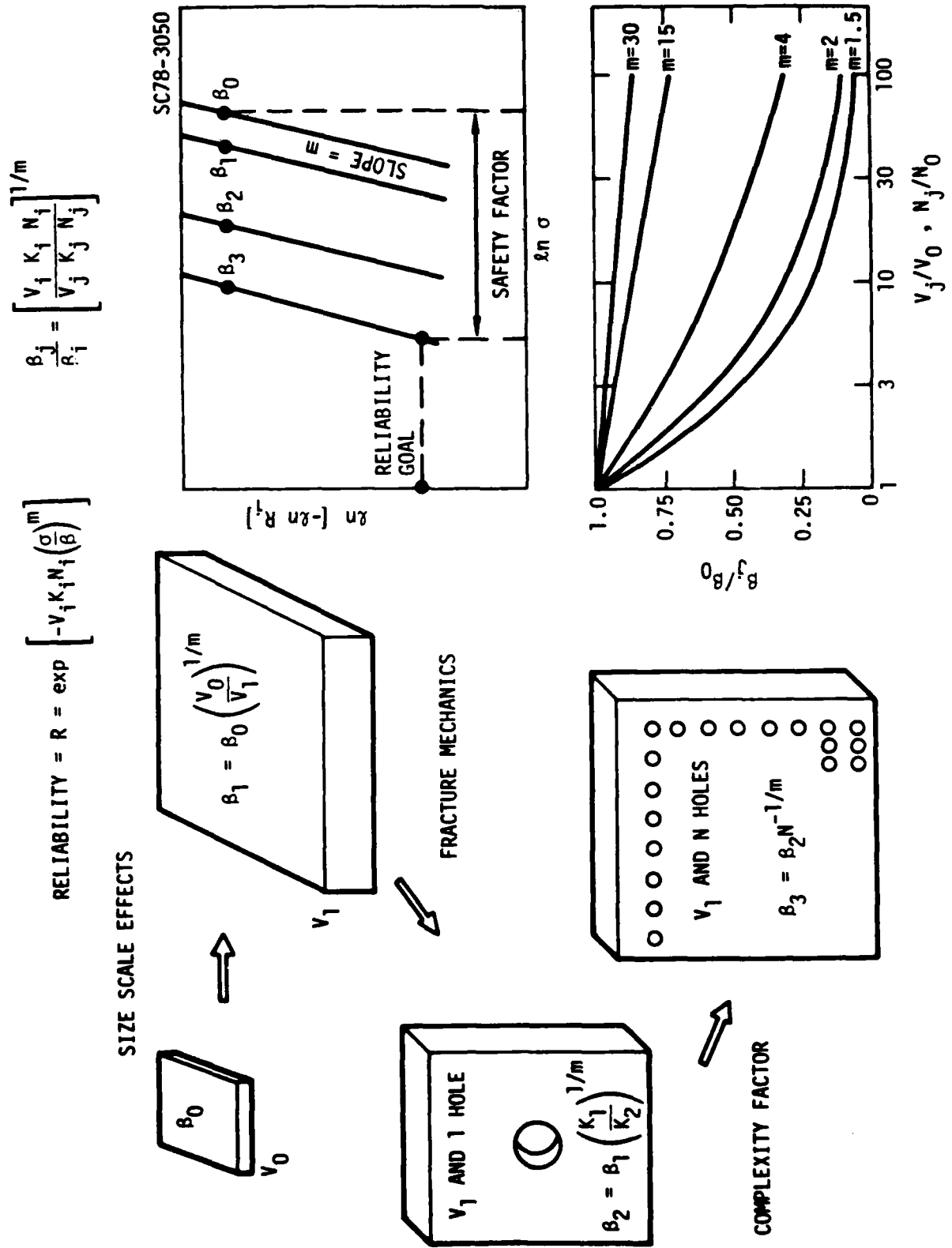


Fig. 1-4 Weibull criteria for structure reliability.



SC78-3051

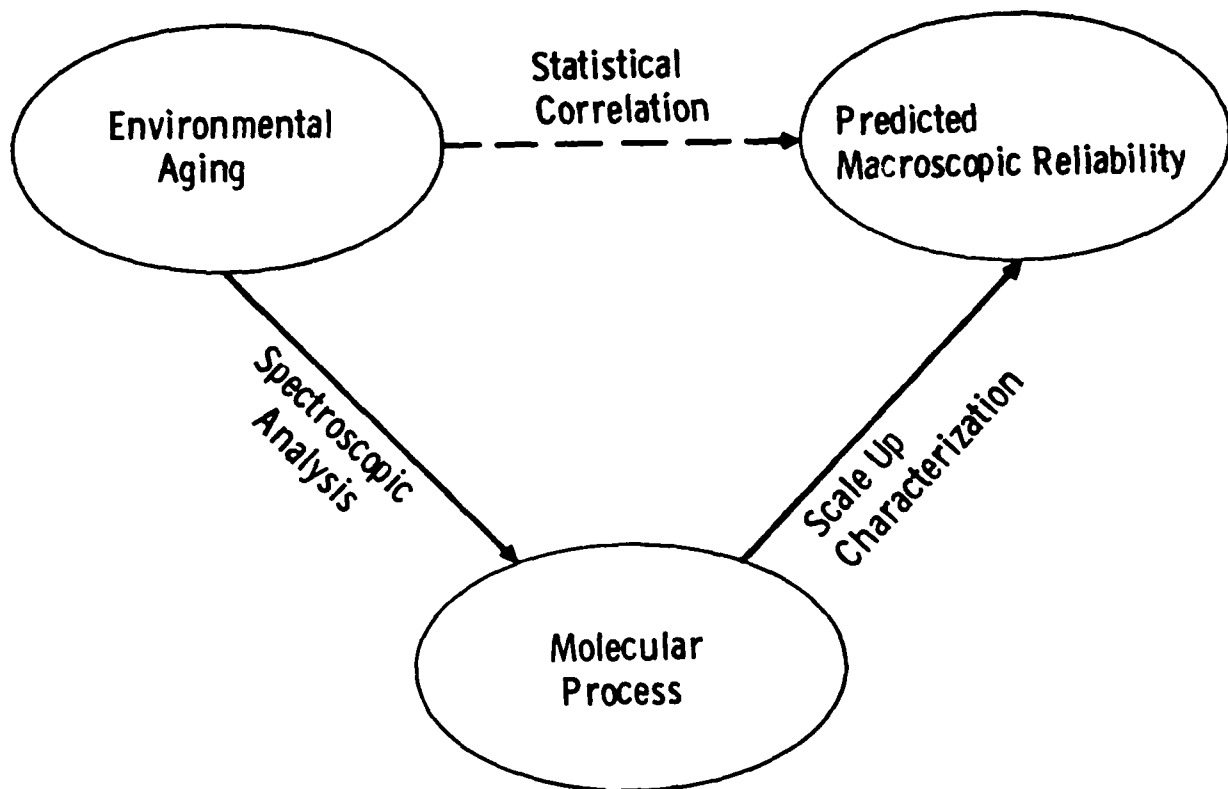


Fig. 1-5 Preferred dual path for correlating environmental aging with macroscopic strength.

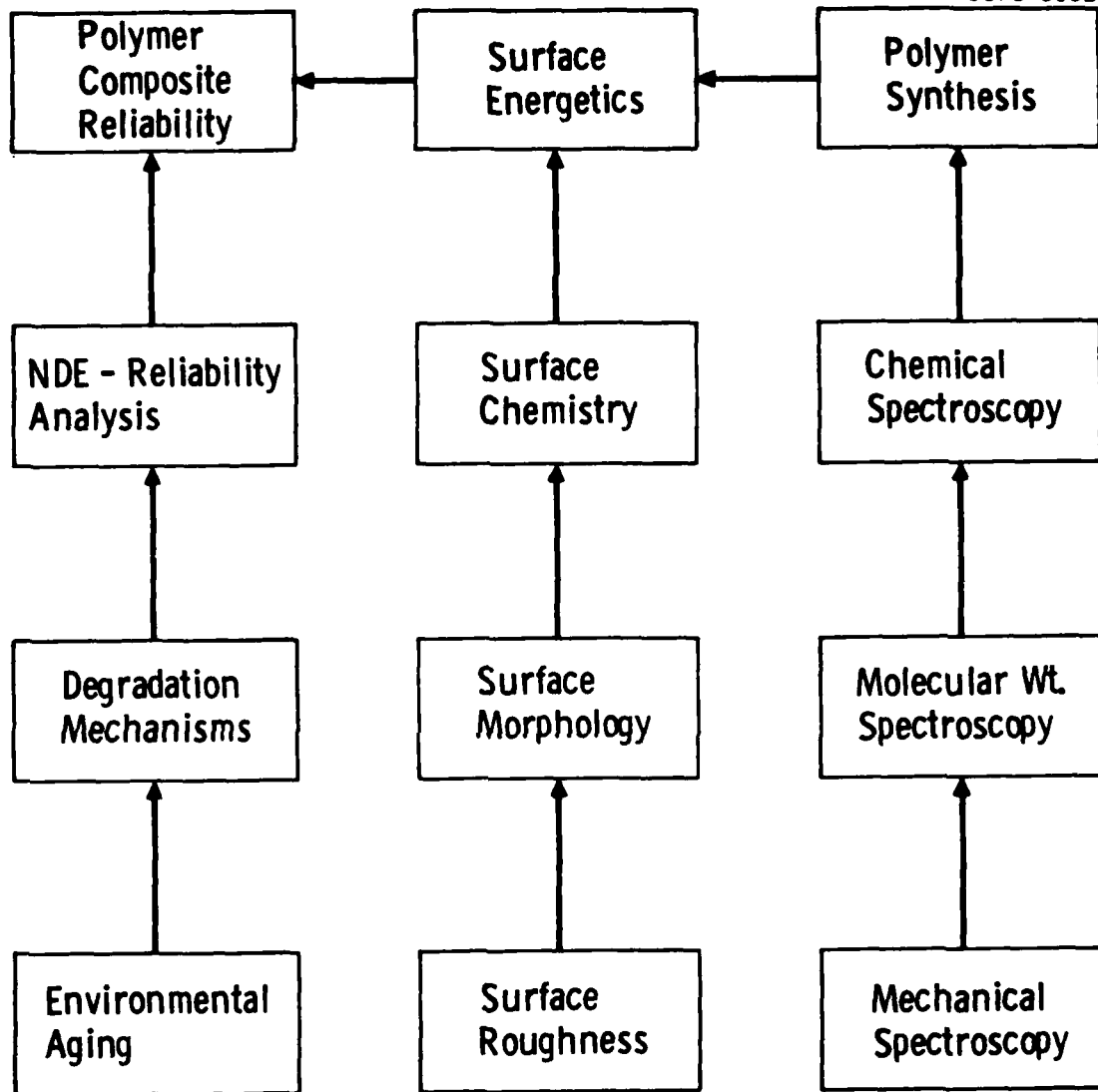


Fig. 1-6 Technical approach to polymer composite reliability.

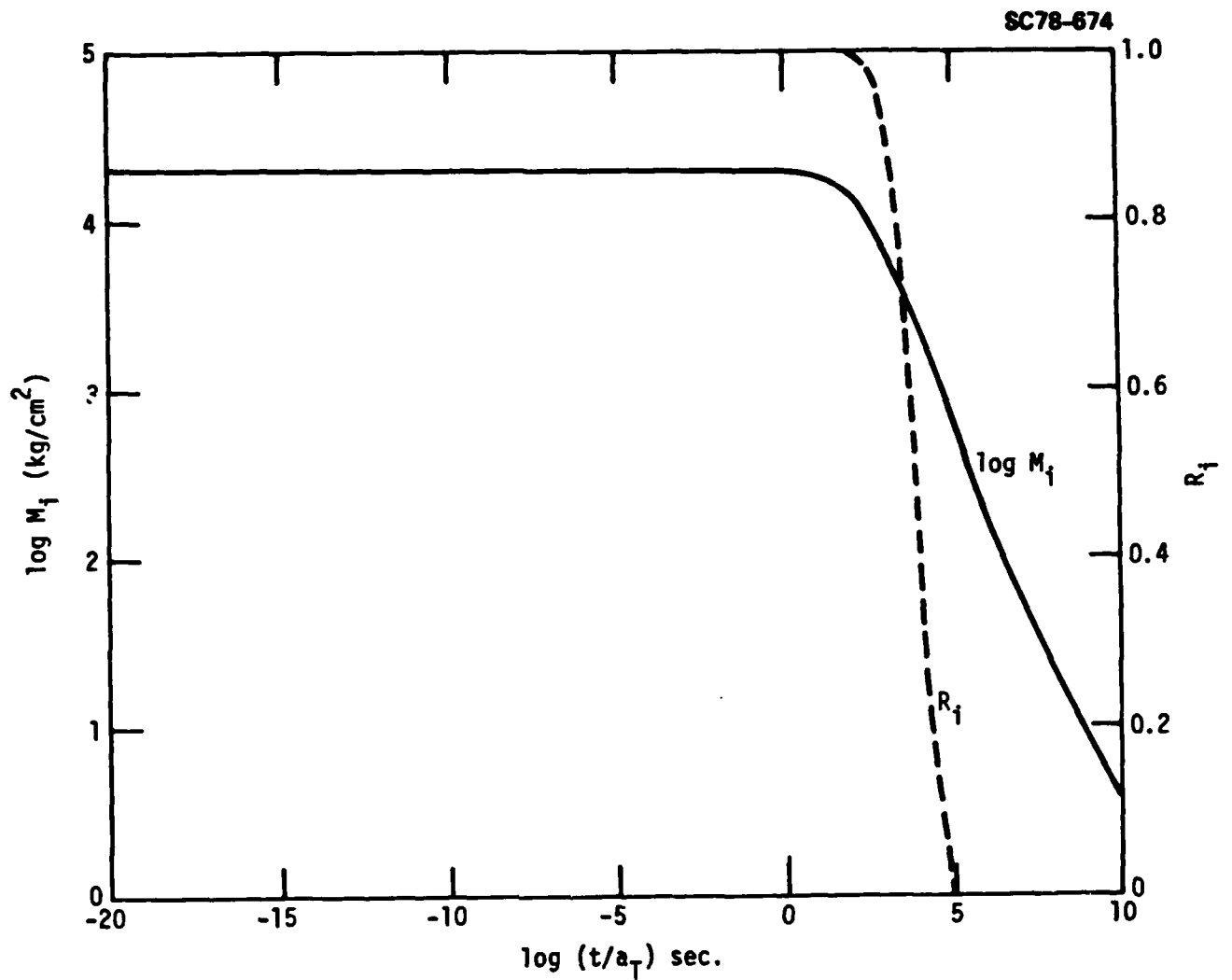


Fig. 1-7 Calculated function of M_i and R_i for $M_0 = 20,000$ kg/cm², $M_\infty = 2.0$ kg/cm², $\tau = 100$ s, $R_0 = 0$, $\tau_0 = 10^4$ s, $m = 1.0$.

SC78-672

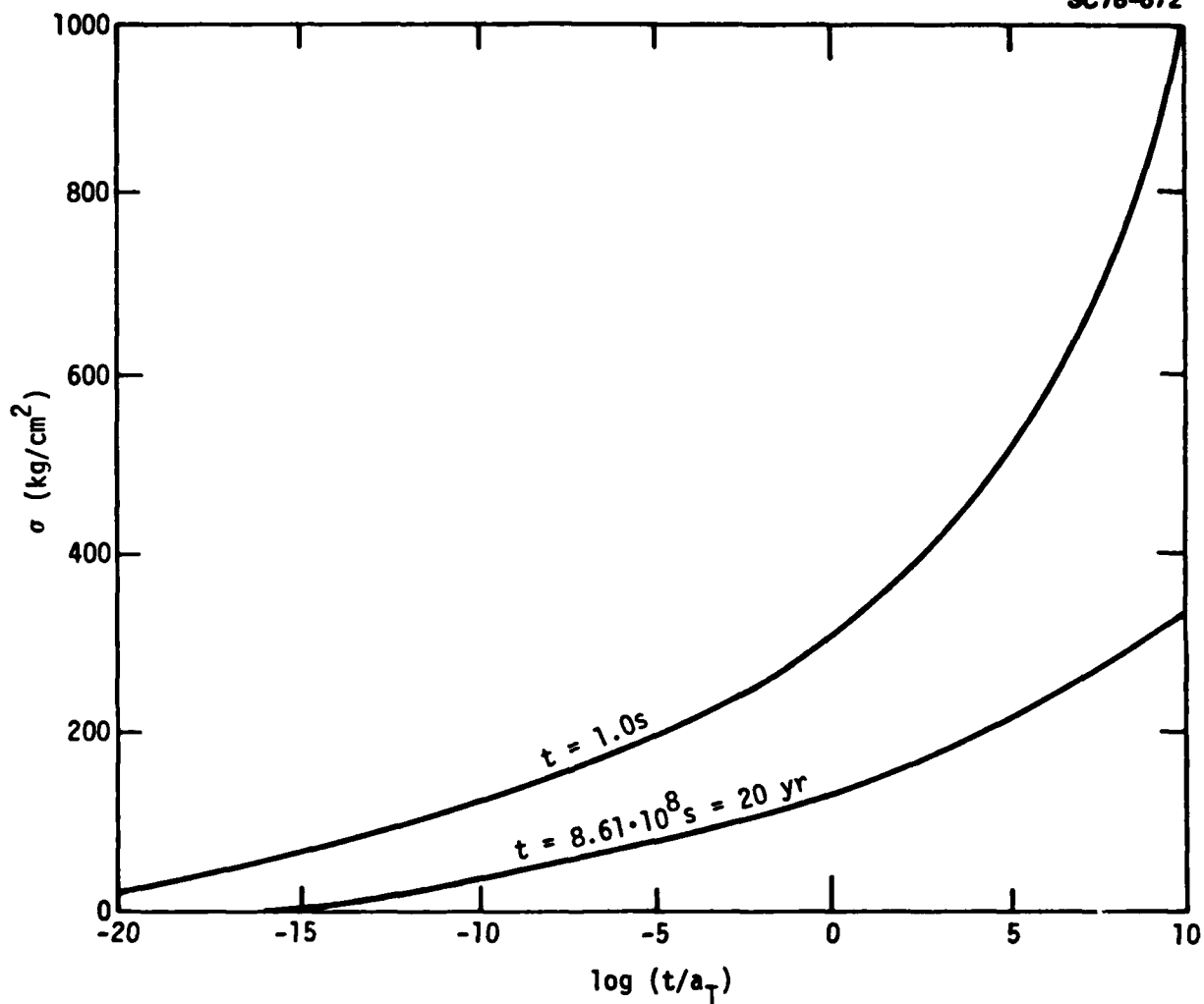


Fig. 1-8 Illustrative relations between tensile stress σ and time shift factor $\log(t/a_T)$.

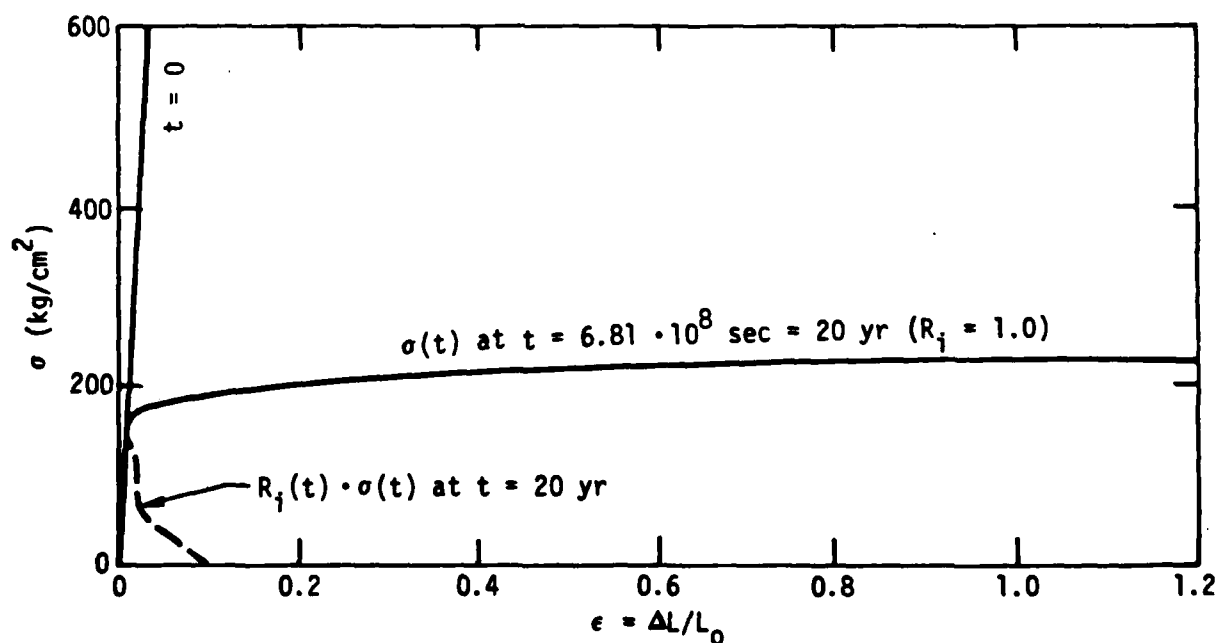
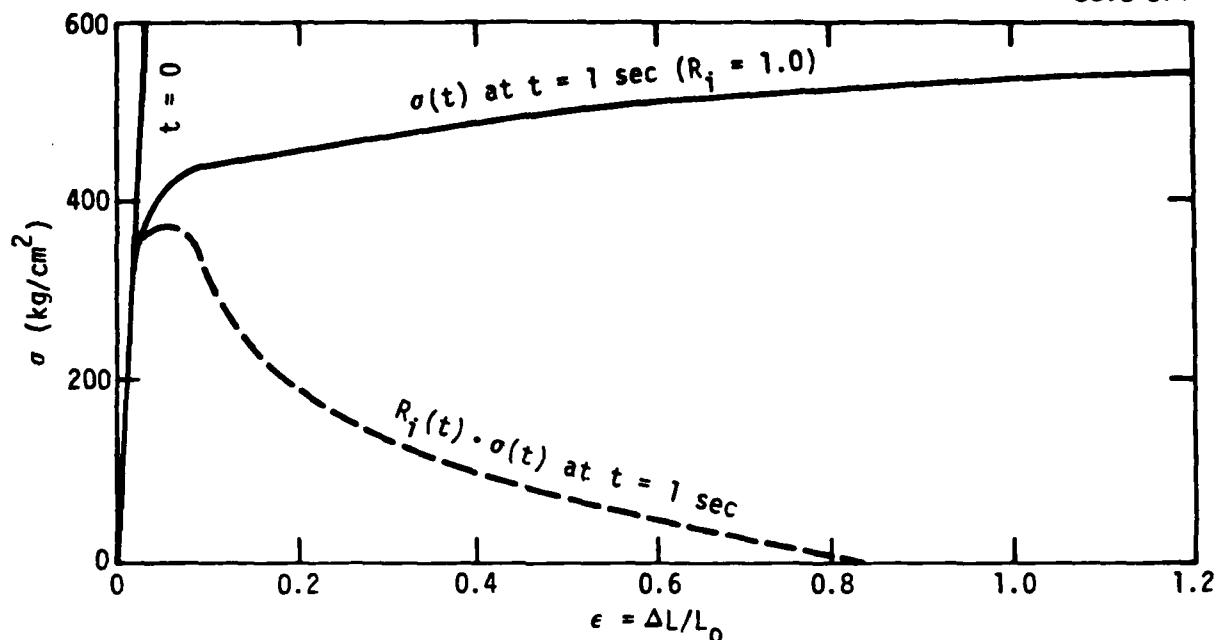


Fig. 1-9

Calculated tensile creep stress $\sigma(t)$ vs strain $\epsilon(t)$ (solid curves) and reliability $R_i(t)$ reduced stress $R_i(t) \cdot \sigma_i(t)$ vs strain $\epsilon(t)$ (dashed curves) at $t = 1$ s (upper view) and $t = 20$ yr (lower view).

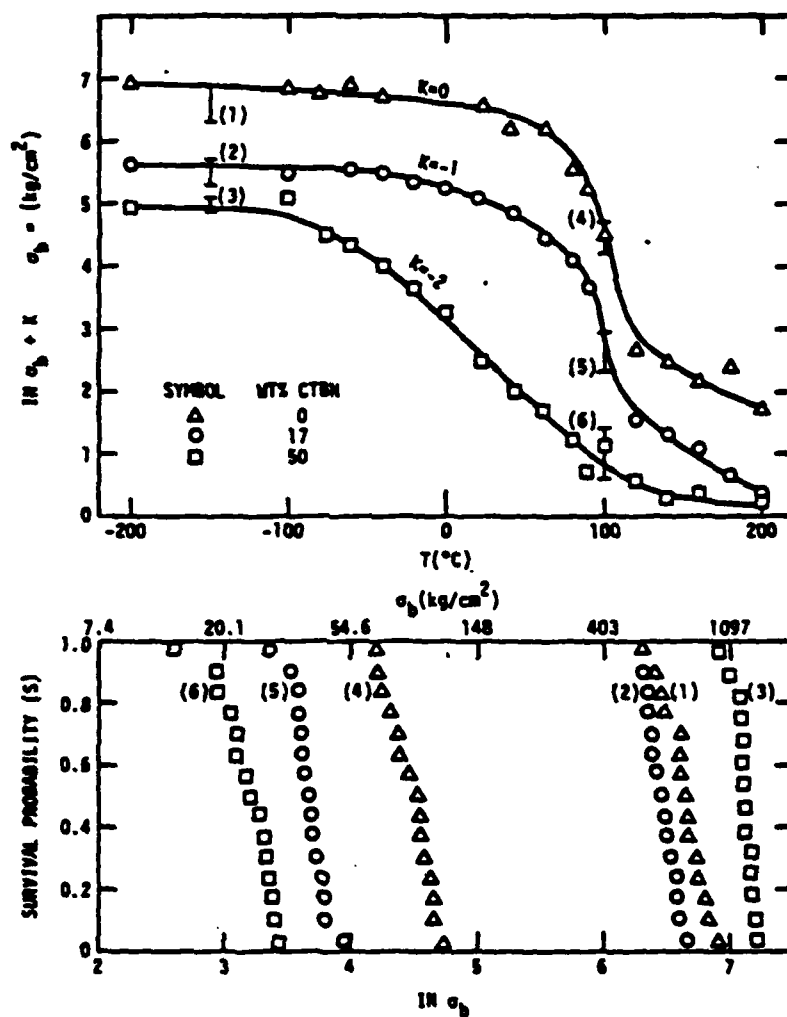


Fig. 1-10 (a) The temperature and composition dependence of the tensile strength for a rubber modified epoxy.
 (b) The stress dependence of the survival probability for rubber modified epoxy at -150°C and 100°C.

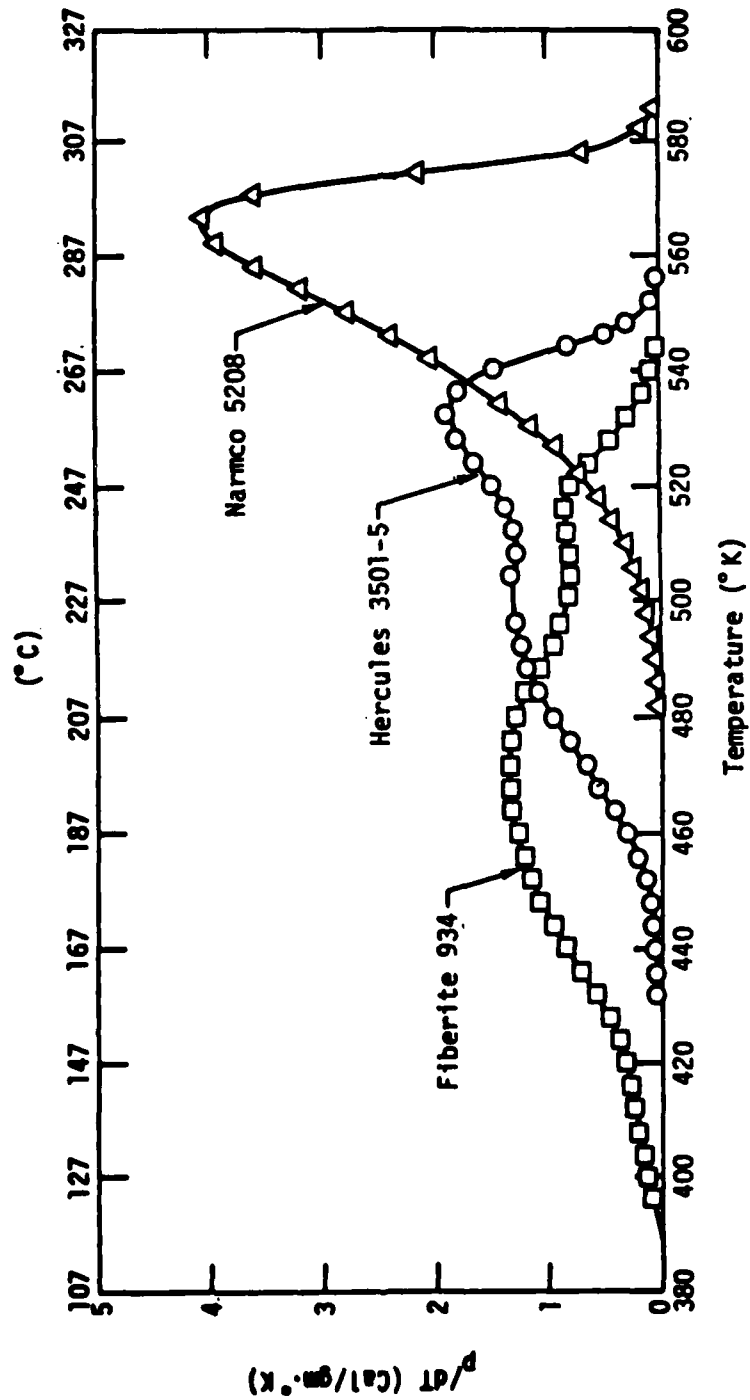


Fig. 1-11 DSC thermograms for curing reactions of commercial epoxy matrix materials extracted from prepreg (DSC scan rate $\dot{\phi} = 20^{\circ}\text{C}/\text{min}$).

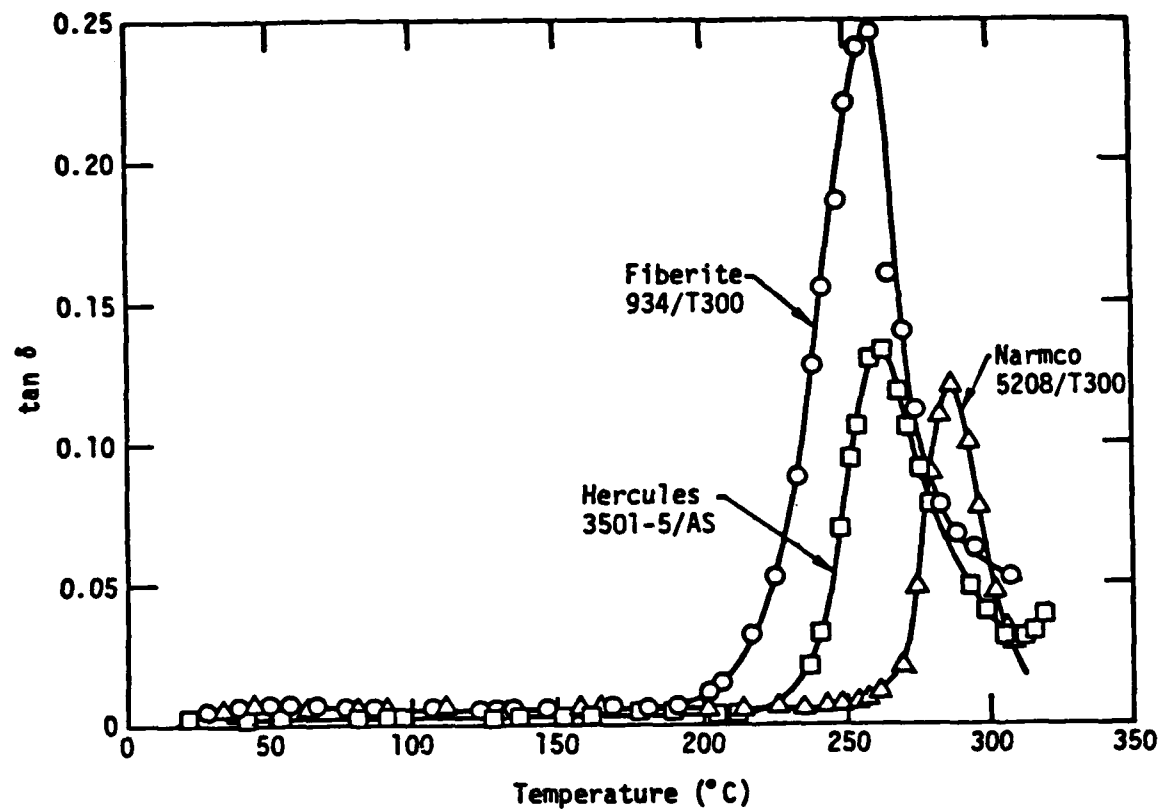


Fig. 1-12 Rheovibron thermal scans for flexural damping in cured reinforced graphite-epoxy composite in the dry unaged condition.

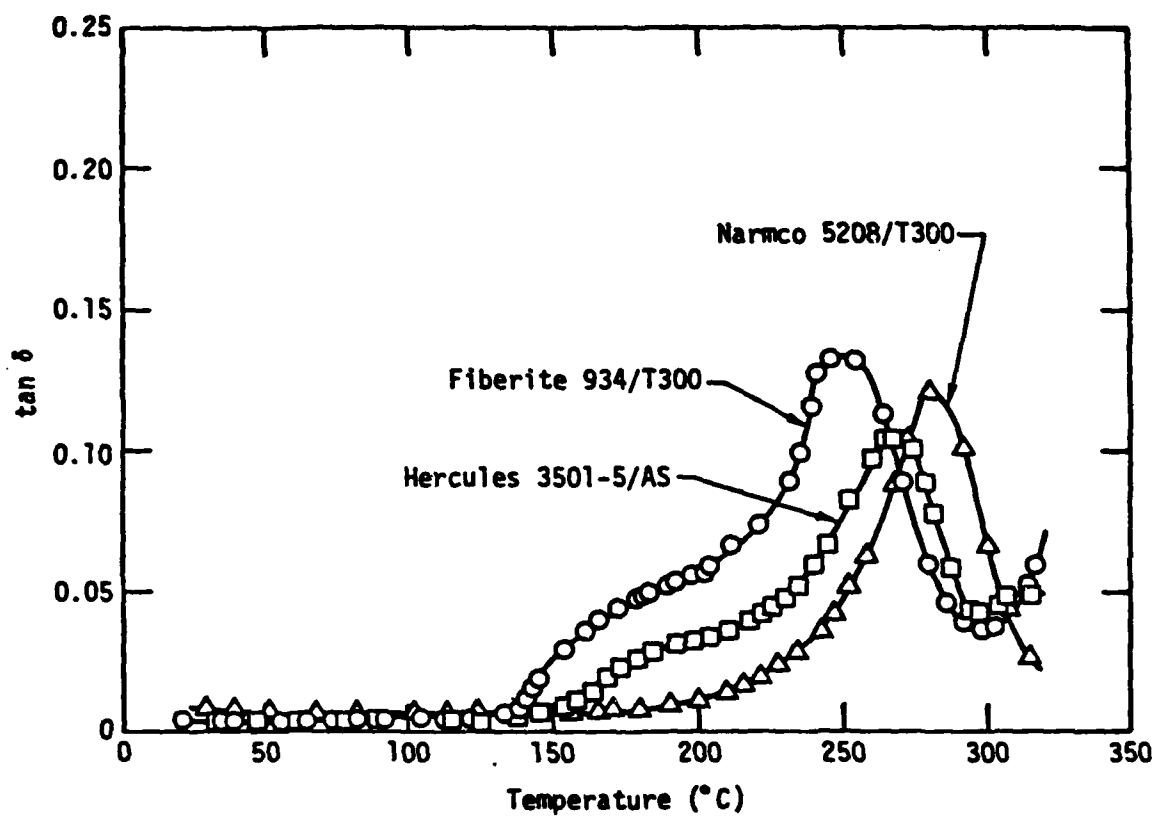


Fig. 1-13 Rheovibron thermal scans for flexural damping in cured uniaxial reinforced graphite-epoxy composite in the wet-aged condition.

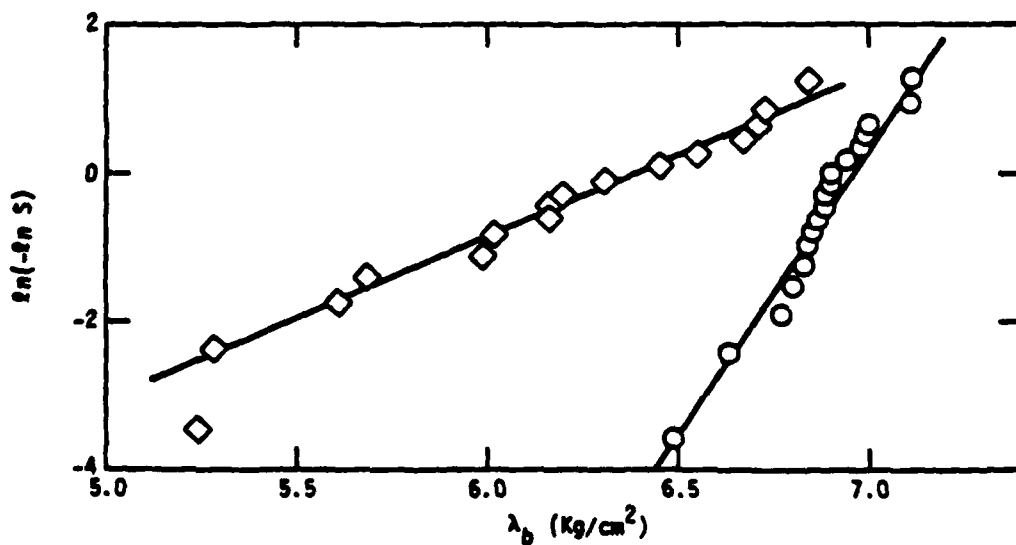
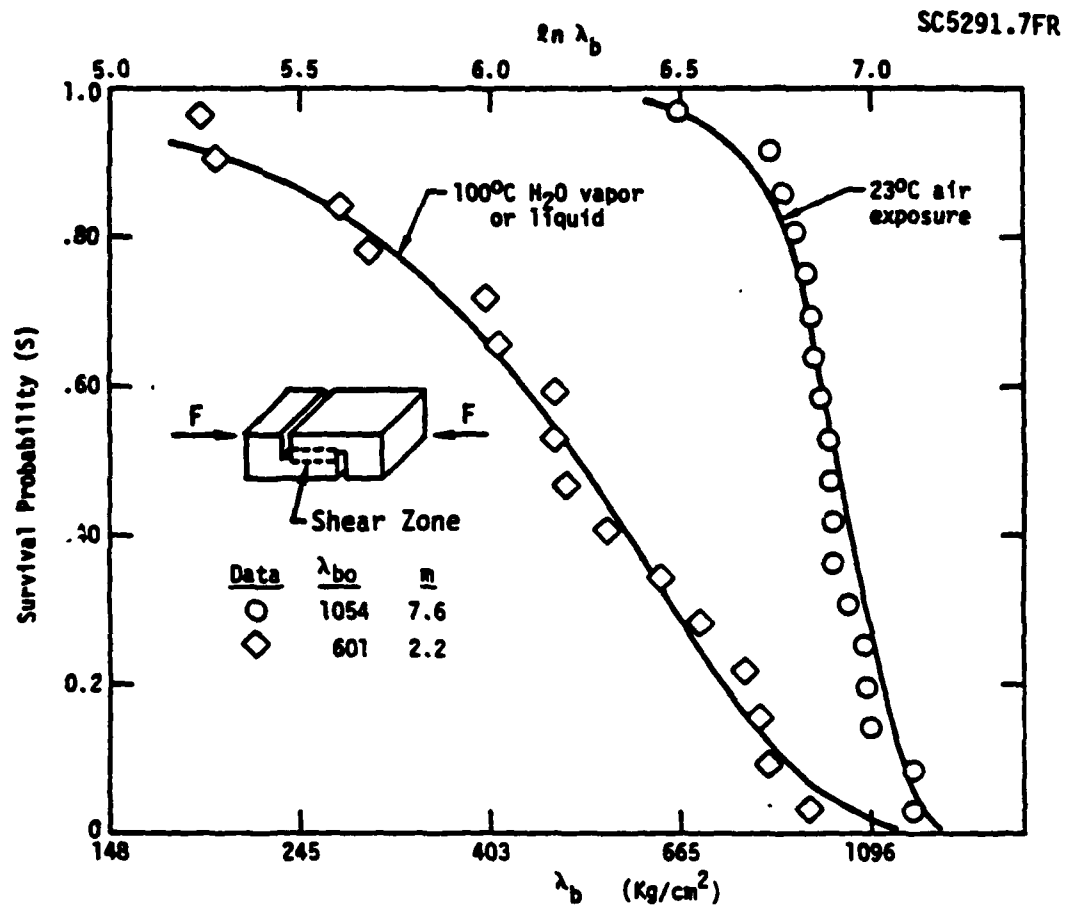


Fig. 1-14 Cumulative distribution function of survival probability.

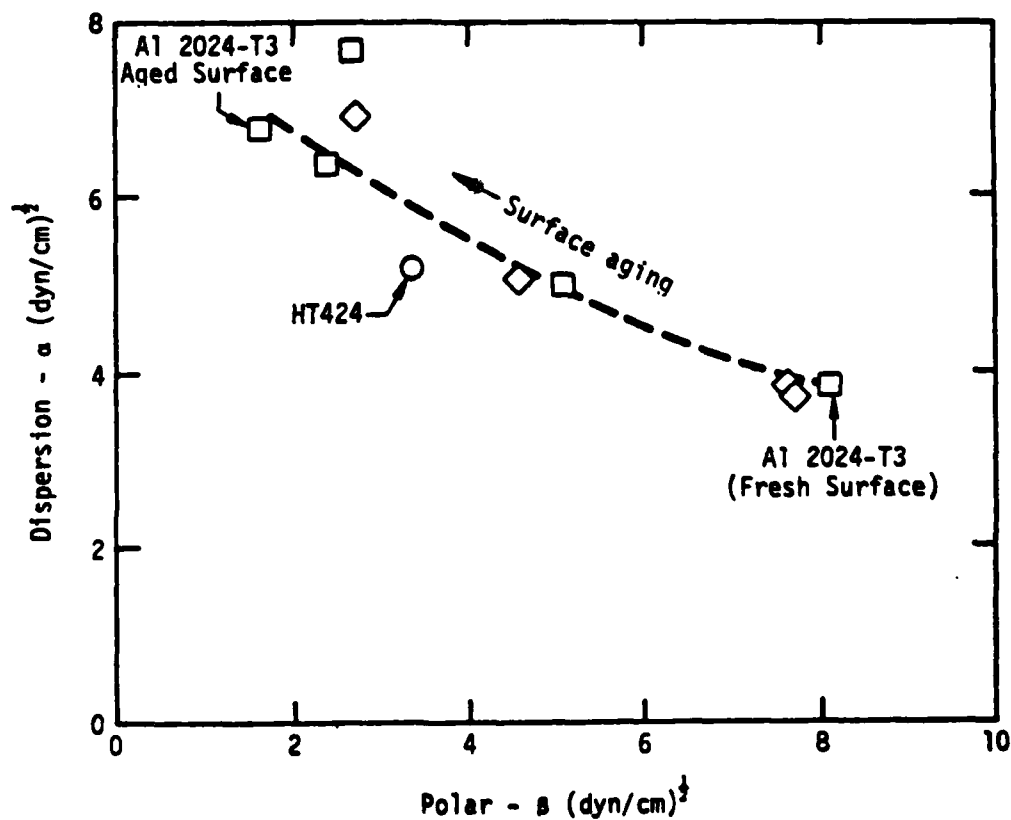


Fig. 1-15 Dispersion (α) and polar (β) components of the solid-vapor surface tension $\gamma_{SV} = \alpha^2 + \beta^2$ for HT424 primer (Phase 1) and Al 2024-T3 adherend (Phase 3).

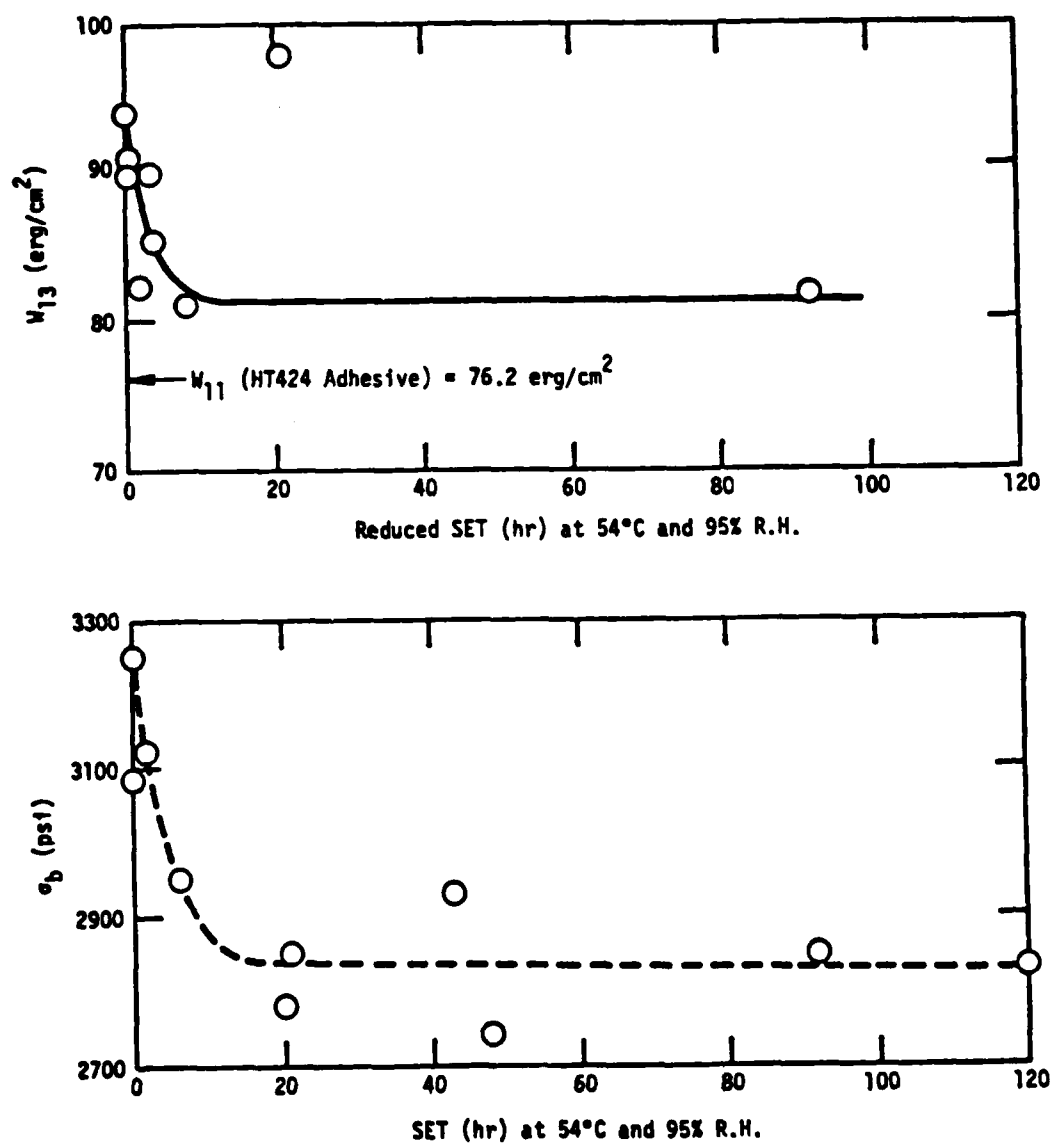


Fig. 1-16 Dependence of interfacial work of adhesion W_{13} (upper curve) and lap shear bond strength σ_b (lower curve) at varied SET.

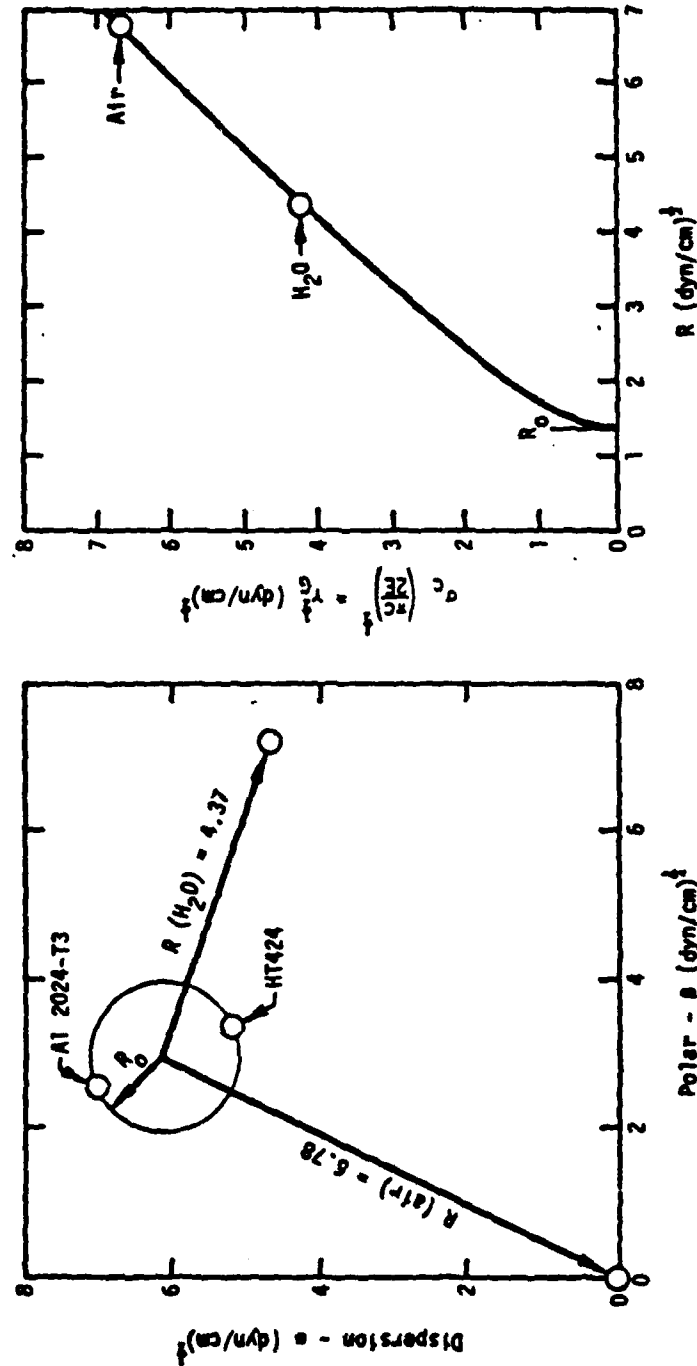


Fig. 1-17 Modified Griffith analysis of the effect of H_2O immersion in reducing the critical interfacial stress σ_c for interfacial failure between HT424 and etched Al 2024-T3 ($\phi_I = 1 - \phi_C = 1.0$).

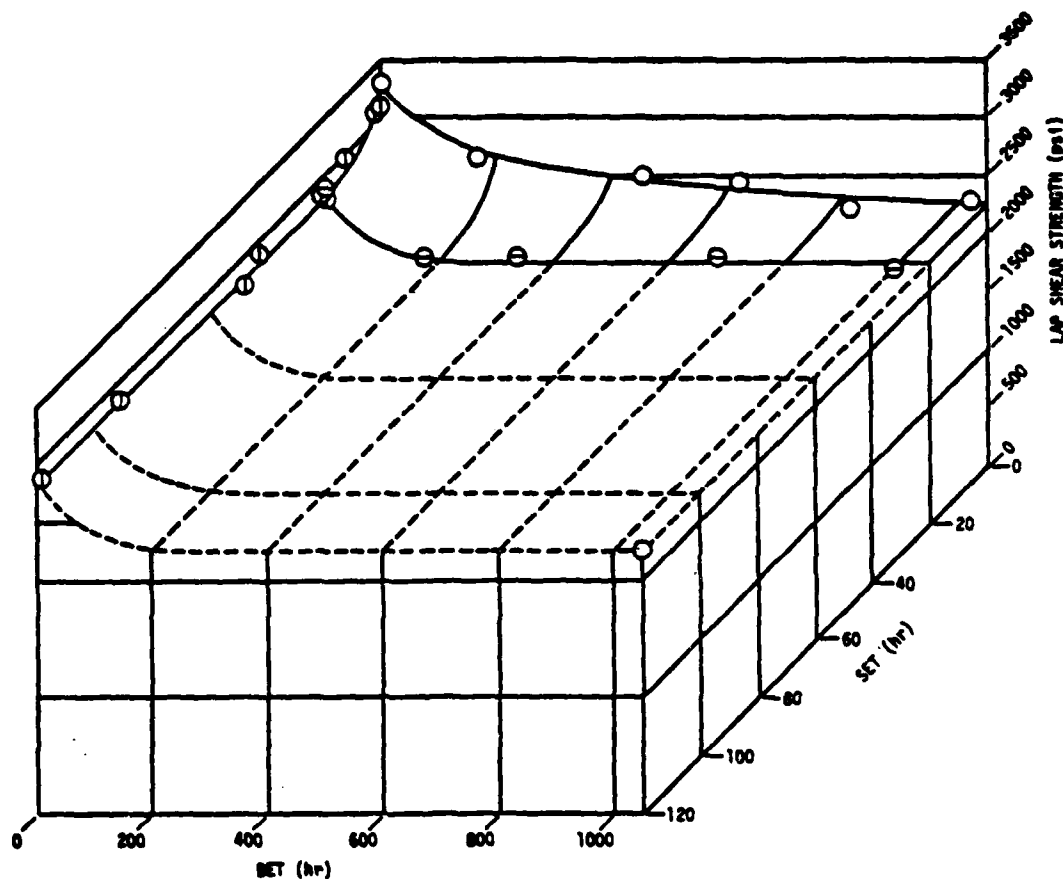


Fig. 1-18 SET and BET response surface for lap shear bond strength for Al 2024-T3 - HT424.

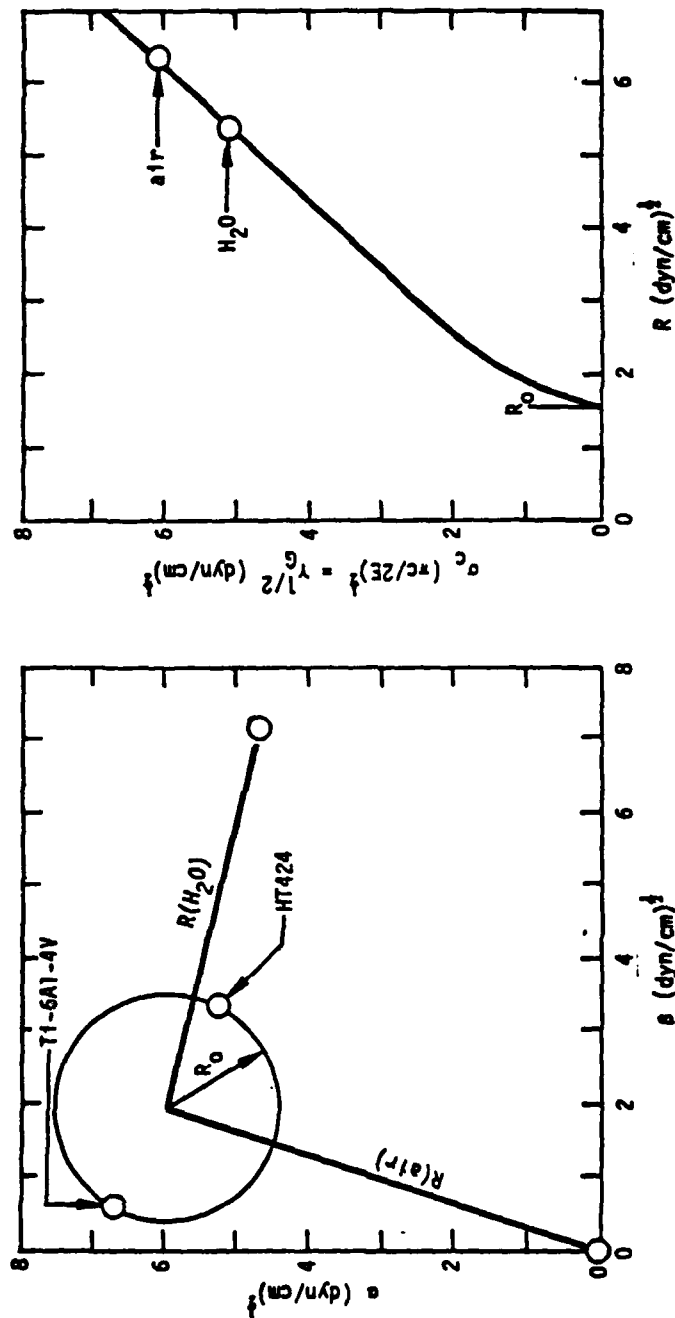


Fig. 1-19 Modified Griffith analysis of the effect of H_2O immersion in reducing critical failure stress σ_i for interfacial failure between HT424 and phosphate-fluoride treated Ti-6Al-4V ($\phi_I = 1 - \phi_C = 1.0$).

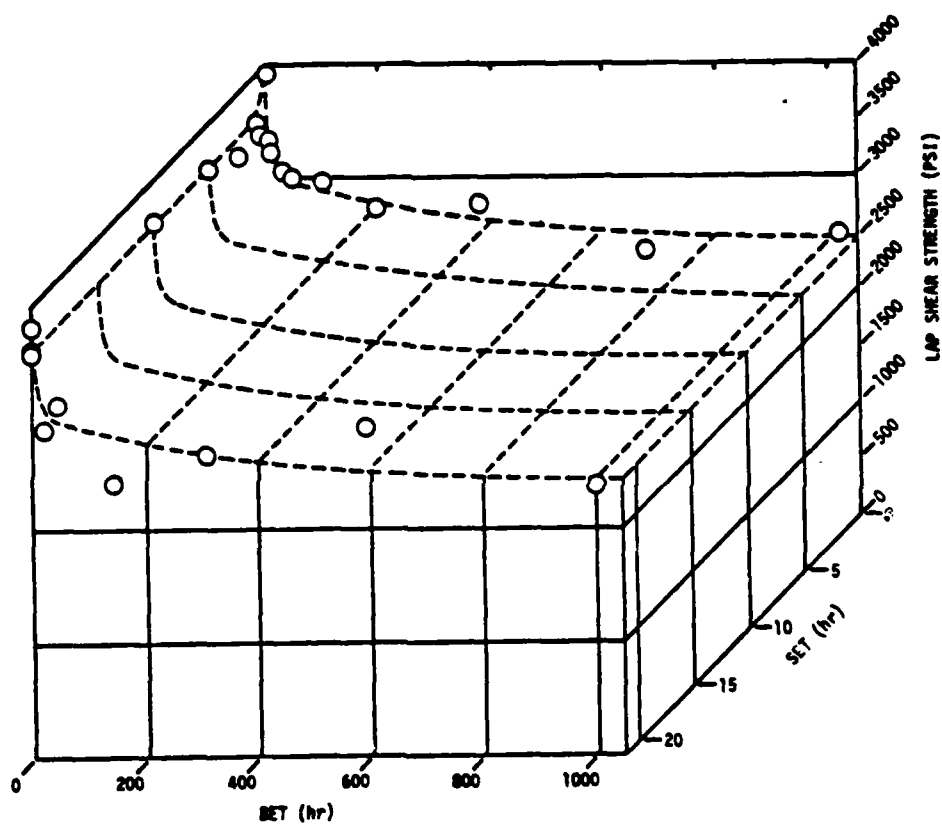


Fig. 1-20 SET vs BET response surface for lap shear bond strength for Ti-6Al-4V - HT424.

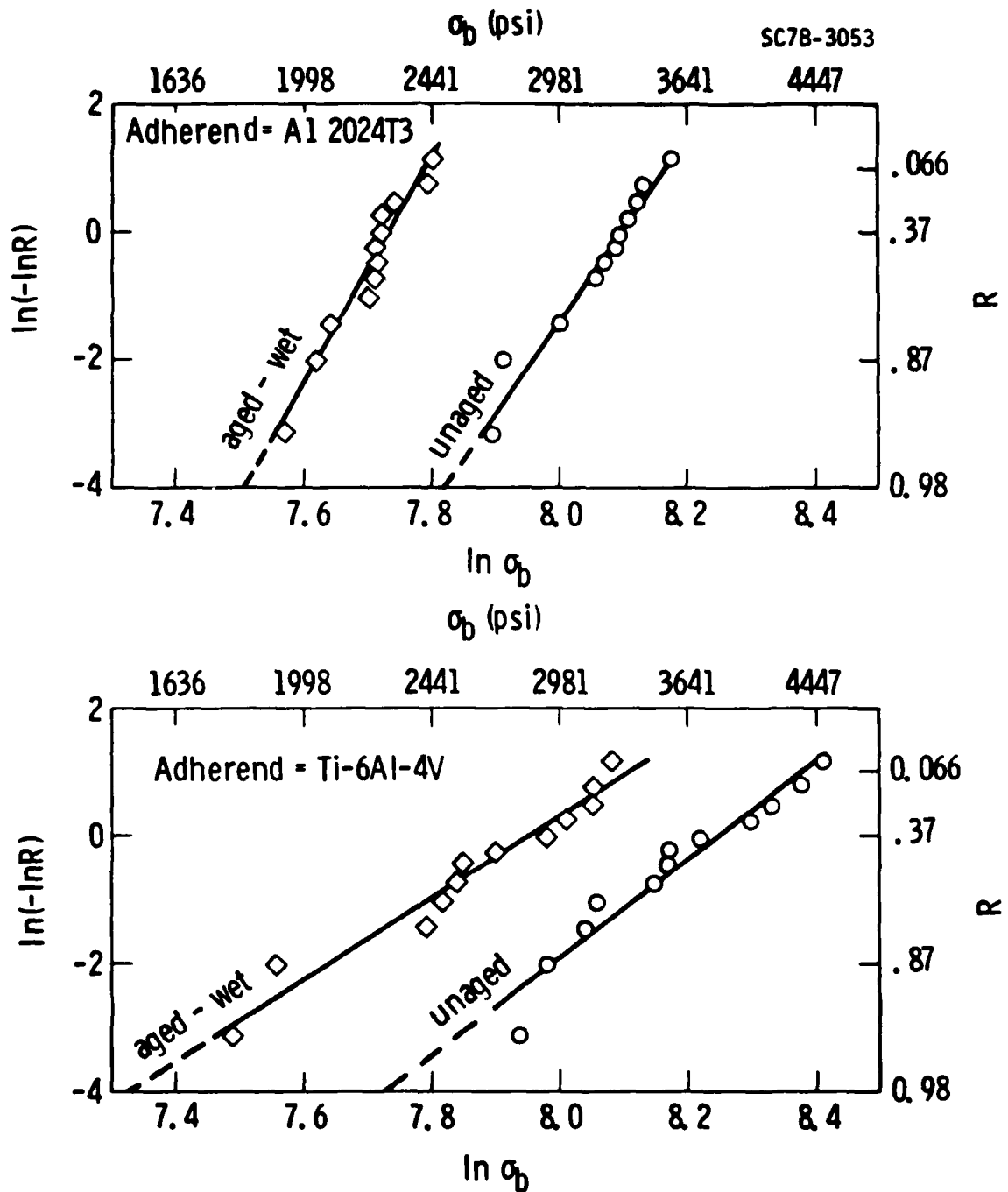


Fig. 1-21 Comparison of Weibull shear strength distributions for aluminum (upper view) and titanium (lower view) adherends.

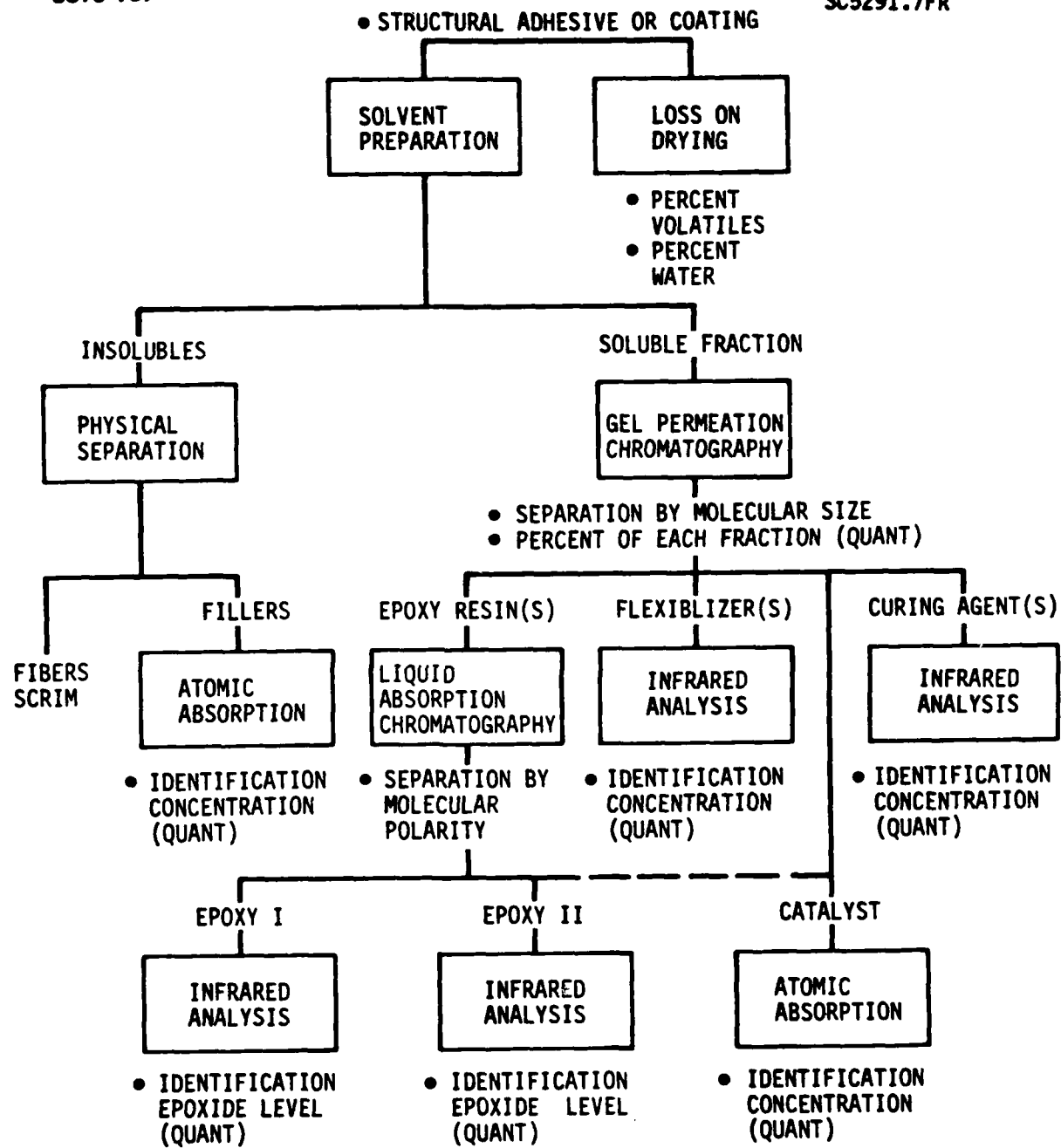


Fig. 1-22 Chemical analysis flow chart.



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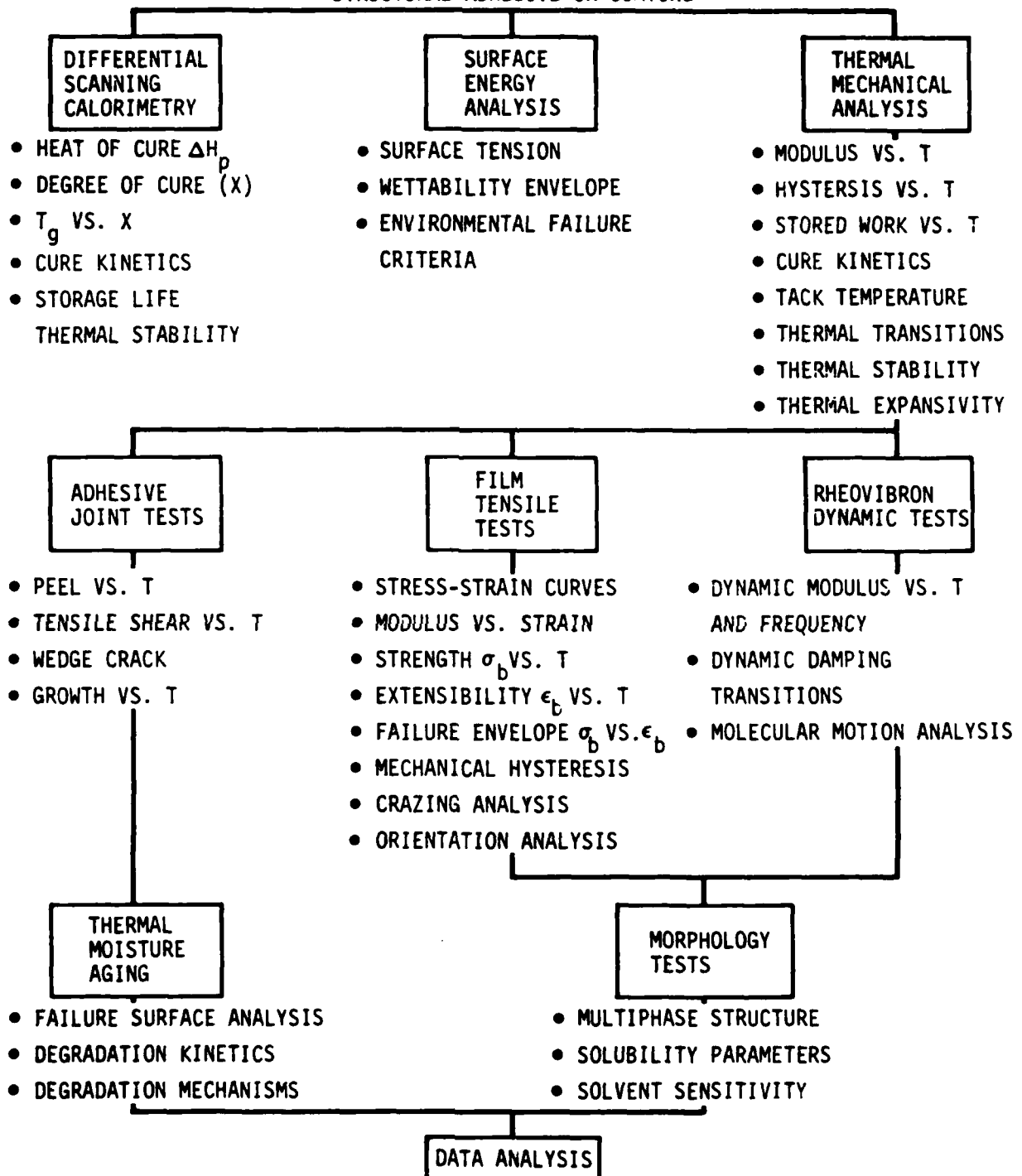


Fig. 1-23 Physical and mechanical analysis flow chart.



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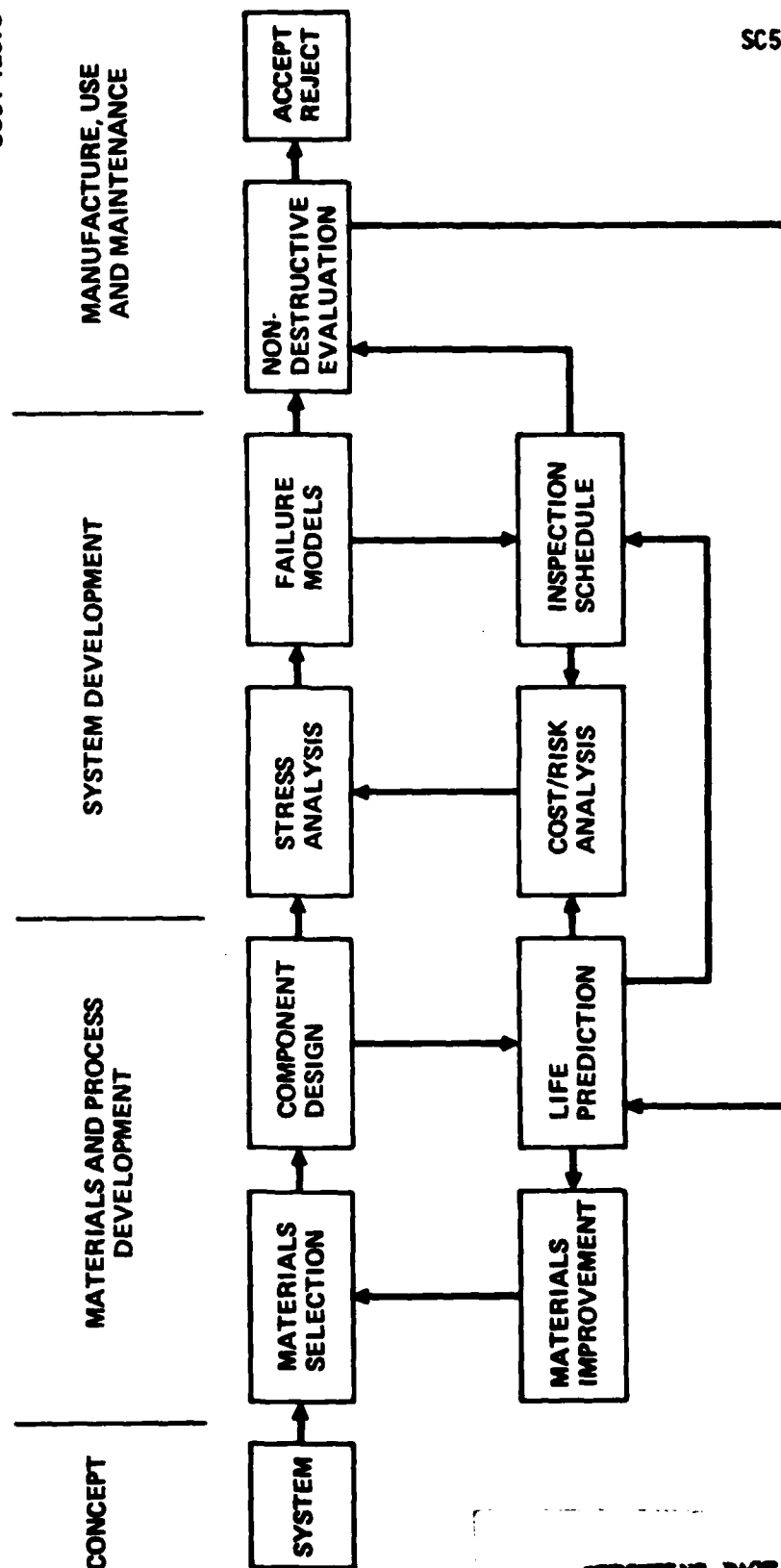


Fig. 2-1 Logic flow chart for predictive design methodology.

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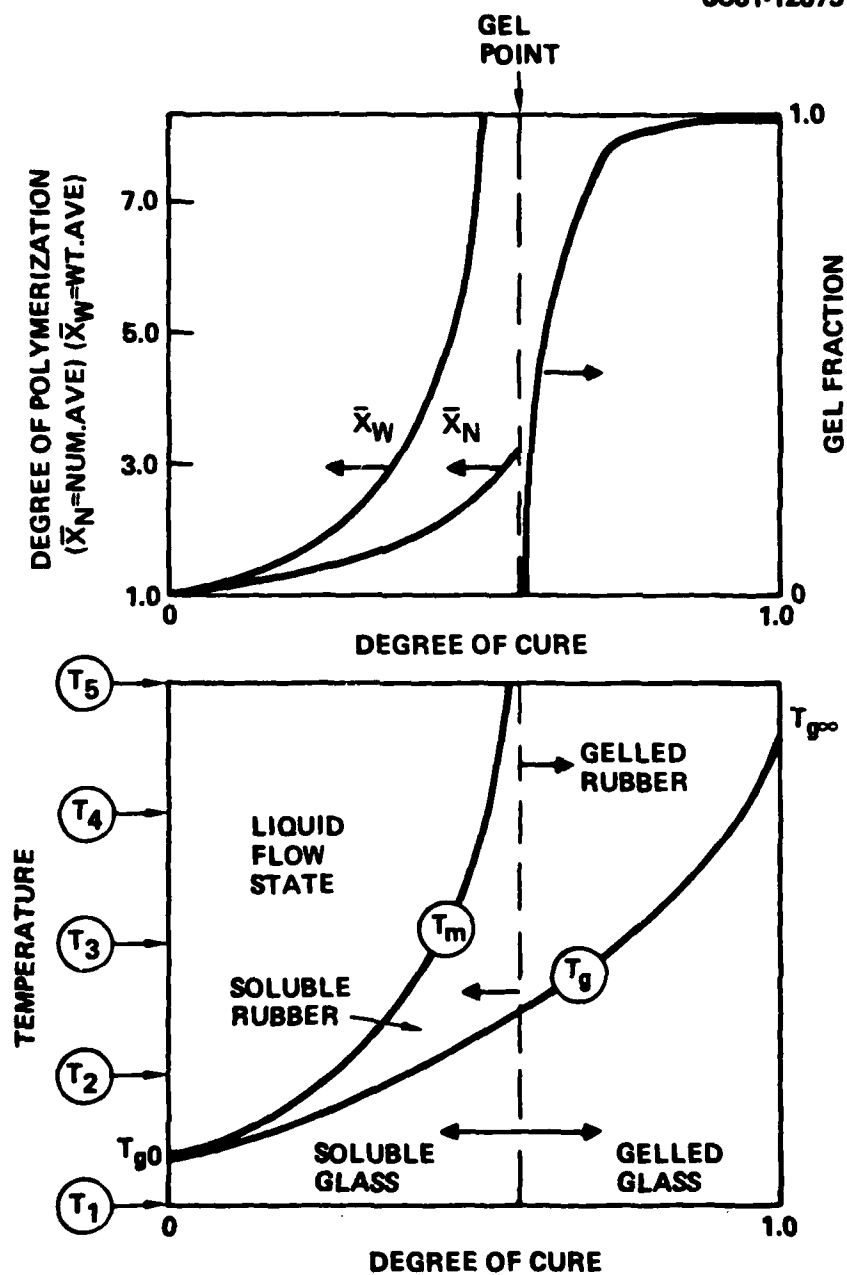


Fig. 2-2 (Upper): Change in molecular weight distribution and sol-gel state with degree of cure (idealized). (Lower): The effect of degree upon glass transition temperature T_g and melt temperature T_m for liquid flow (idealized).



SC81-12677

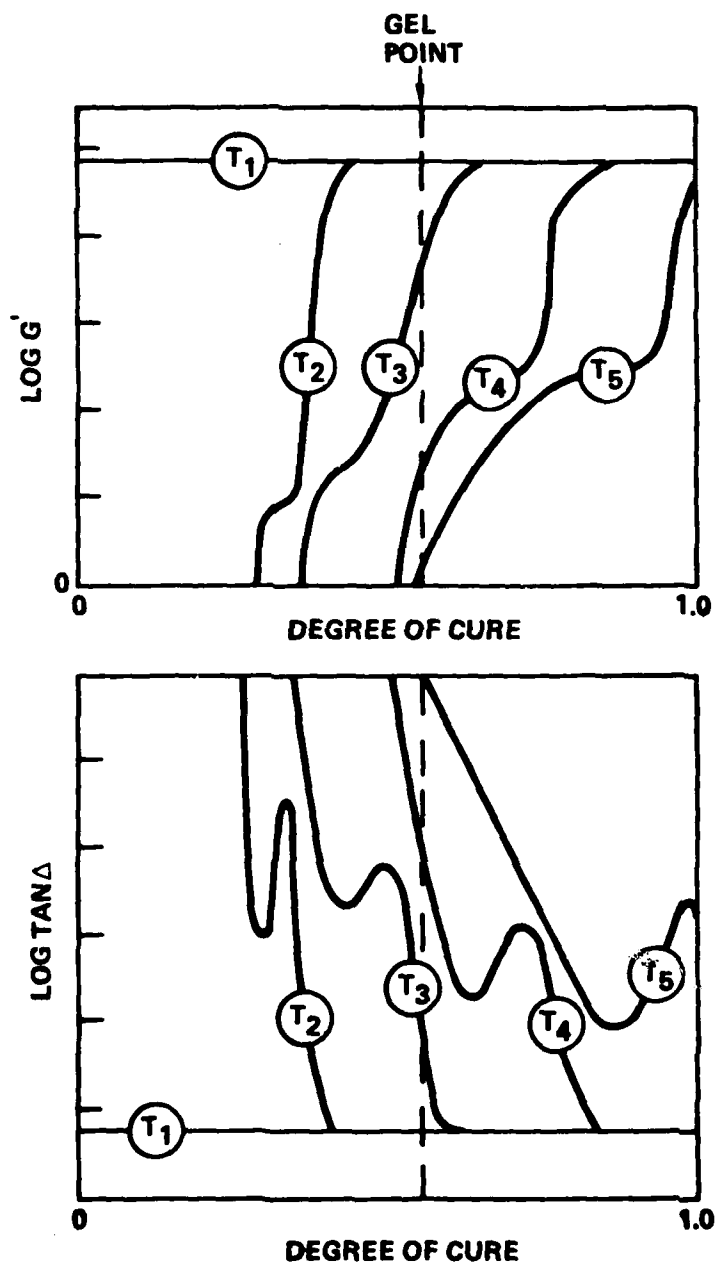


Fig. 2-3

Idealized isothermal dynamic mechanical monitoring of degree of cure in terms of shear storage modulus G' (upper view) and loss tangent $\tan \delta$ (lower view).

SC81-12676

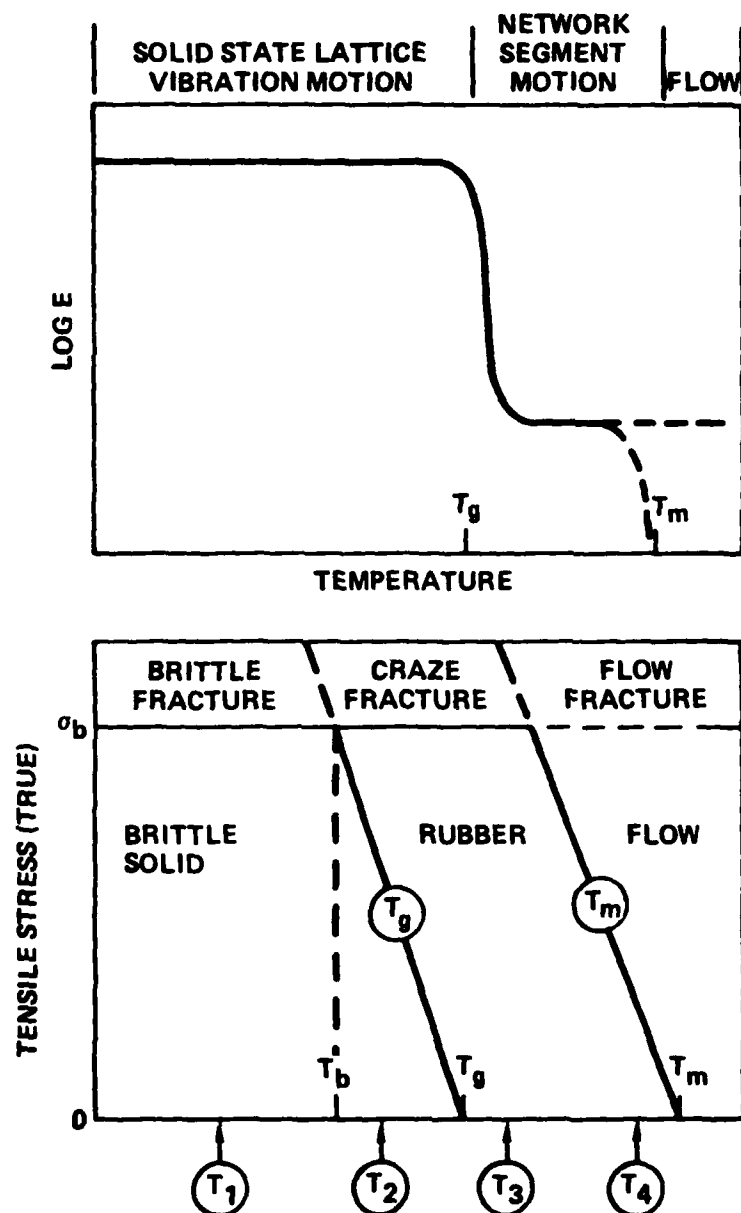


Fig. 2-4 Thermal scanning of fully cured matrix for tensile modulus (upper view) and stress-temperature response (lower view) at constant time of loading (idealized).



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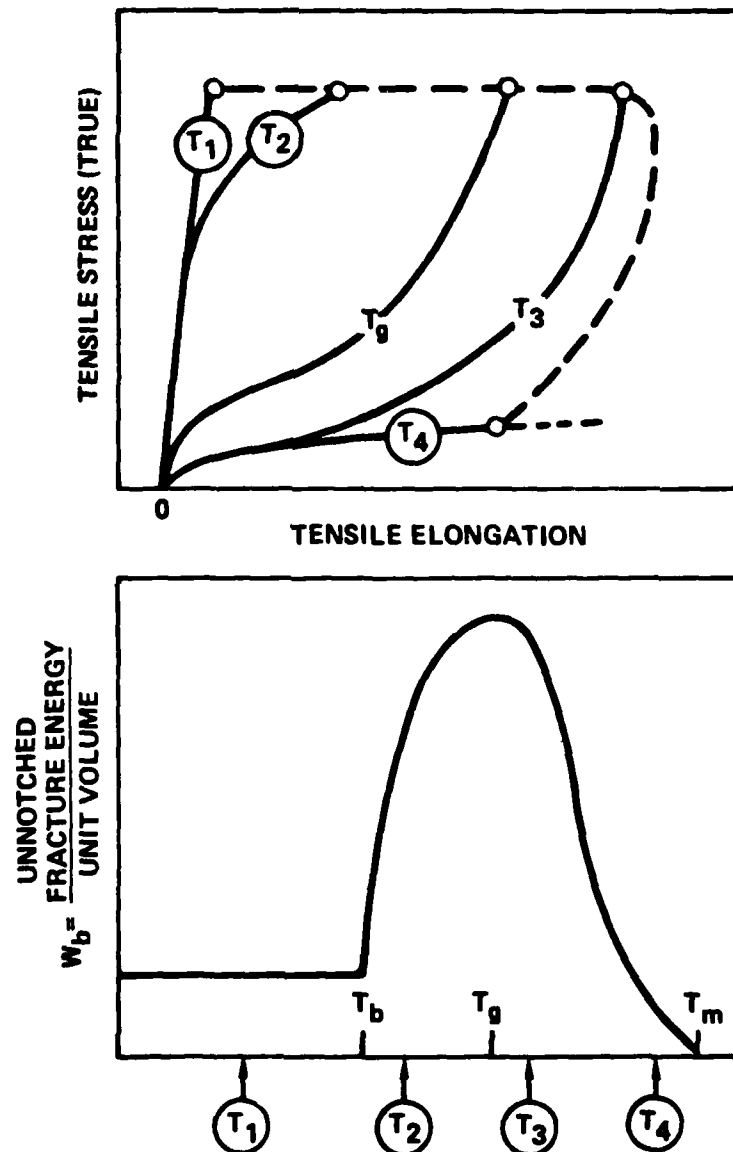
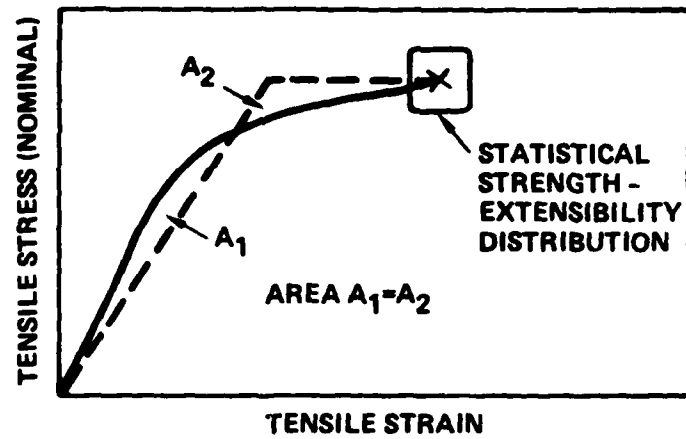


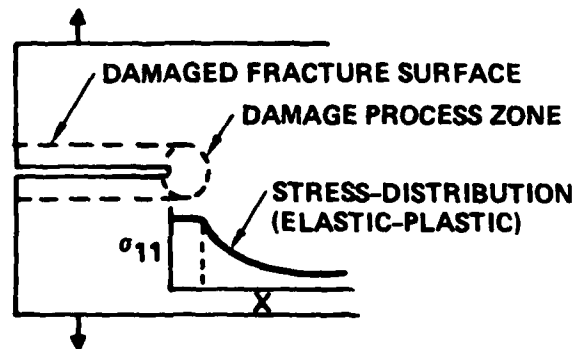
Fig. 2-5

Characteristic tensile stress-strain and fracture response (upper view) and temperature profile of unnotched tensile fracture energy (lower view).

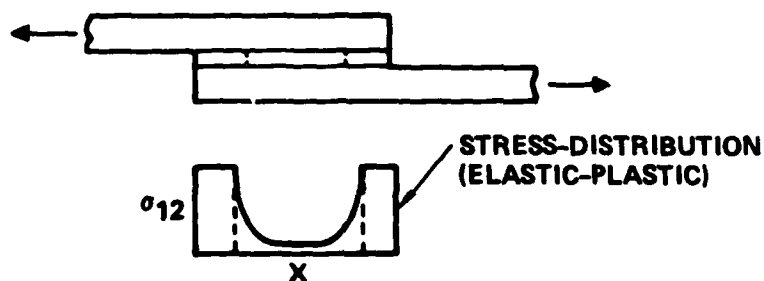
SC81-12674



I. ELASTIC-PLASTIC ANALOG STRESS-STRAIN CURVE



II. FRACTURE MECHANICS (DUGDALE MODEL)



III. STRESS ANALYSIS (HART-SMITH MODEL)

Fig. 2-6

Conversion of measured stress-strain to elastic-plastic analog (I) and introduction into fracture mechanics (II) and stress analysis (III) predictive models.



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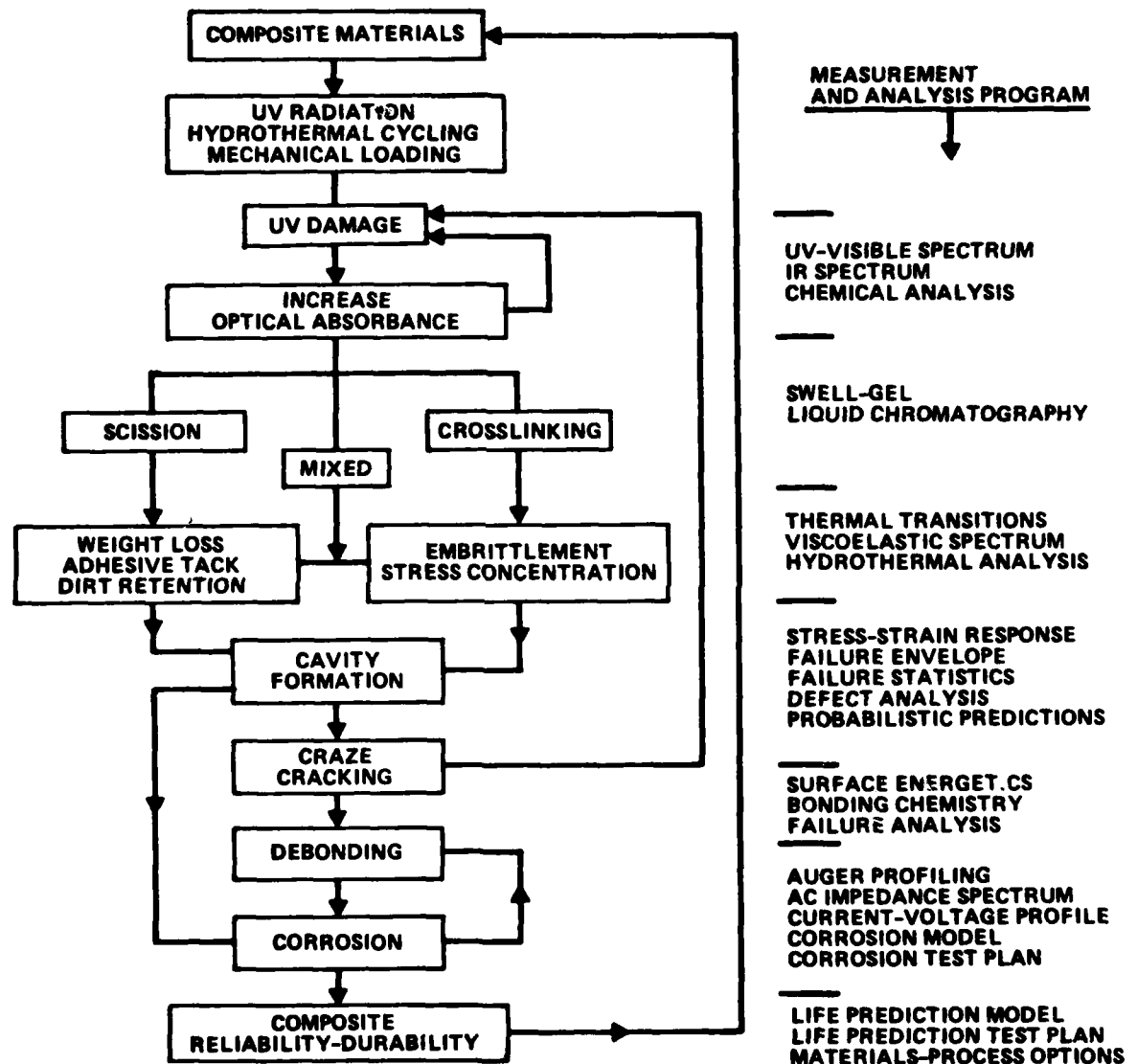


Fig. 2-7 General laminate life prediction program.



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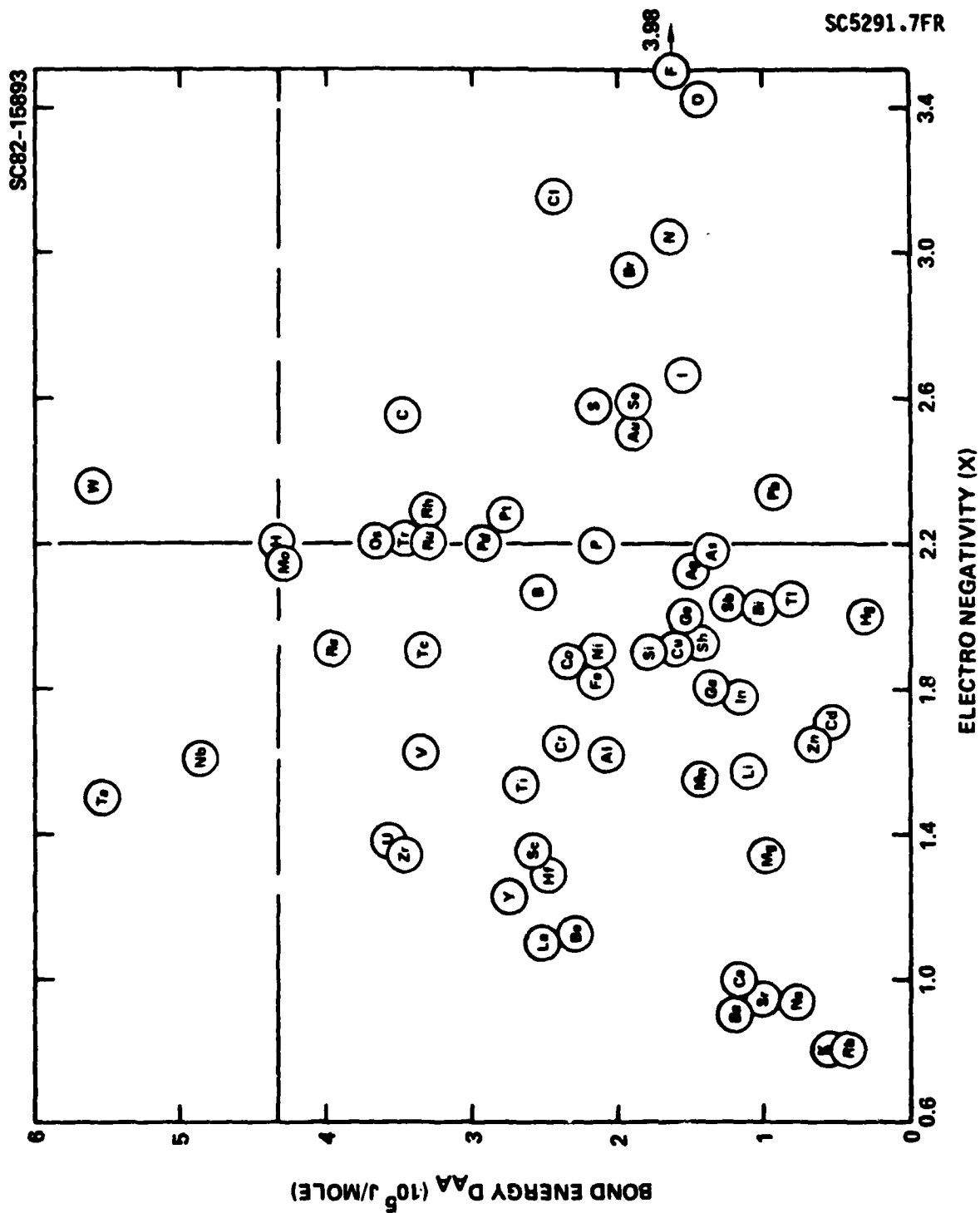


Fig. 3-1 Covalent bond energy D_{AA} and electronegativity X for the elements.

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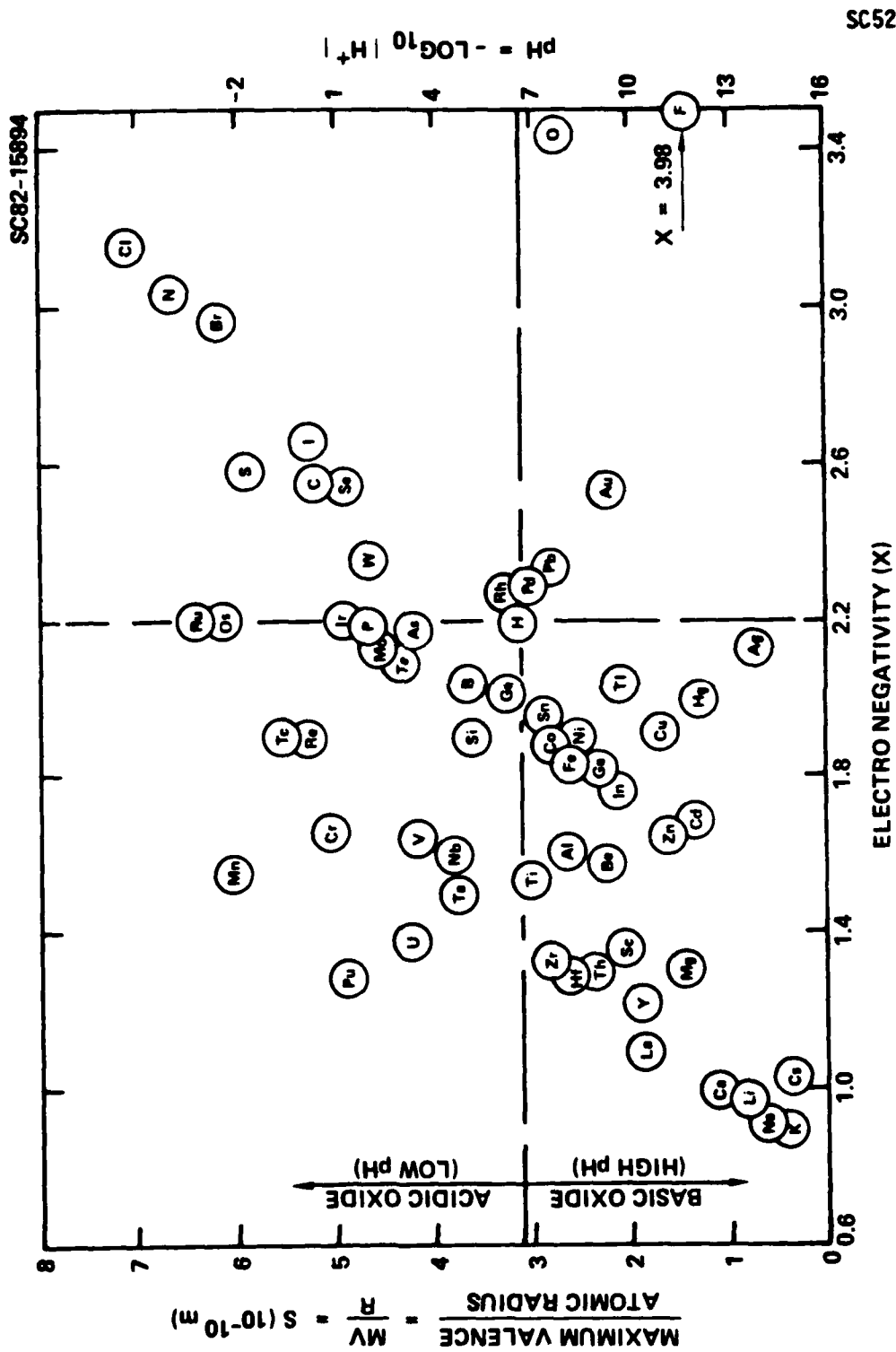


Fig. 3-2 The maximum valence to atomic radius ratio, MV/R vs electronegativity.

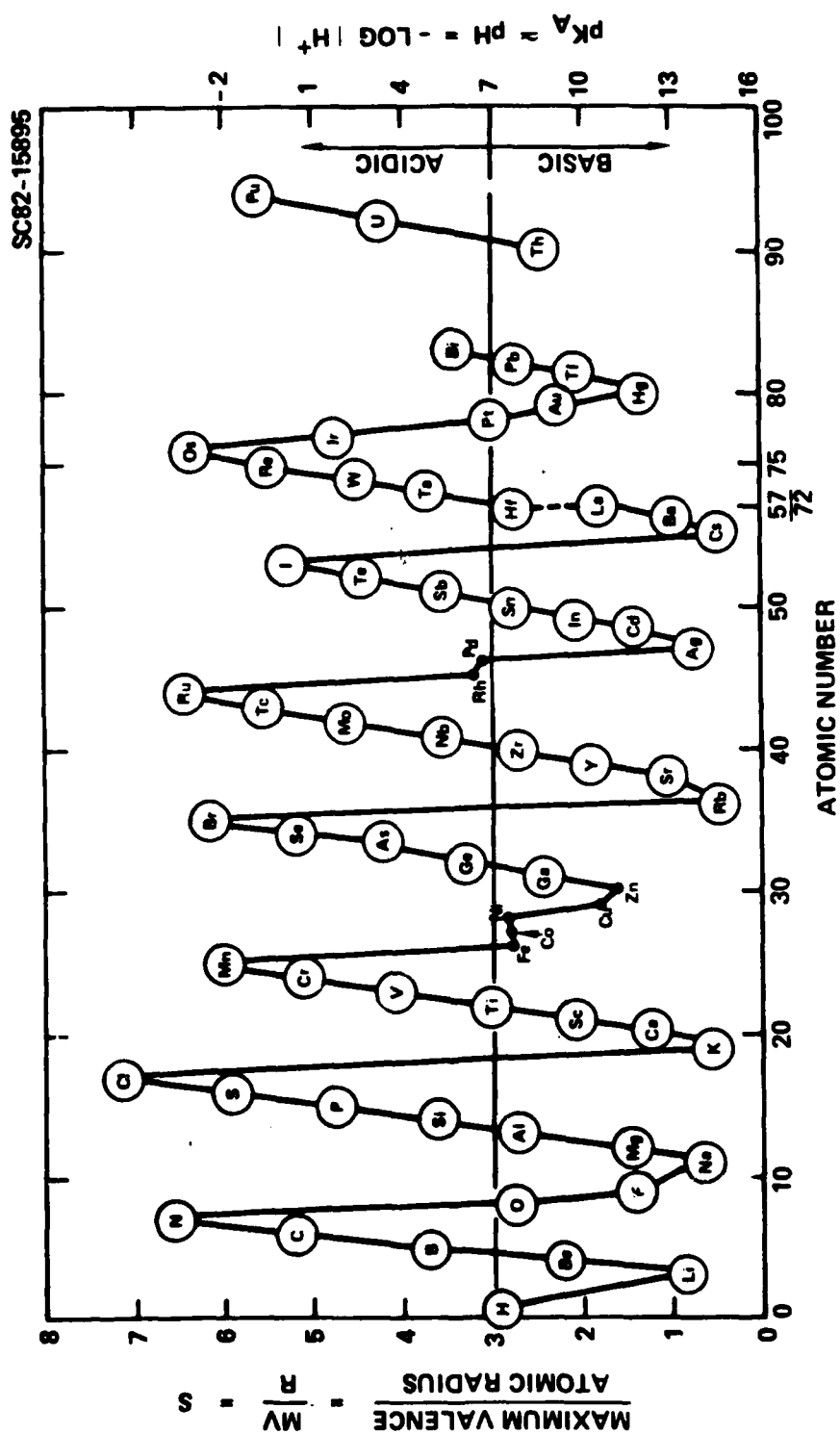


Fig. 3-3 Acidity index $pH = 16 - 3S$ vs atomic number.

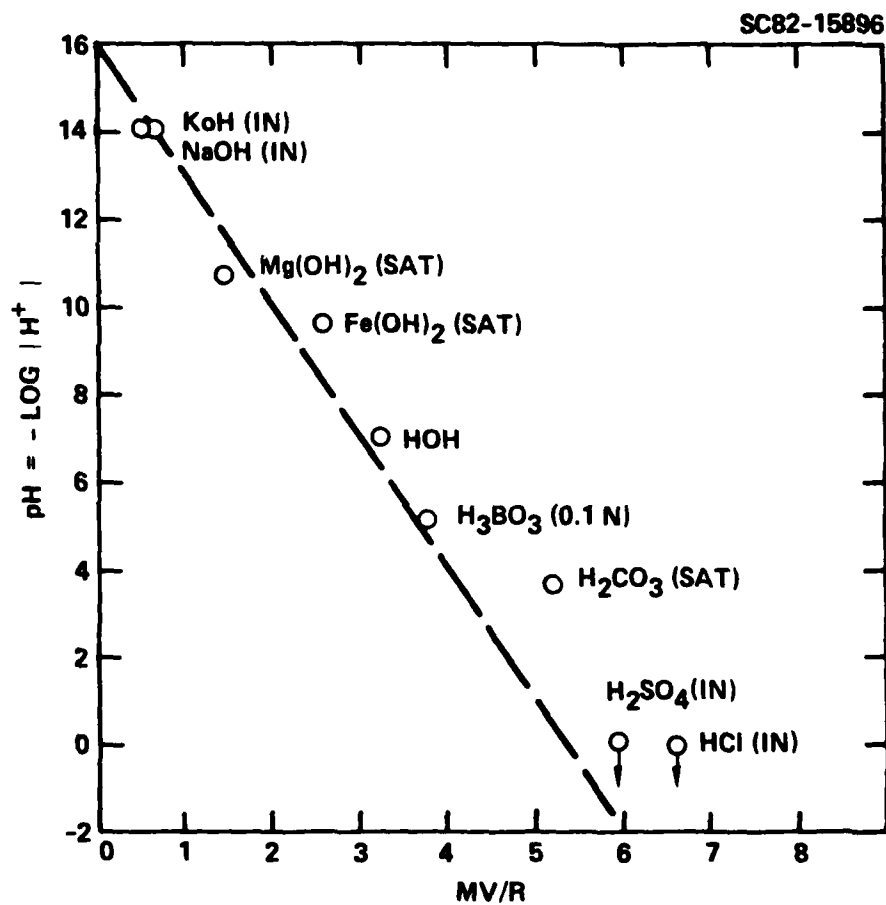


Fig. 3-4 pH vs (MV/R) for acids and bases.

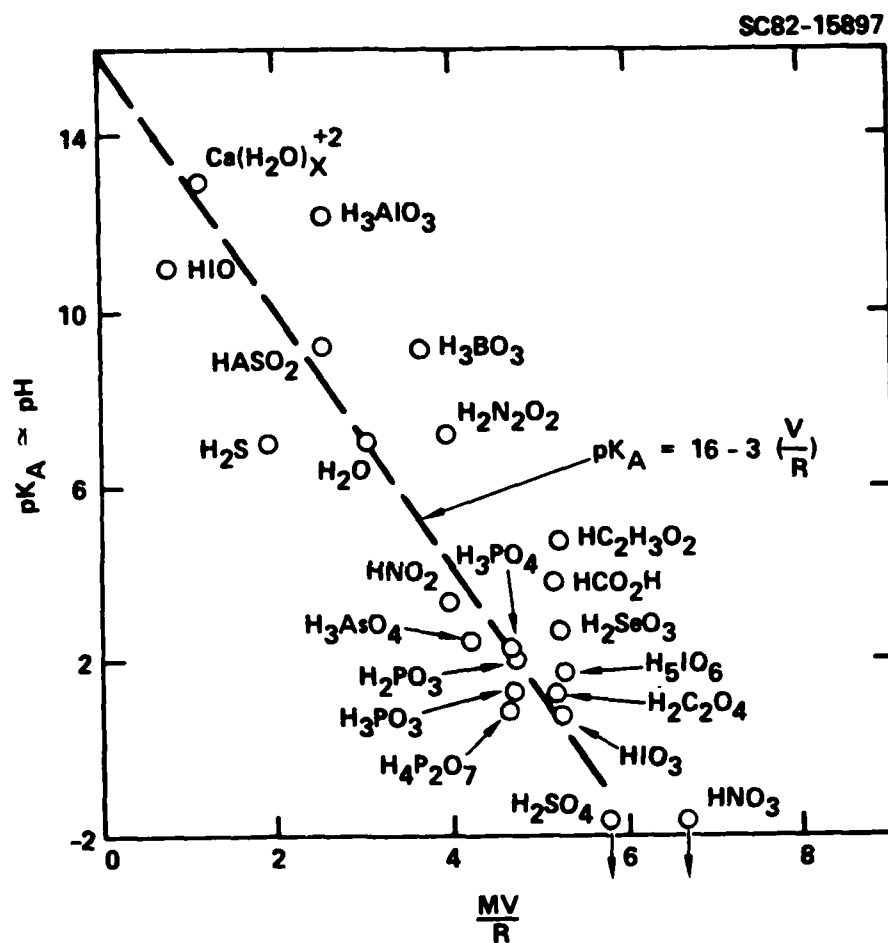


Fig. 3-5 Acid dissociation index pK_A vs (V/R) for miscellaneous acids and bases at varied valence.

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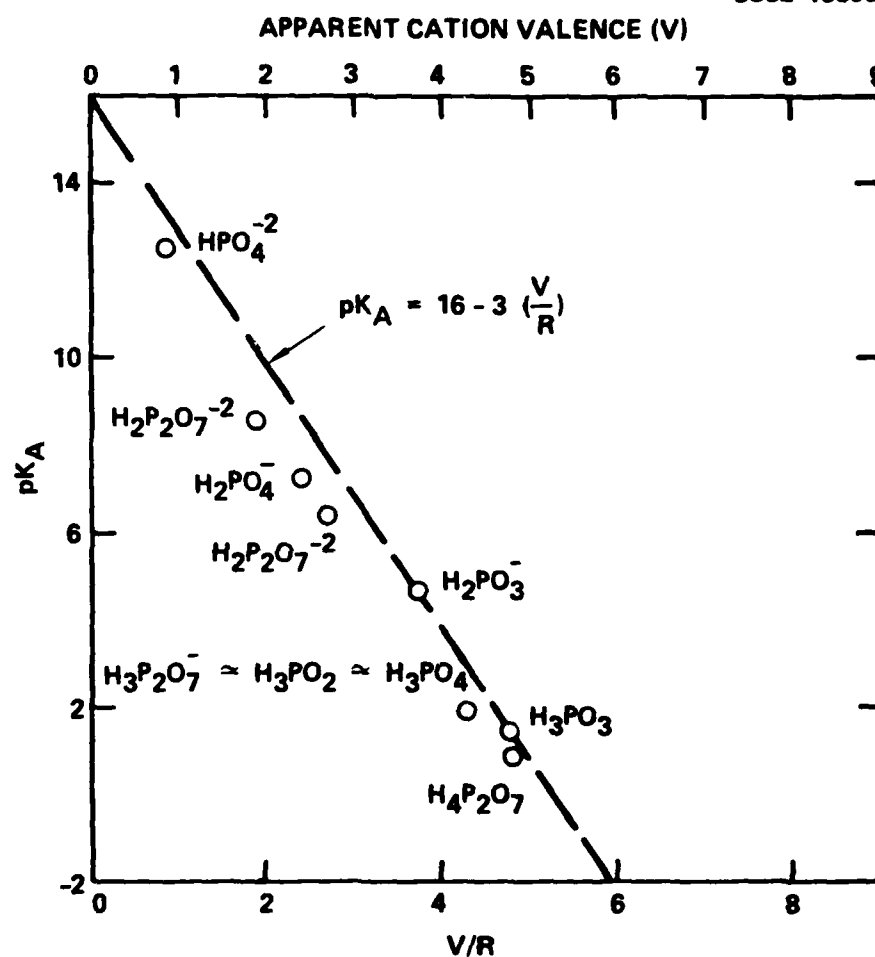


Fig. 3-6 Acid dissociation index pK_A vs apparent cation valence V and V/R .

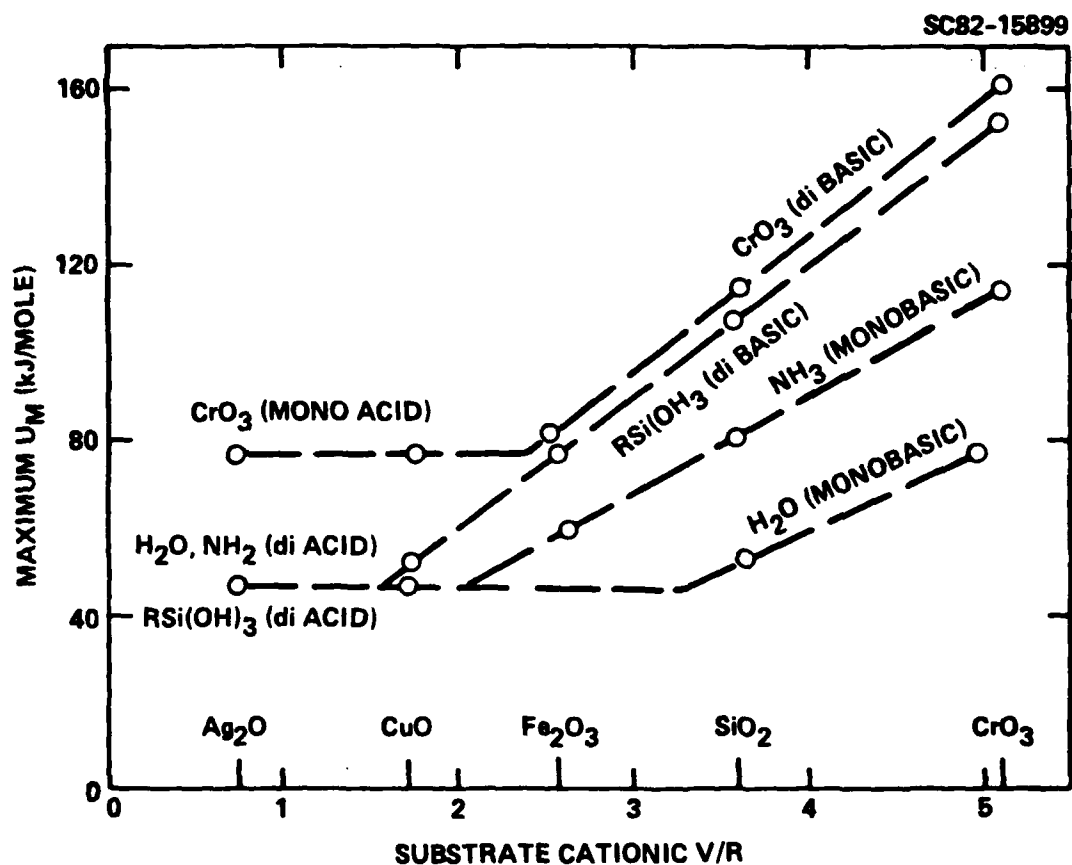


Fig. 3-7 Calculated maximum Coulomb energy U_m between adsorbate and substrate oxides.

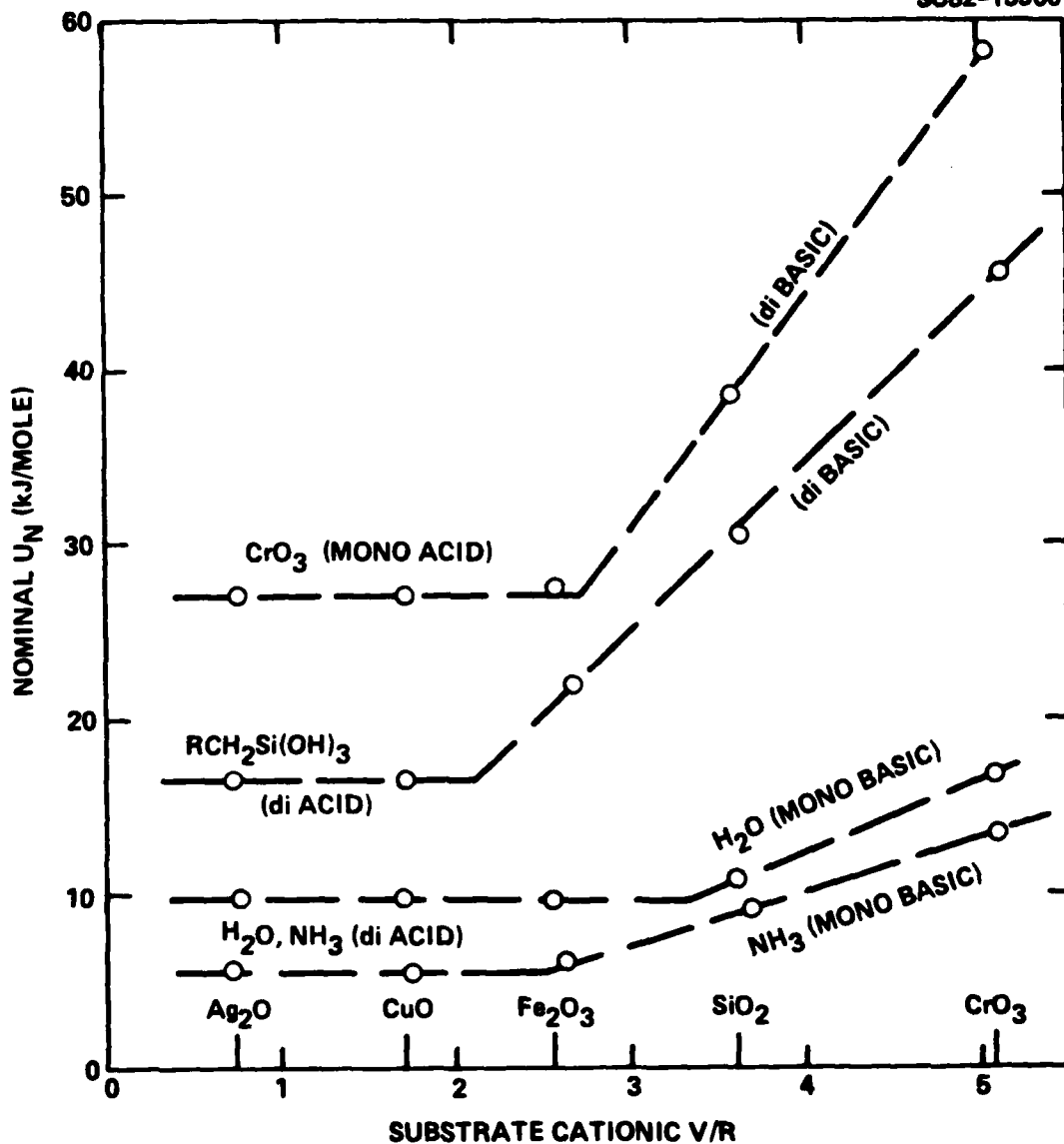


Fig. 3-8

Calculated nominal Coulomb energy U_N between absorbate and substrate oxides.



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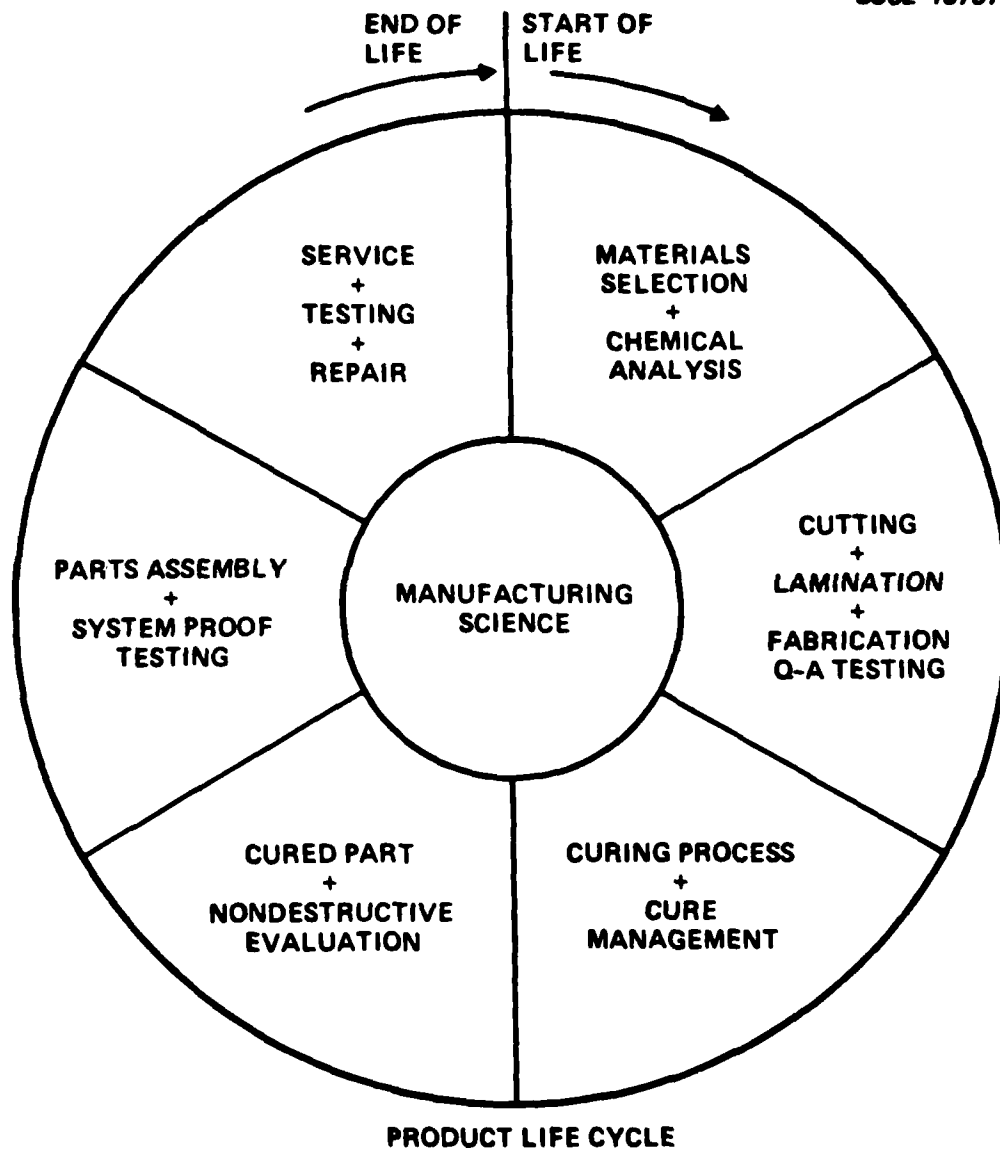


Fig. 4-1 Central role of manufacturing science in the product life cycle.

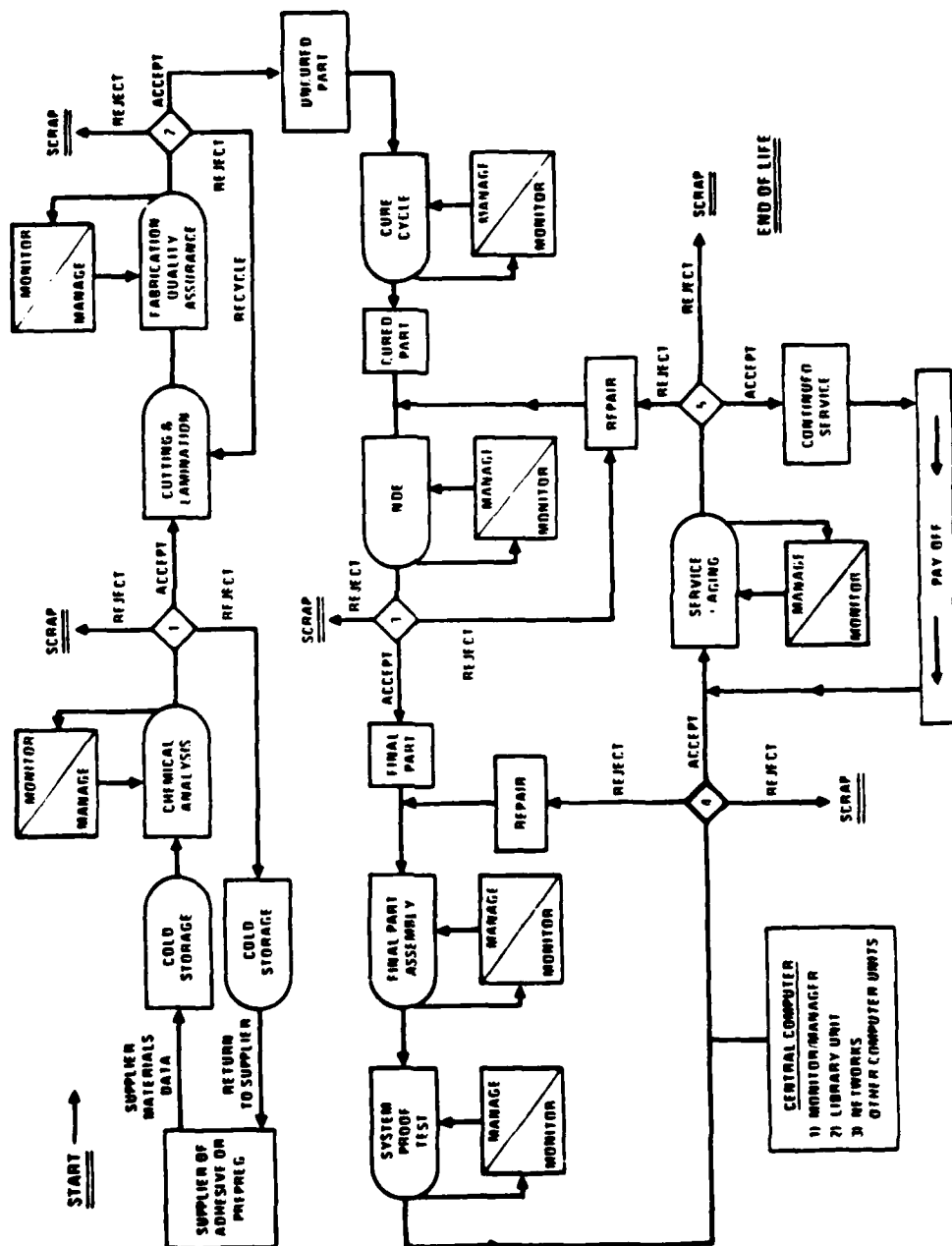


Fig. 4-2 Illustrative computer aided manufacture-service-repair cycle.

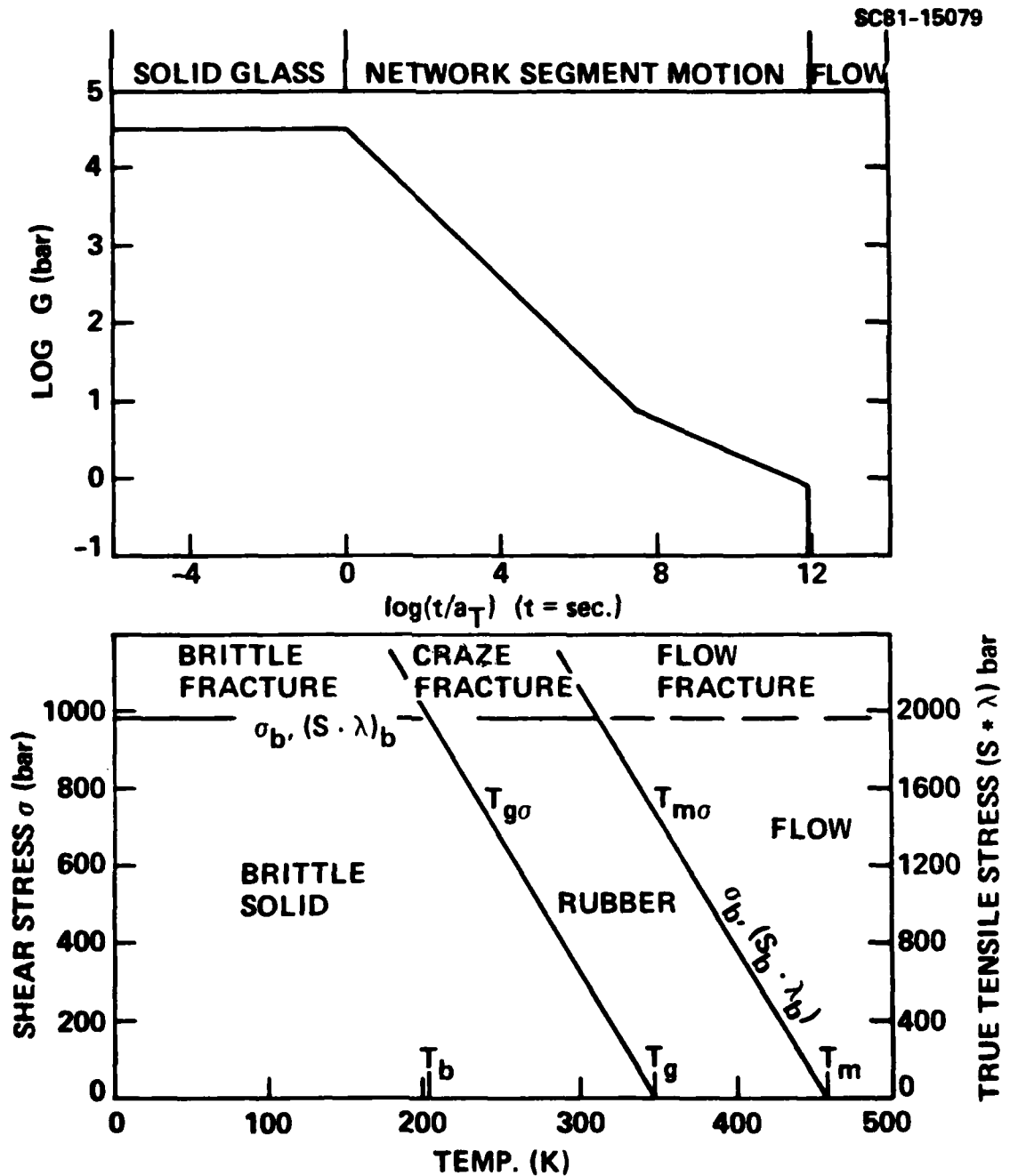
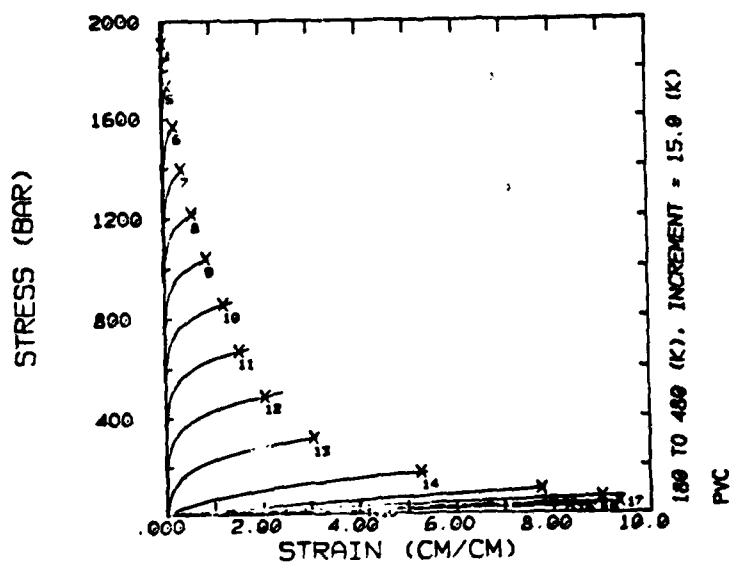
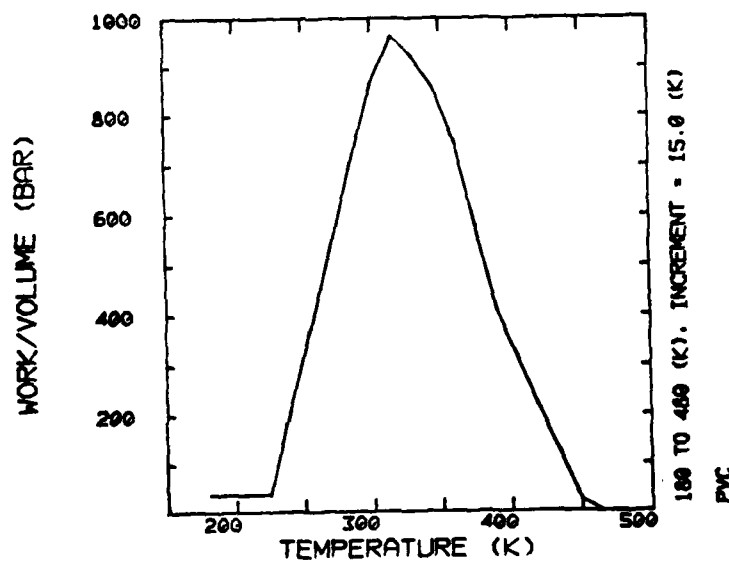


Fig. 4-3

Calculated shear modulus G vs reduced relaxation time t/a_T (upper curve) and stress-temperature functions for yield and fracture (lower curves).



STRESS VS STRAIN - TENSILE - FIXED T=1.00 SEC



WORK VS TEMP - TENSILE - FIXED T=1.00 SEC

Fig. 4-4

Computed estimates of nominal tensile stress vs strain response and failure (indicated by X in upper curves) and fracture energy (lower curve) of linear polyvinyl chloride ($T_g = 348$ K, $M_n = 8.53E5$ gm/mole).

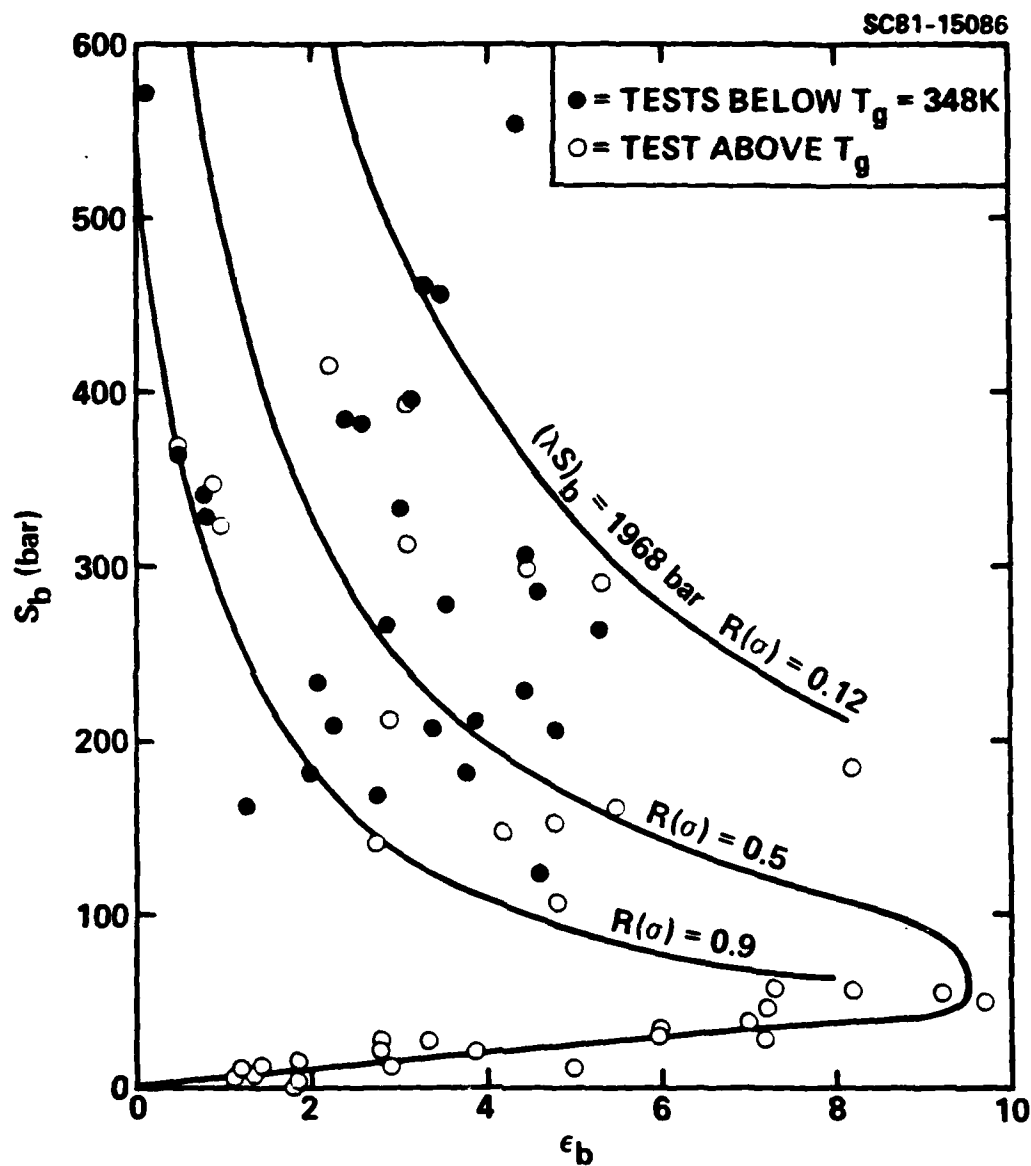


Fig. 4-5 Experimental values of nominal tensile stress S_b vs extensibility ϵ_b for polyvinyl chloride film ($T_g = 346 K$, $M_w = 1.16E6 \text{ gm/mole}$).

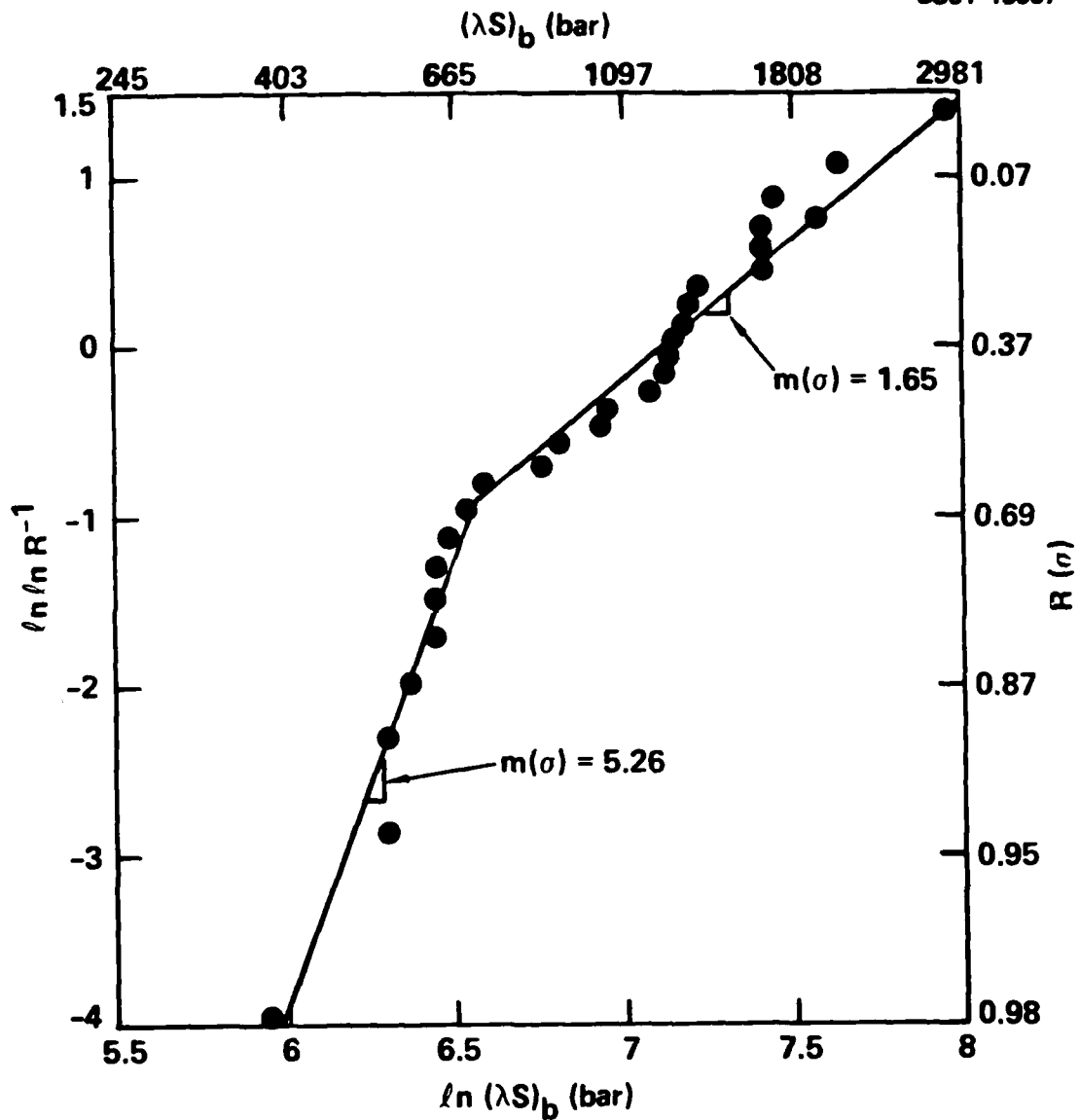


Fig. 4-6 Experimental reliability distribution $R(\sigma)$ for true tensile strength $(\lambda S)_b$ of polyvinyl chloride below T_g .

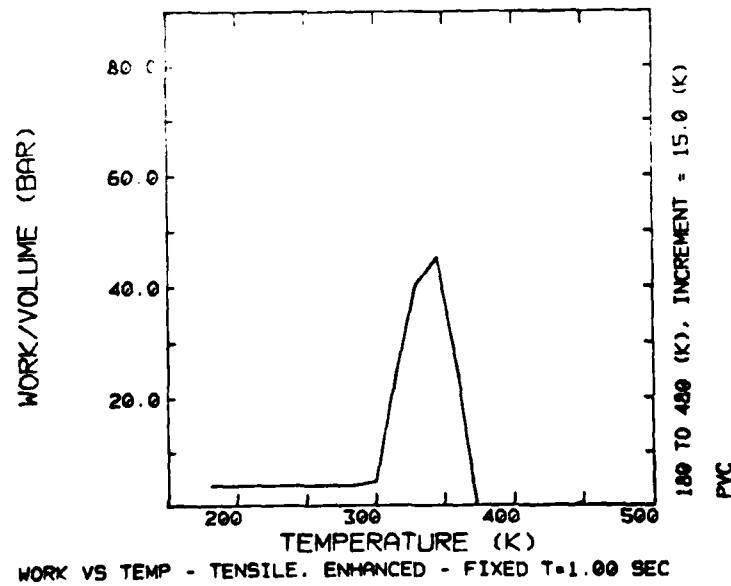
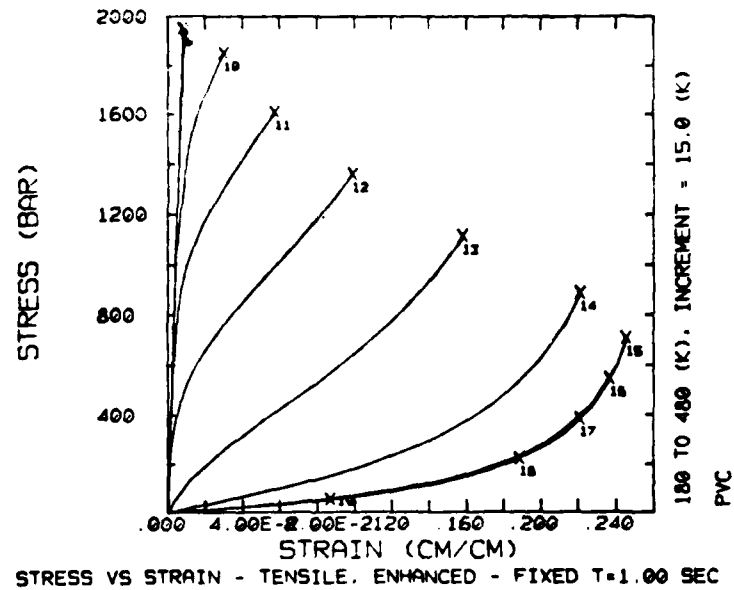


Fig. 4-7 Computed estimates of nominal tensile stress vs strain response (upper curves) and fracture energy (lower curve) for crosslinked PVC.

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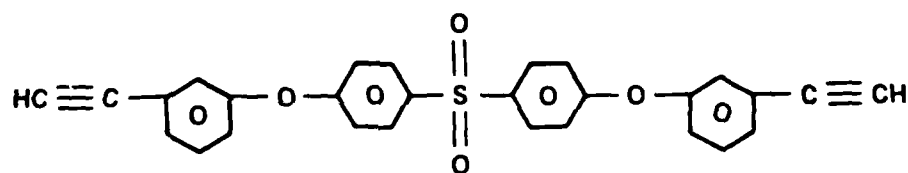


Fig. 4-8 Model ATS oligomer structure.



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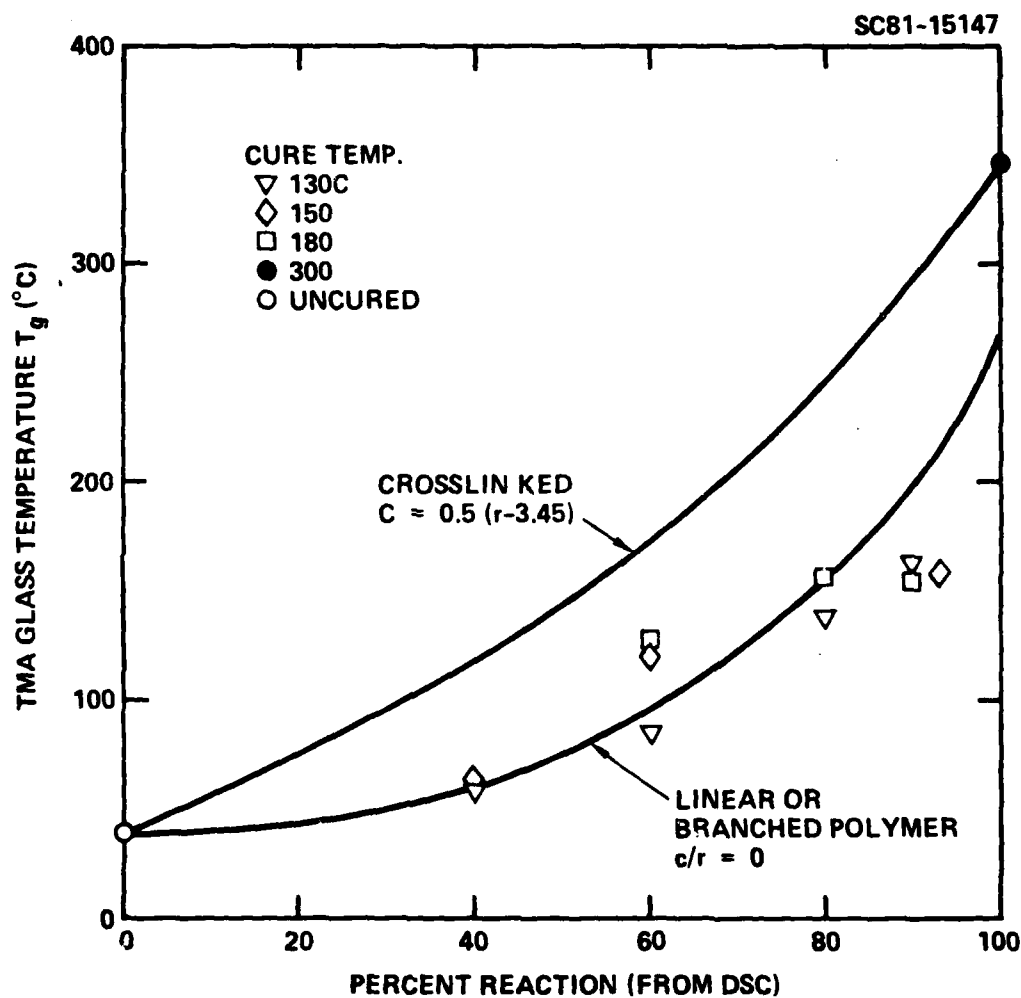


Fig 4-9

Experimental and theoretical (solid curves) values of T_g for ATS as a function of cure path.

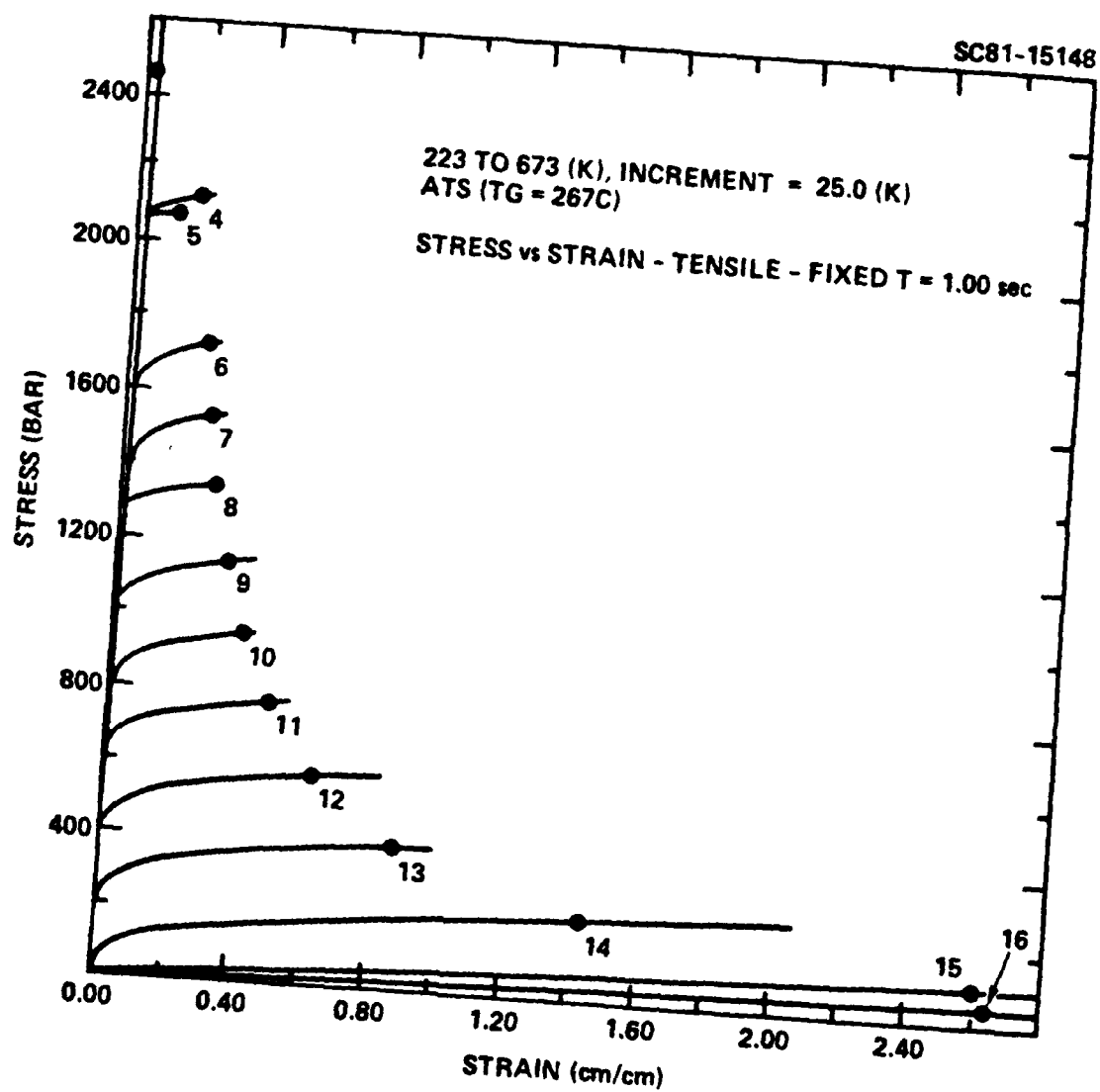


Fig. 4-10 Calculated curves of nominal tensile stress vs strain for linear ATS polymer with $T_g = 267^\circ\text{C}$ and $M_p = 2.26\text{E5 gm/mole}$ (see Table 4-8 for temperatures).



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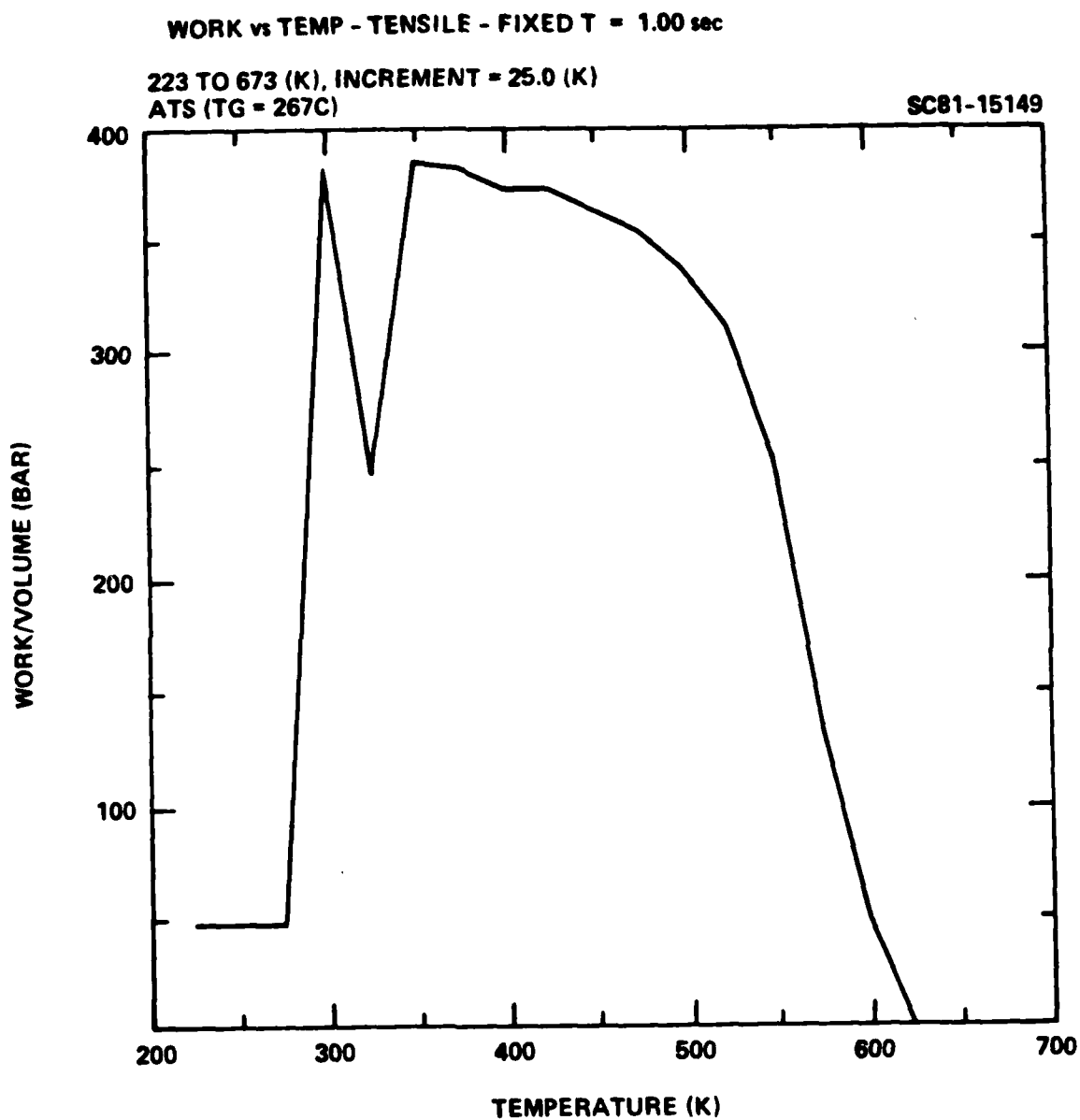


Fig. 4-11 Calculated temperature dependence of tensile fracture energy W_T per unit volume of unnotched linear ATS polymer.

STRESS vs STRAIN - TENSILE, ENHANCED - FIXED T = 1.00 sec
 223 TO 673 (K), INCREMENT = 25.0 (K)
 ATS (TG = 344C)

SC81-15150

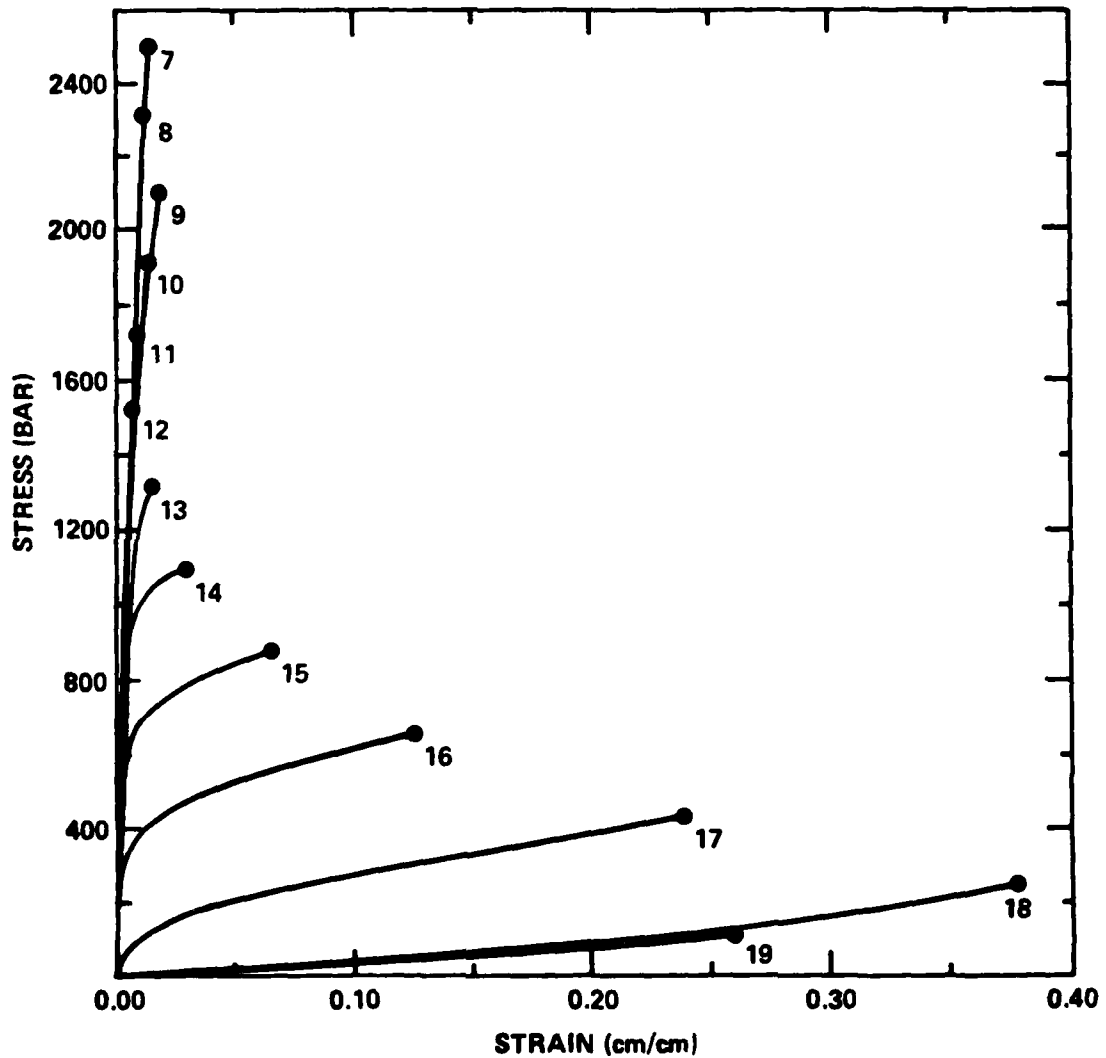


Fig. 4-12 Calculated curves of nominal tensile stress vs strain for crosslinked ATS with $T_g = 344^\circ\text{C}$ and $M_p = 2.26\text{E}5$ and $M_c = 1817$ gm/mole (see Table 4-8 for temperatures).



WORK vs TEMP - TENSILE, ENHANCED - FIXED T = 1.00 sec

223 TO 673 (K), INCREMENT = 25.0 (K)
ATS (TG = 344C)

SC81-15151

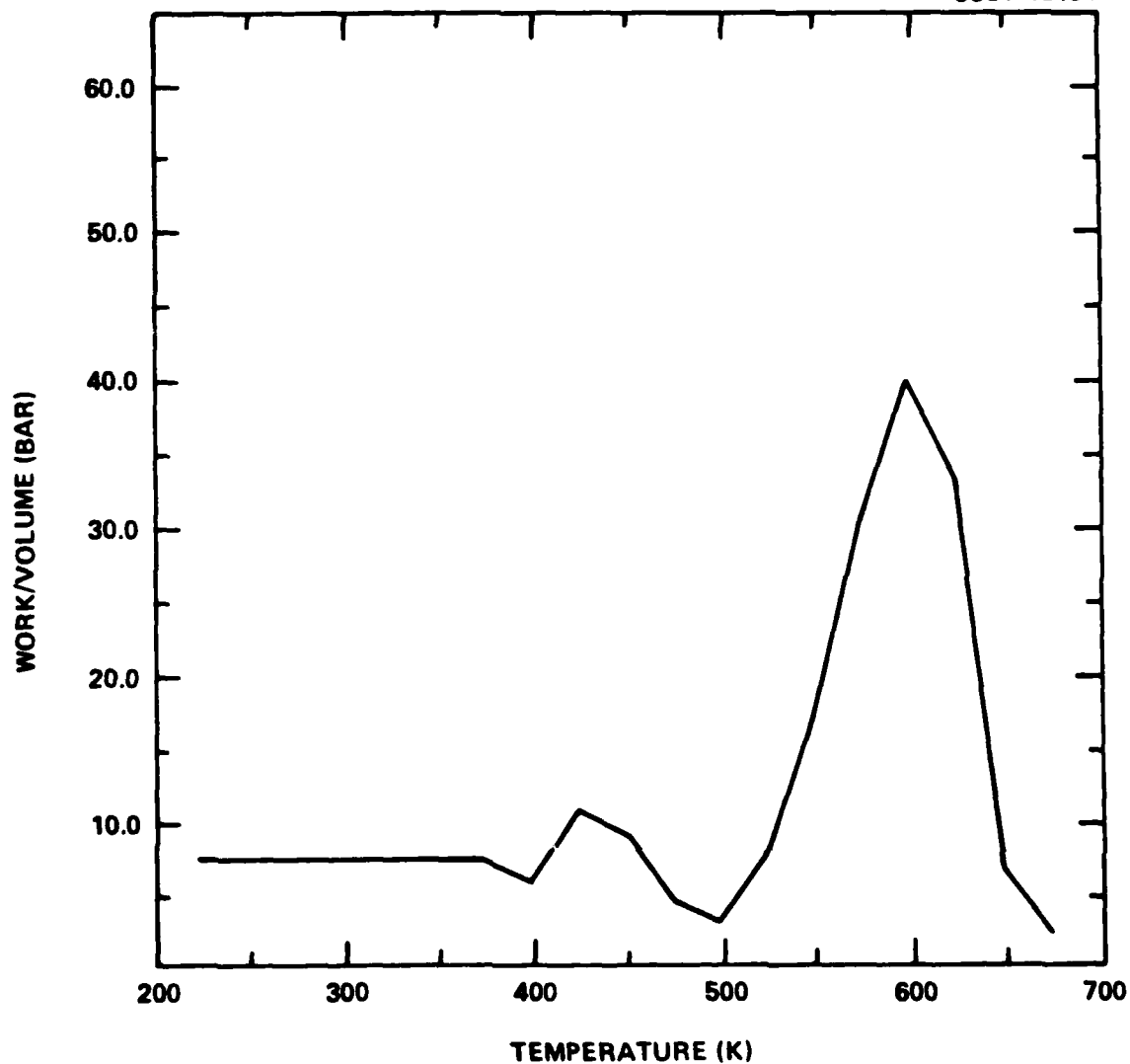


Fig. 4-13 Calculated temperature dependence of tensile fracture energy W_T per unit volume of unnotched crosslinked ATS polymer.

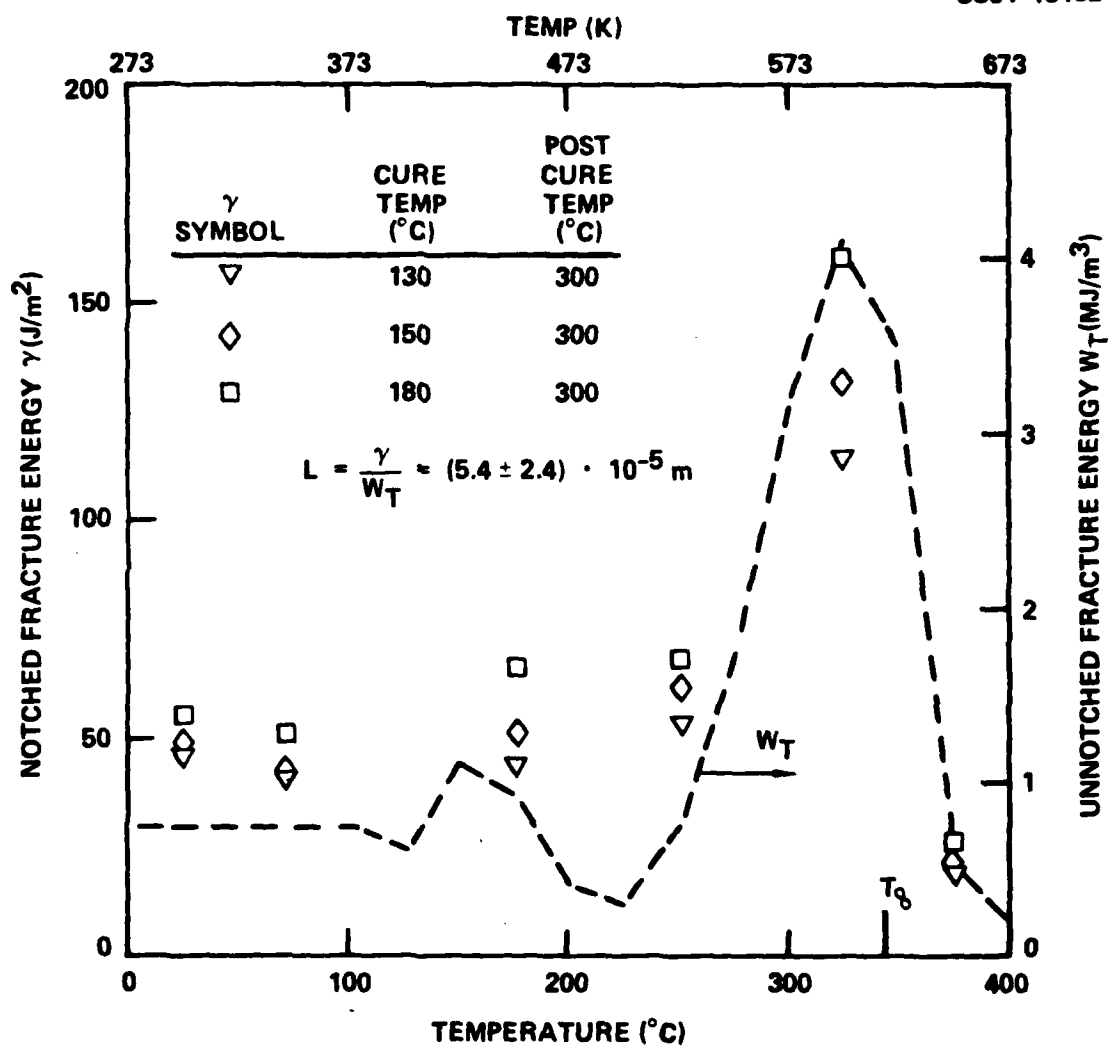


Fig. 4-14 Comparison of experimental notched fracture energy (γ) with unnotched fracture energy W_T from 25°C to 375°C.



SC82-20535

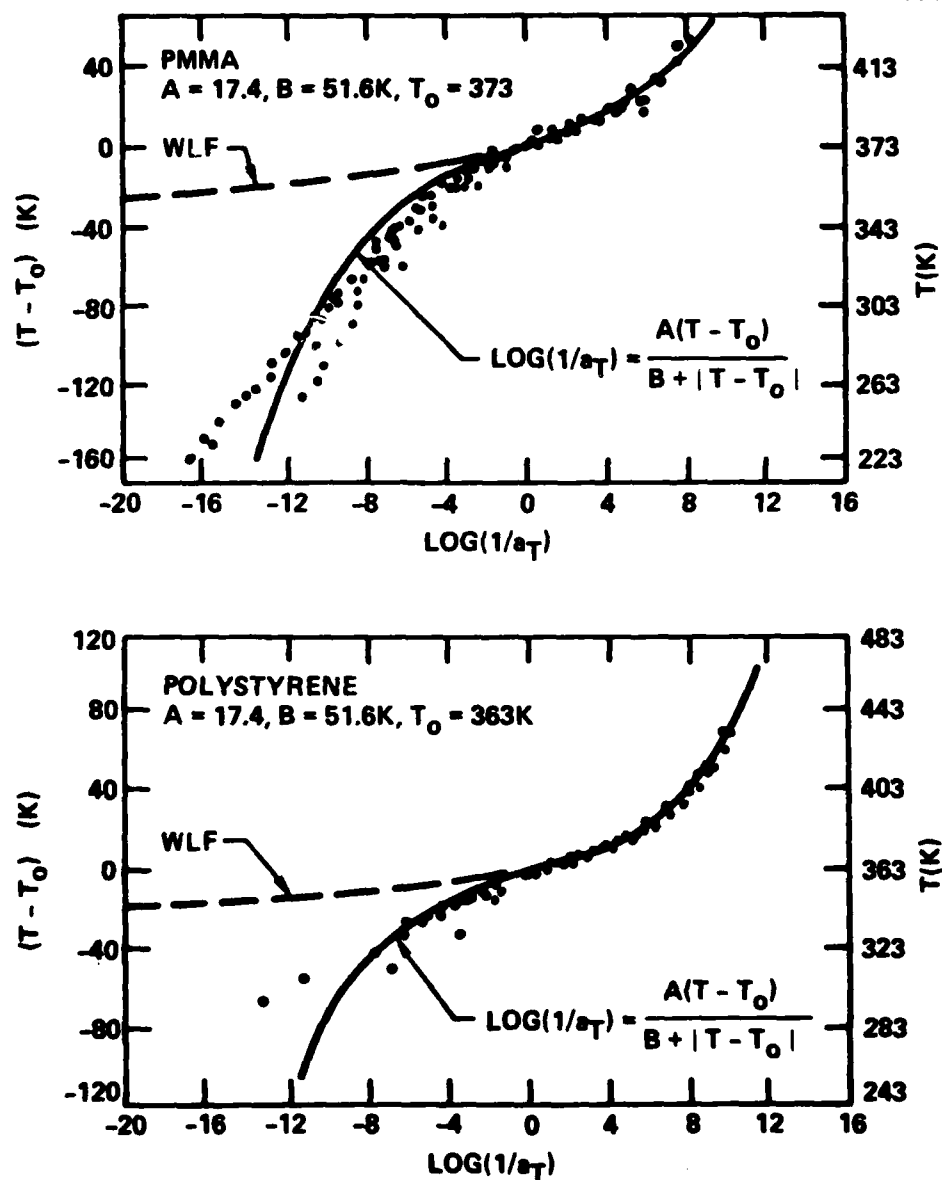


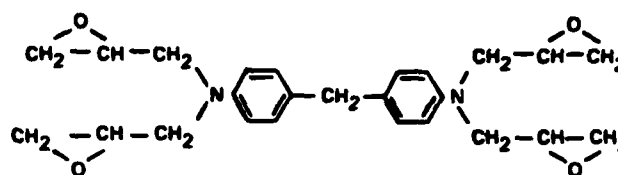
Fig. 4-15 Comparison of standard (dashed) and revised (solid curve) forms of WLF equations. (For summary of experimental time-temperature shift factors a_T , see Ref. 31, 32).



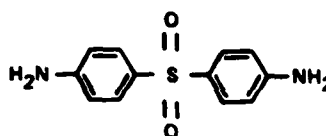
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EPOXY (E): TETRAGLYCIDYL METHYLENE DIANILINE (TGMDA);
M. W. $\approx$ 422 gm/MOLE

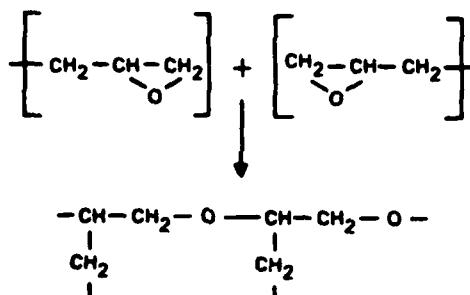
SC52-20340



CURATIVE (C): DIAMINODIPHENYLSULFONE (DDS);
M. W. $\approx$ 248 GM/MOLE



CROSSLINK REACTION 1: (100% BY WEIGHT E)



CROSSLINK REACTION 2: (83% BY WEIGHT E + 37% BY WEIGHT C)

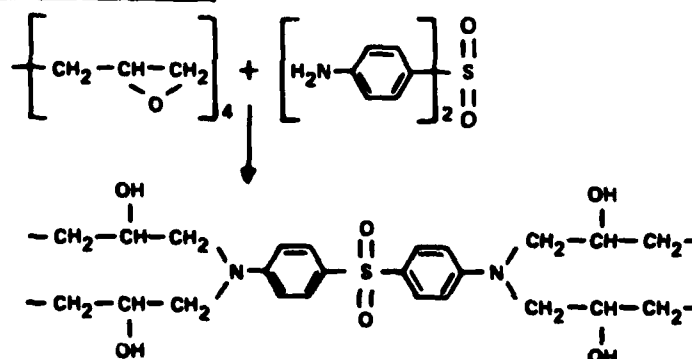


Fig. 5-1

Composition and suggested curing mechanisms for 177°C
(350°F) service temperature epoxy resins.

SC82-20342

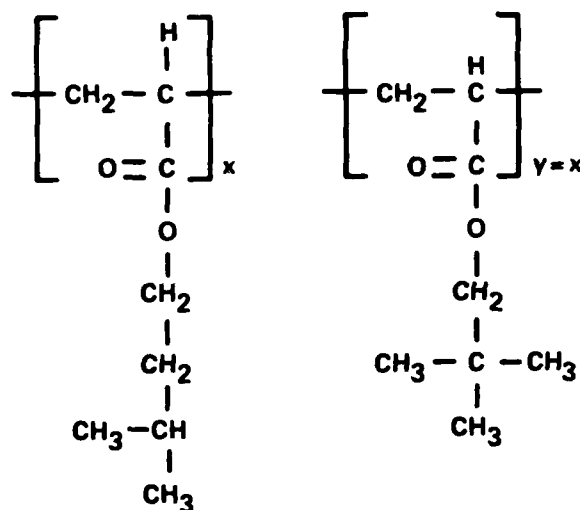


Fig. 5-2

Repeat structure for 50:50 mole % isoamyl acrylate = Neopentyl acrylate of number average molecular weight $M_n = 1.03E6$ g/mol, V_p (230K) = 1.01 cc/gm, $T_g = 230K$, and $M_e = 21,000$ gm/mole.

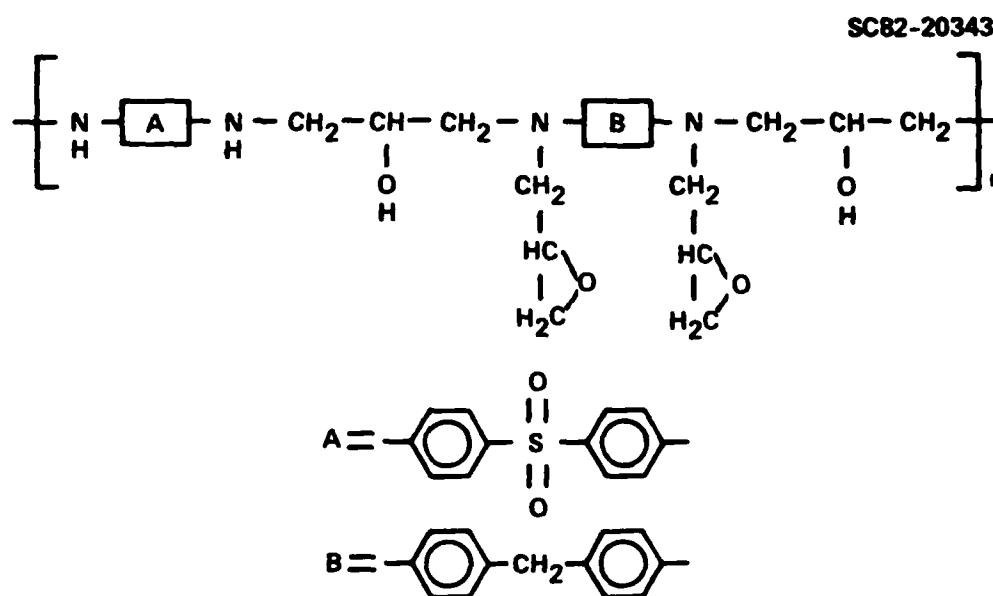


Fig. 5-3 Molecular structure of equimolar amounts of TGDMA and (37 wt%) DDS polymerized by chain extension.

Fig. 5-4



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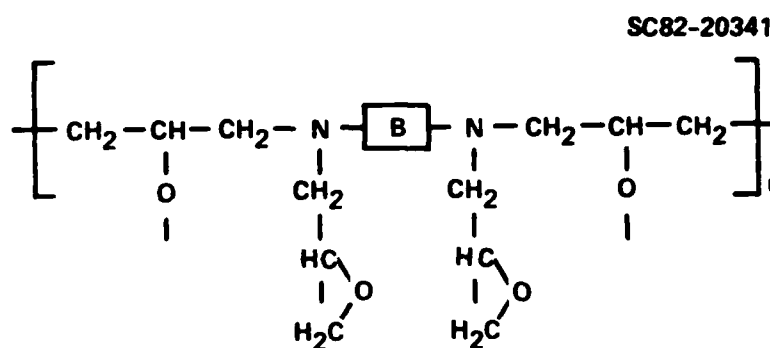


Fig. 5-5 Molecular structure of chain extended TGMDA homopolymer.

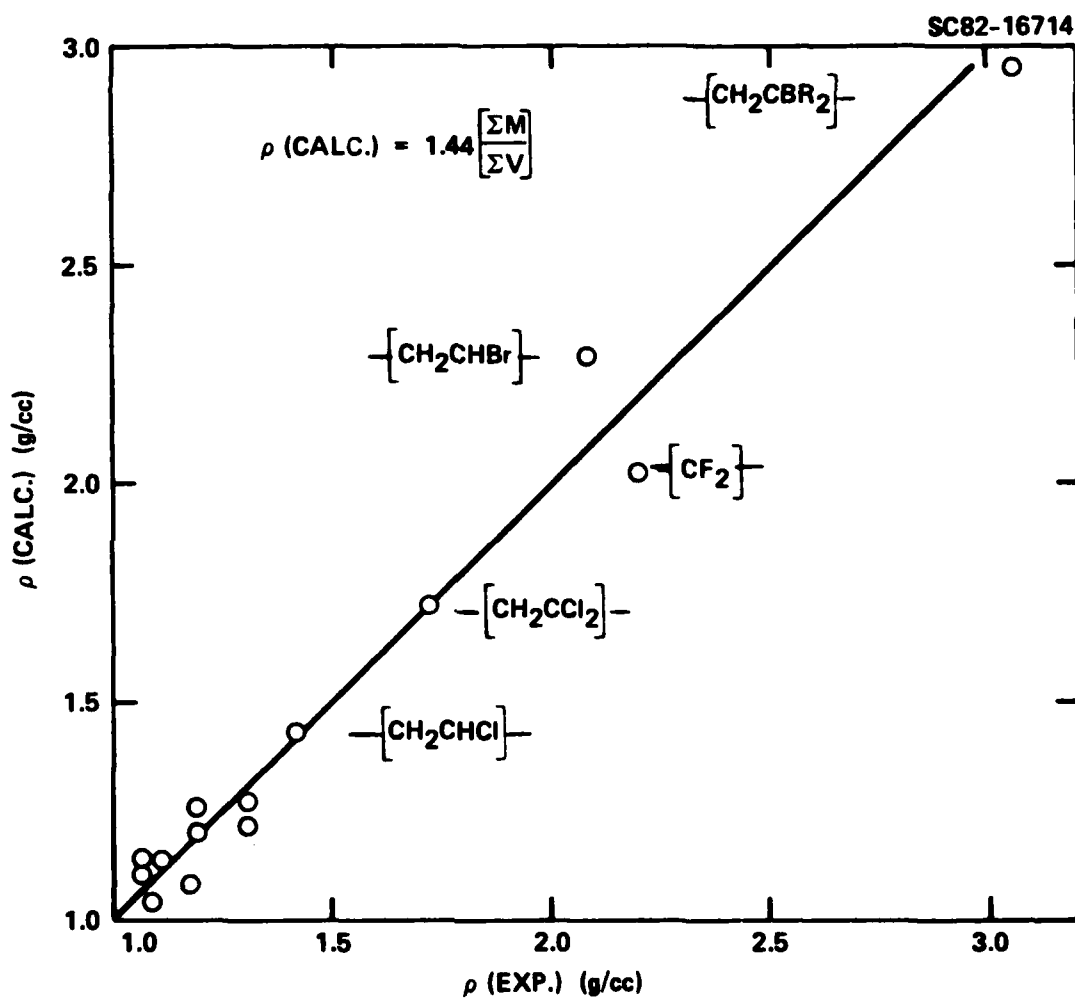


Fig. 5-6

Comparison of calculated and experimental density of solid polymers at 298K (data from Ref. 5).

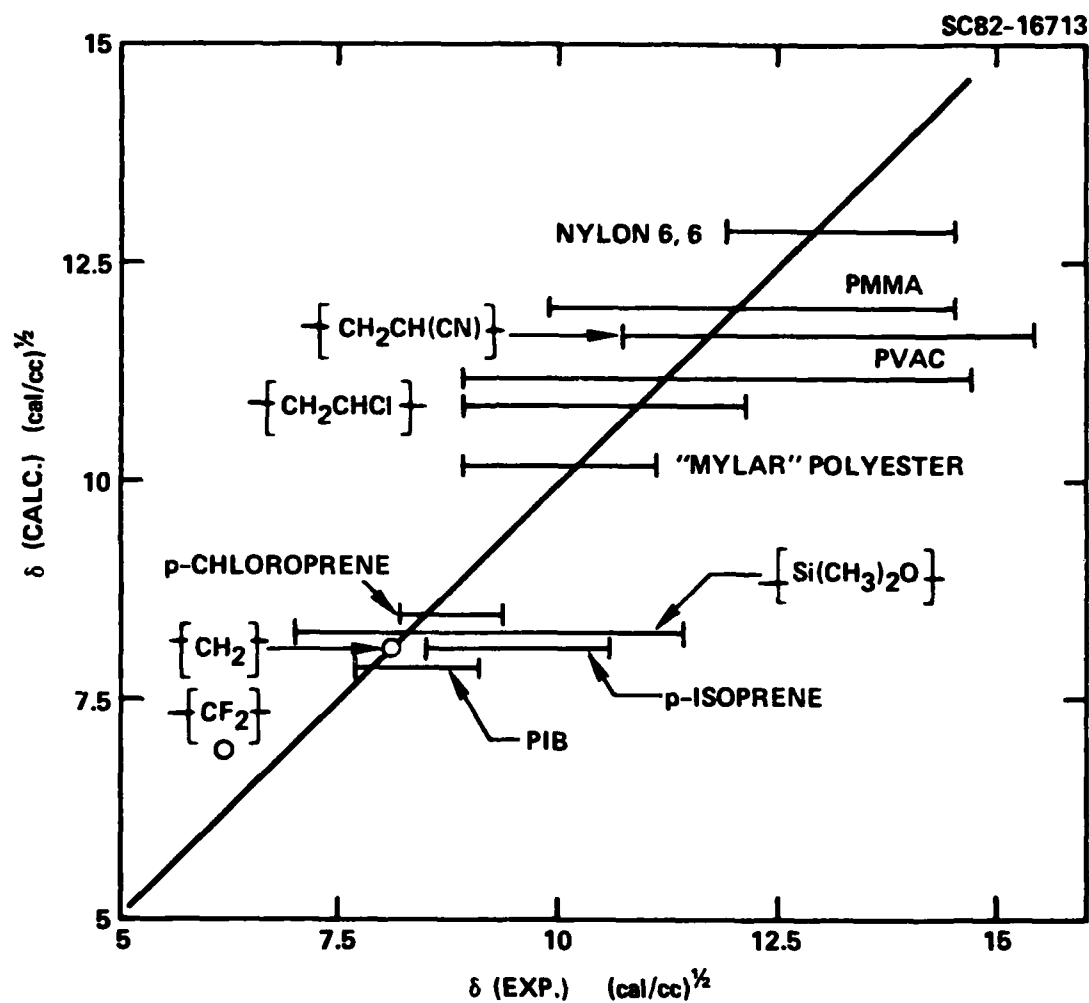


Fig. 5-7

Comparison of calculated and experimental solubility parameter (data from Refs. 9, 10).

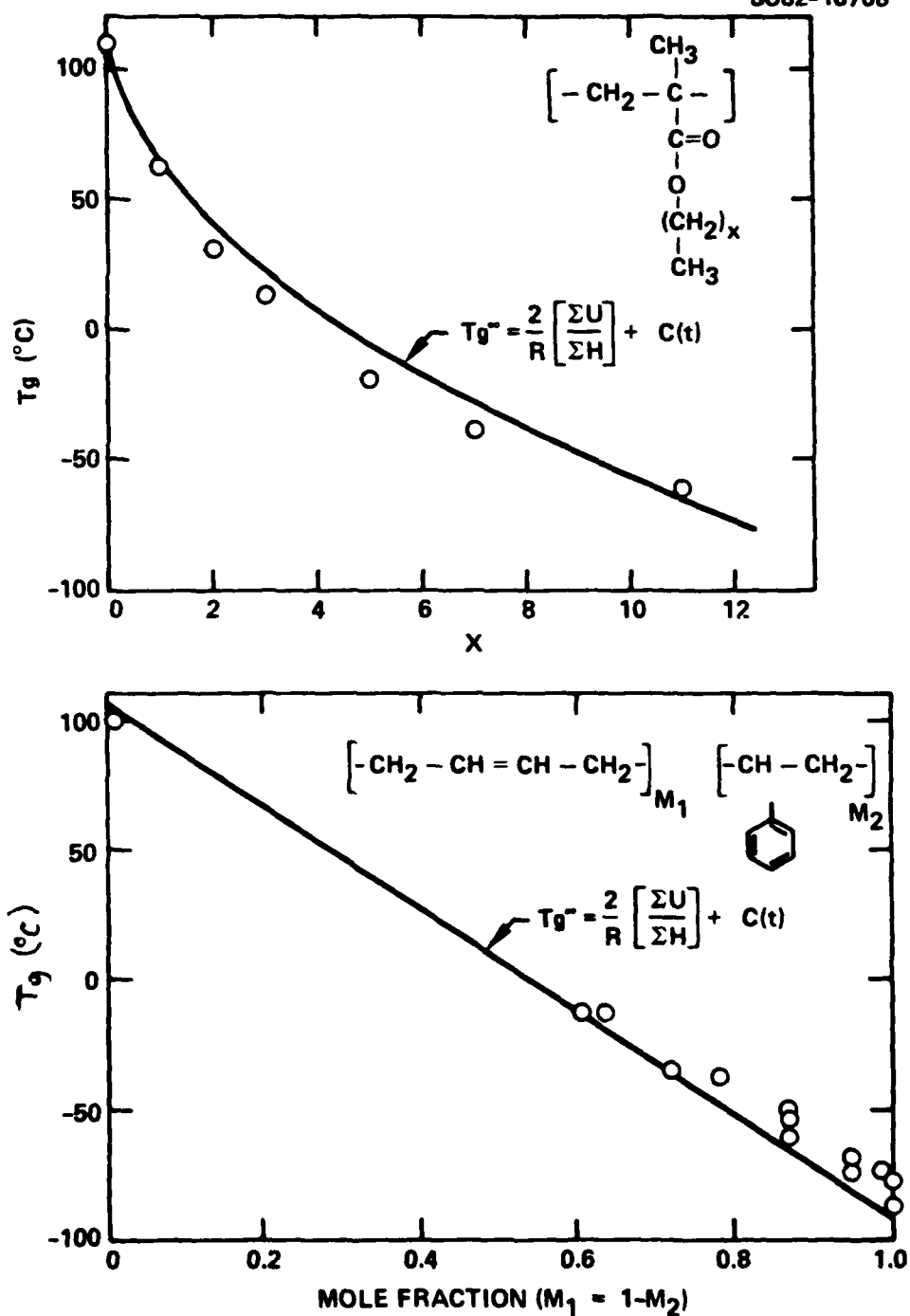


Fig. 5-8 Comparison of calculated and experimental glass temperatures for polyacrylates (upper curve) and butadiene-styrene copolymers (Refs. 11, 12).



SC82-16712

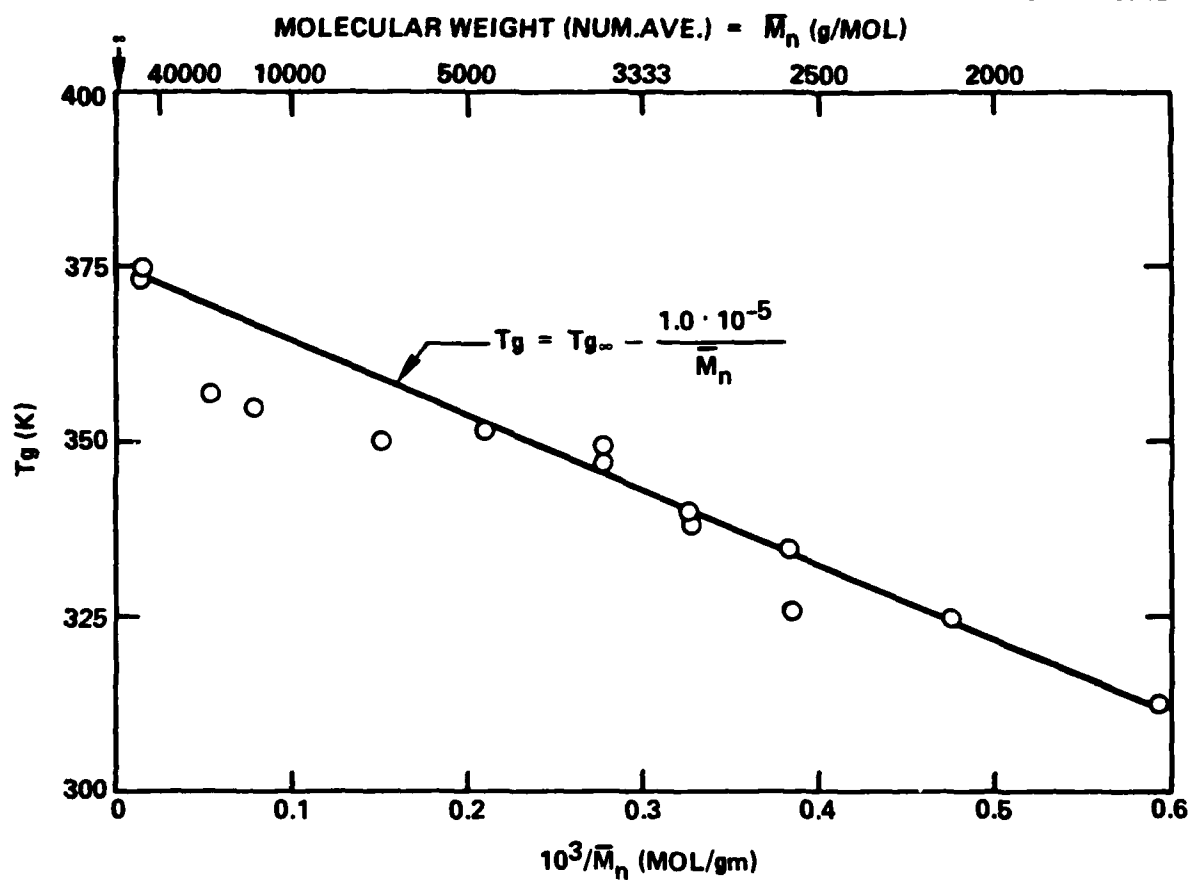


Fig. 5-9 $\bar{M}_n$ vs T_g for atactic polystyrene (data from Refs. 13, 14).

SC82-16711

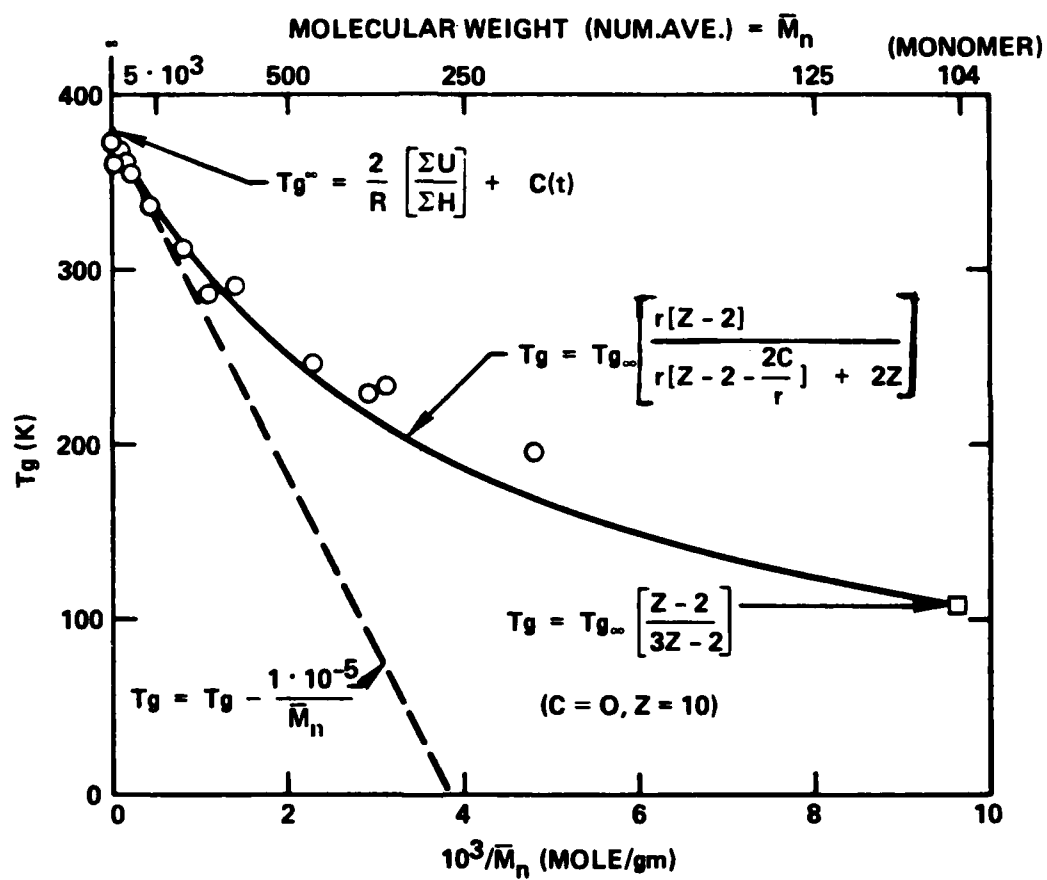


Fig. 5-10 $\bar{M}_n$ vs T_g for atactic polystyrene (data from Refs. 15, 16).



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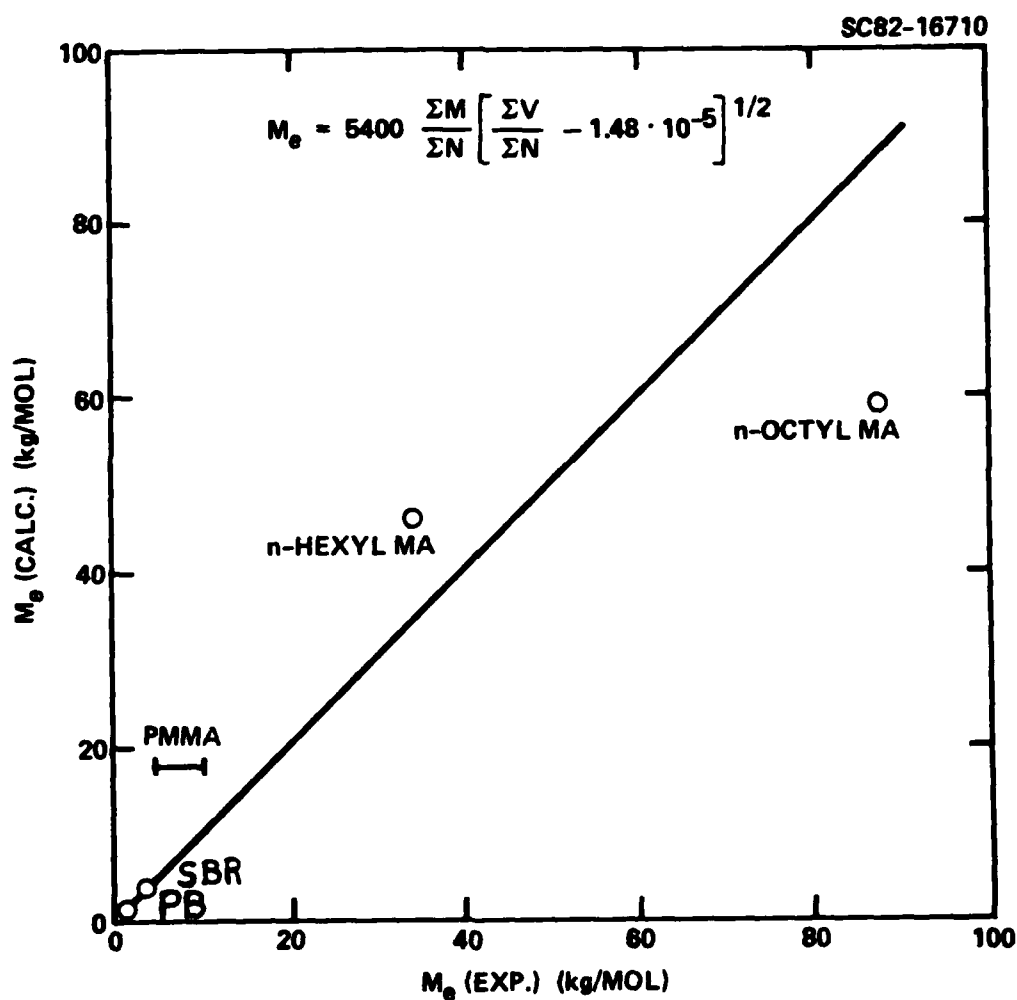


Fig. 5-11 Comparison of calculated and experimental entanglement molecular weight (data from Ref. 17).

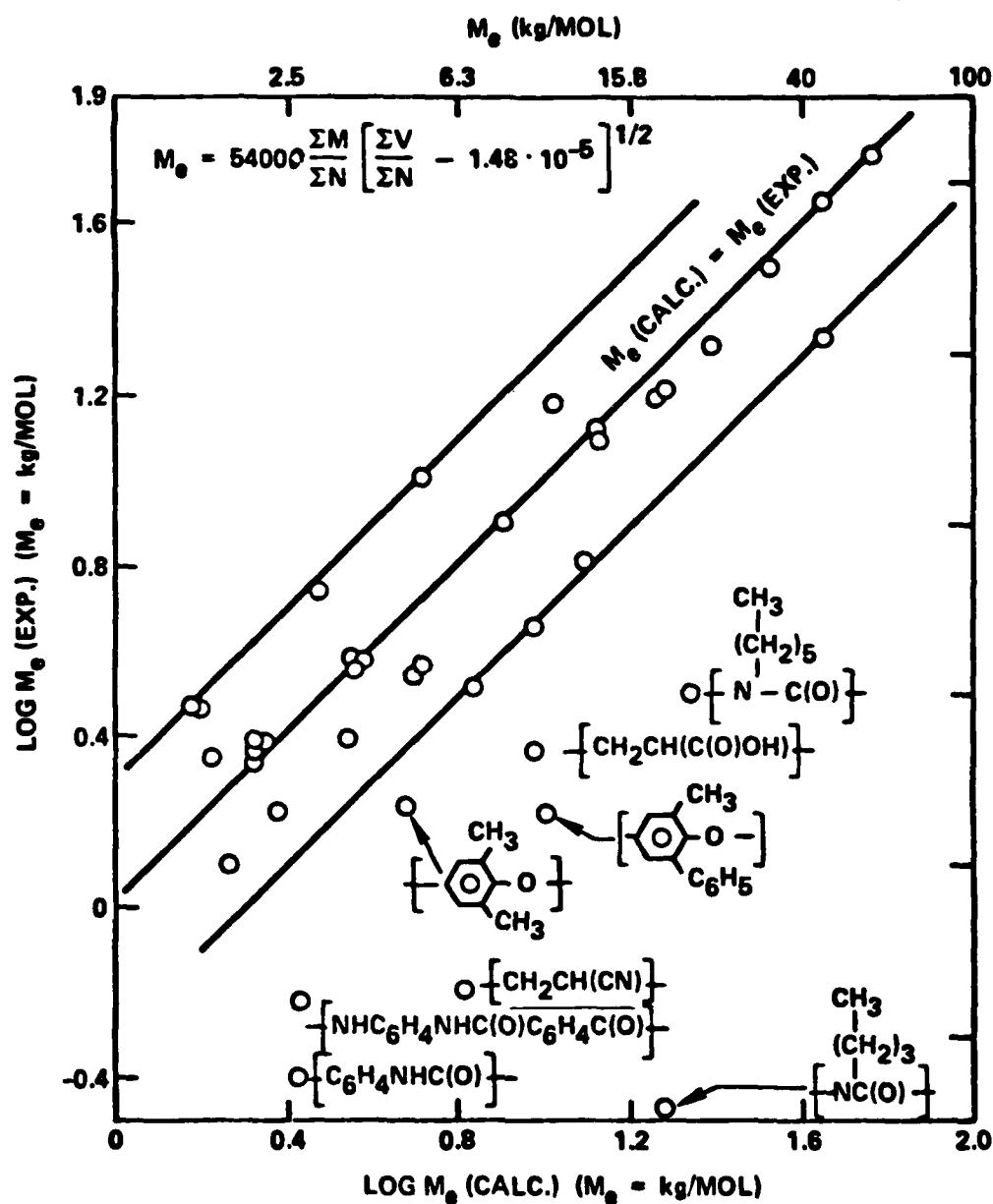


Fig. 5-12 Comparison of calculated and experimental entanglement molecular weight (data from Ref. 18).



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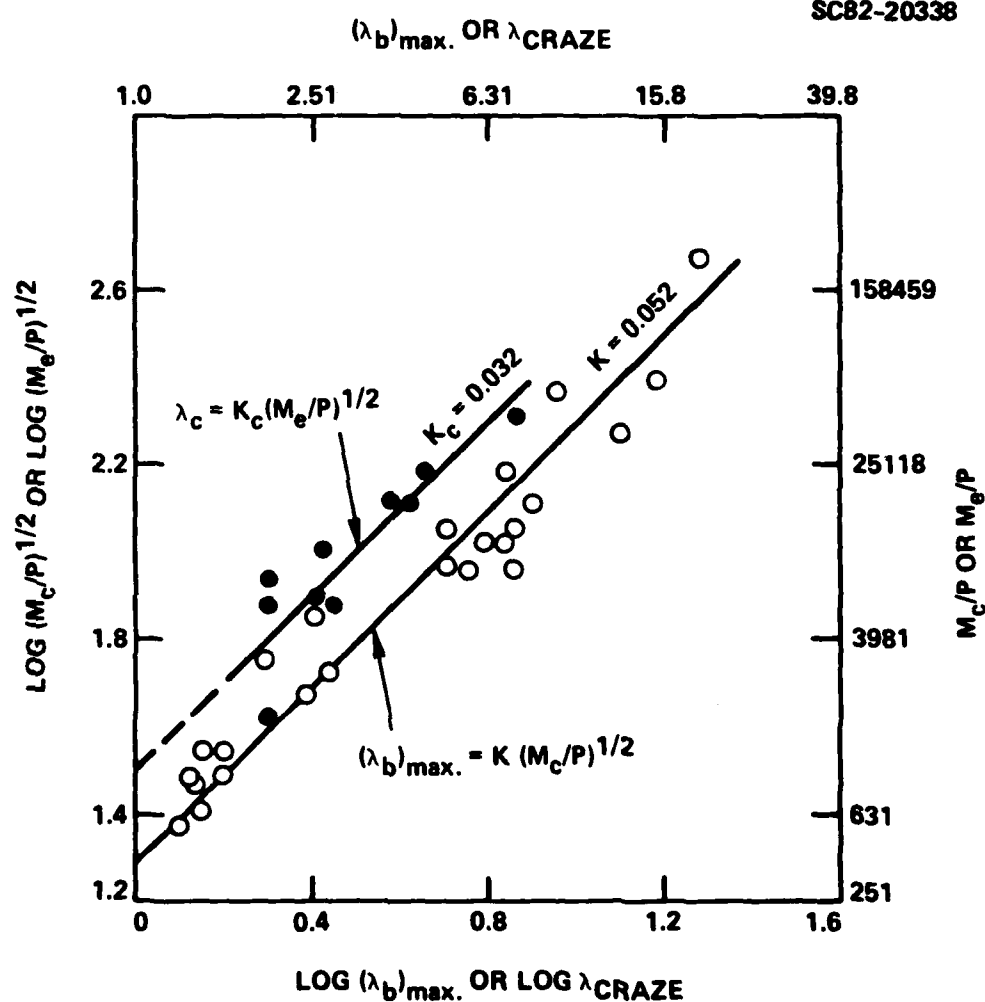


Fig. 5-13

Correlation between entanglement density (ρ/M_e) or chemical crosslink density (ρ/M_c) and maximum extension ratio λ_b or maximum craze extensibility λ_{craze} .

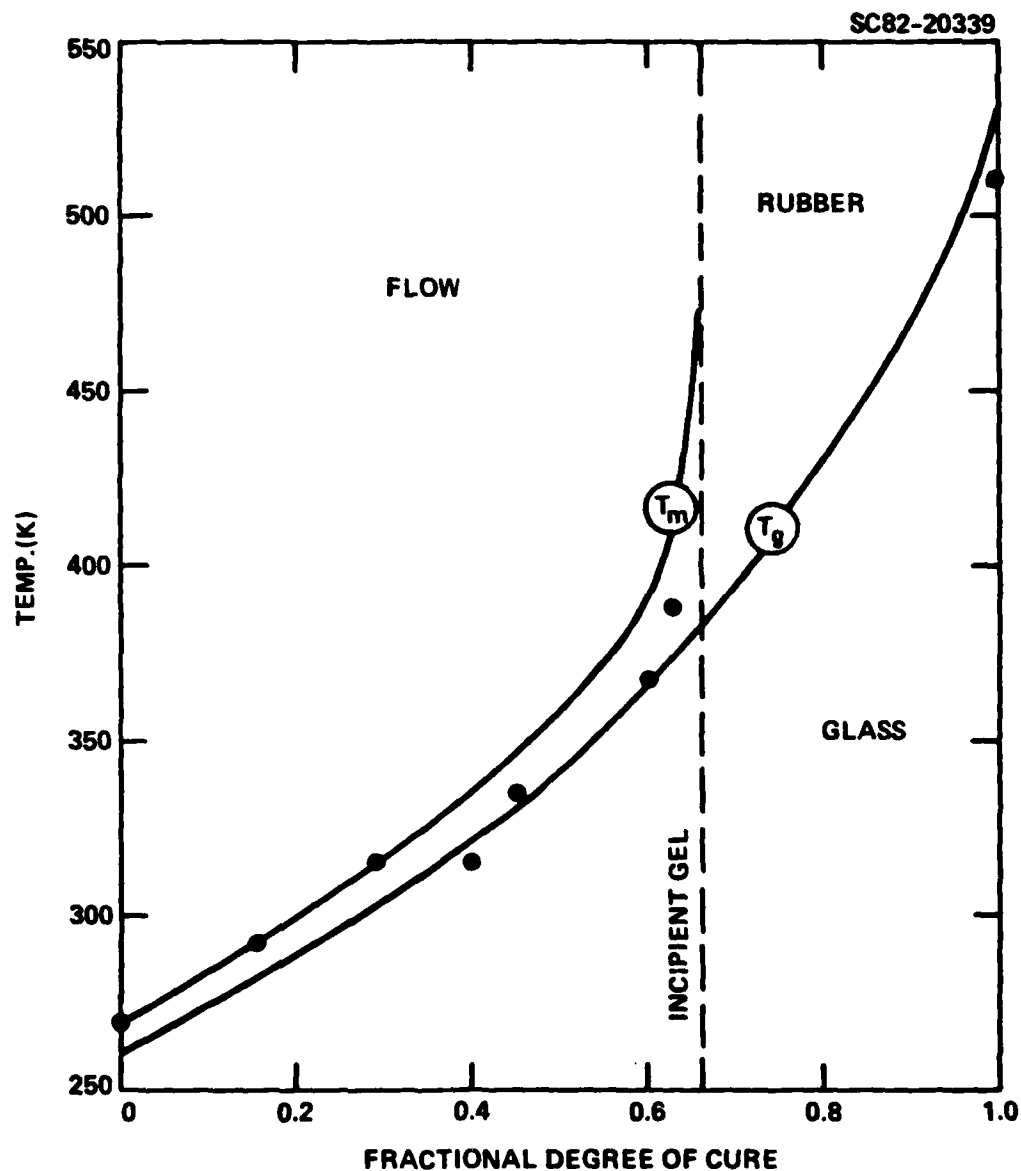


Fig. 5-14 Comparison of computed T_g and T_m curves for nonstoichiometric TGMDA/DDS (see Table 5-22) and measured T_g (X's) for Hercules 3501-5 epoxy resin (see Table 1-6 and Ref. 44).



SC82-20430

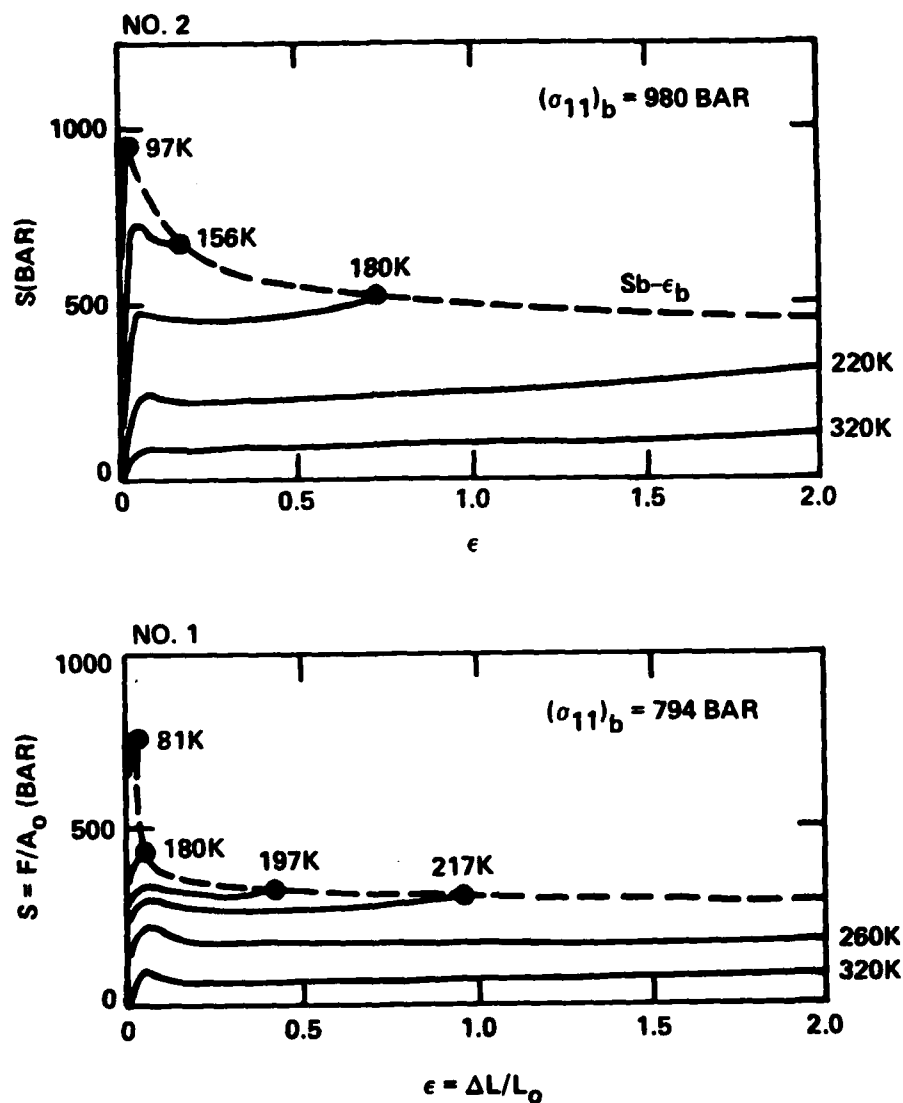


Fig. 6-1 Tensile response of C_2F_4 homopolymer (lower view) and $(C_2F_4)_{1.0} (C_3F_6)_{0.14}$ copolymer (upper view) films.

SC82-20429

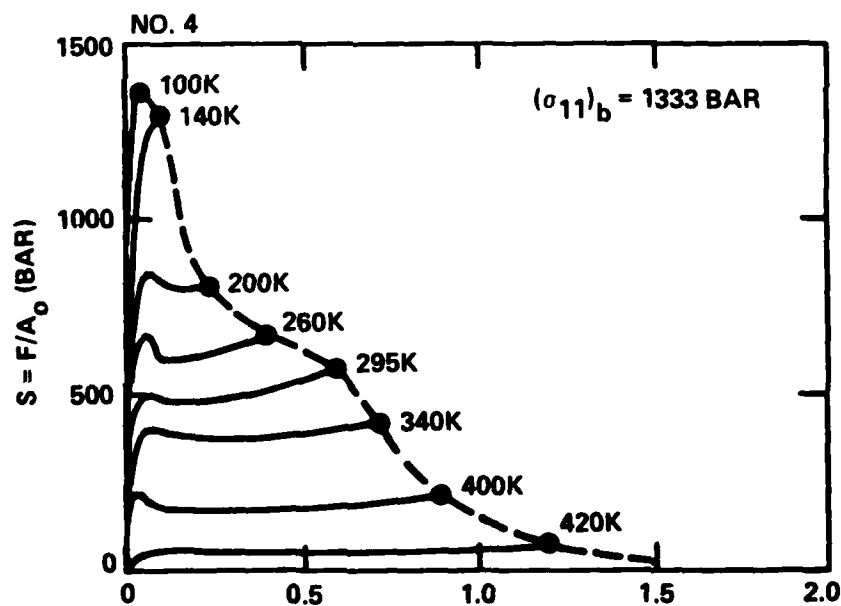
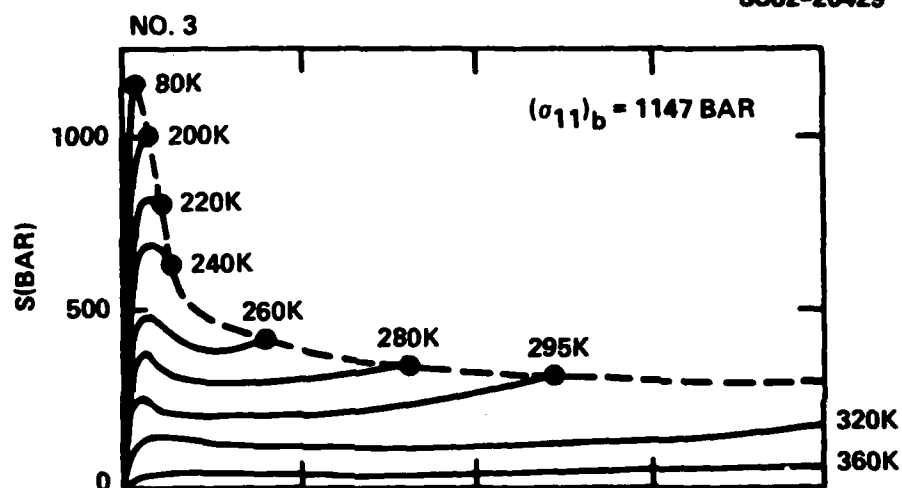


Fig. 6-2 Tensile response of $(\text{CF}_2\text{CFCL})_{1.0}(\text{CF}_2\text{CH}_2)_{0.03}$ copolymer (upper view) and polybisphenol-A carbonate (lower view) films.

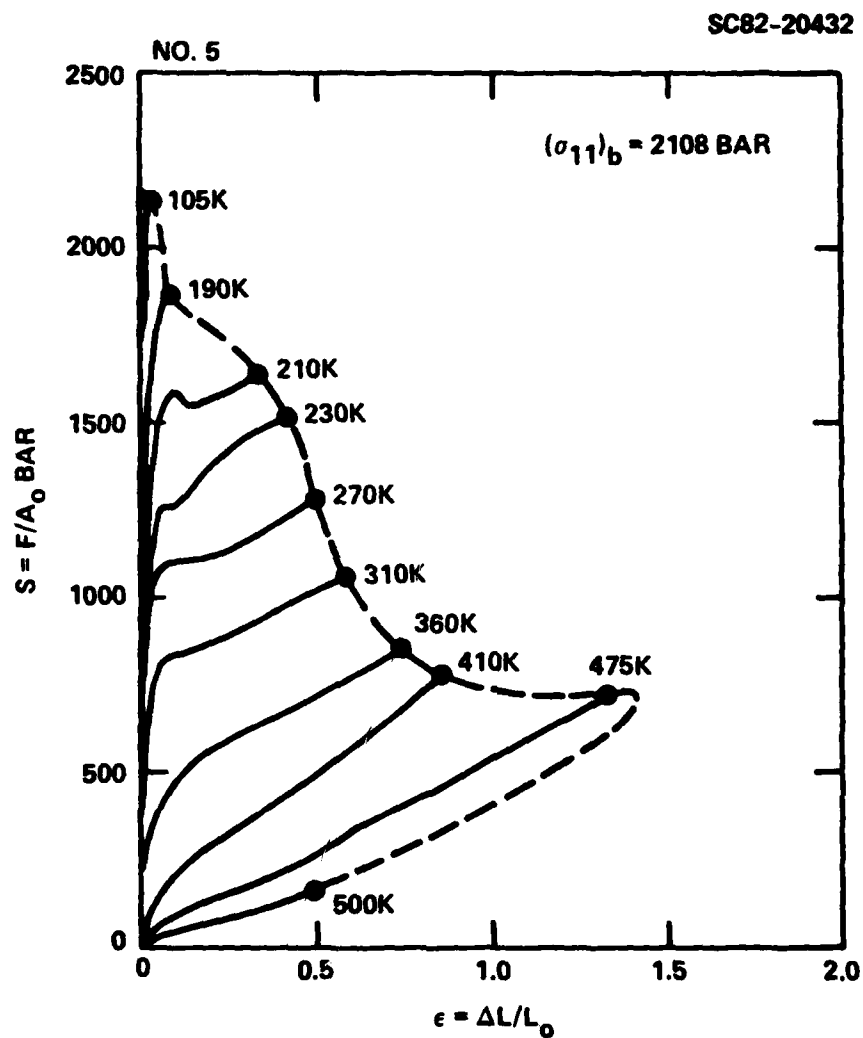


Fig. 6-3 Tensile response of polyethyleneterephthalate film.

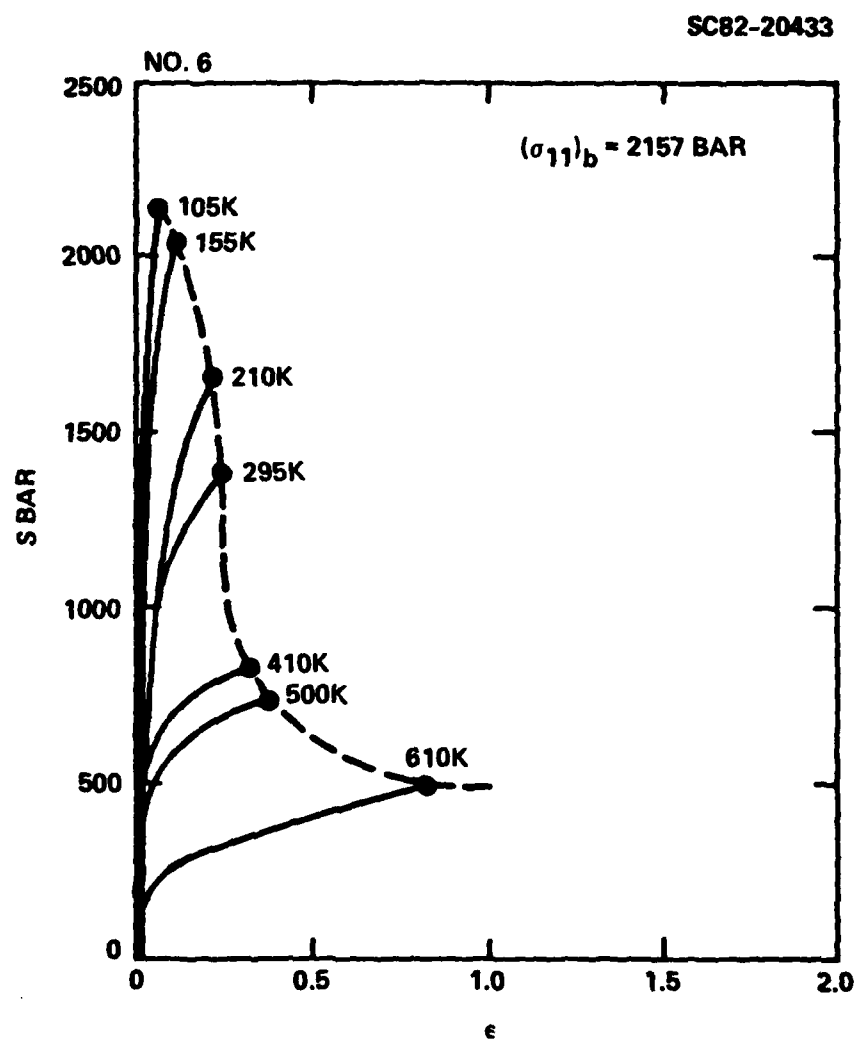


Fig. 6-4 Tensile response of $(\text{N}(\text{CO})_2 \text{C}_6\text{H}_2(\text{CO})_2\text{NC}_6\text{H}_4\text{OC}_6\text{H}_4)$ polyimide film.



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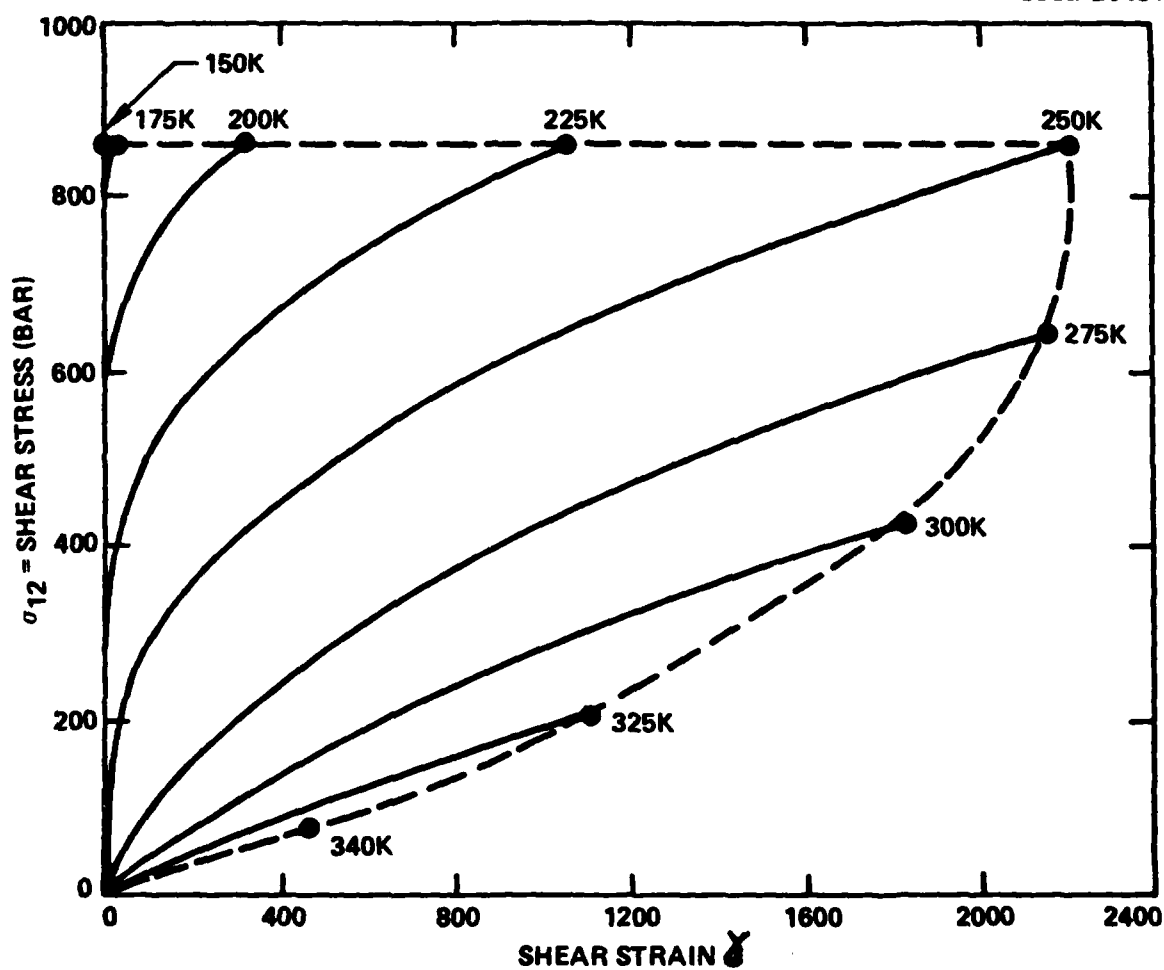


Fig. 6-5

Calculated shear stress vs strain response for equimolar isoamyl-neopentyl acrylate copolymer ($M_n = 1.03E6$ g/mol, $T_g = 230K$).

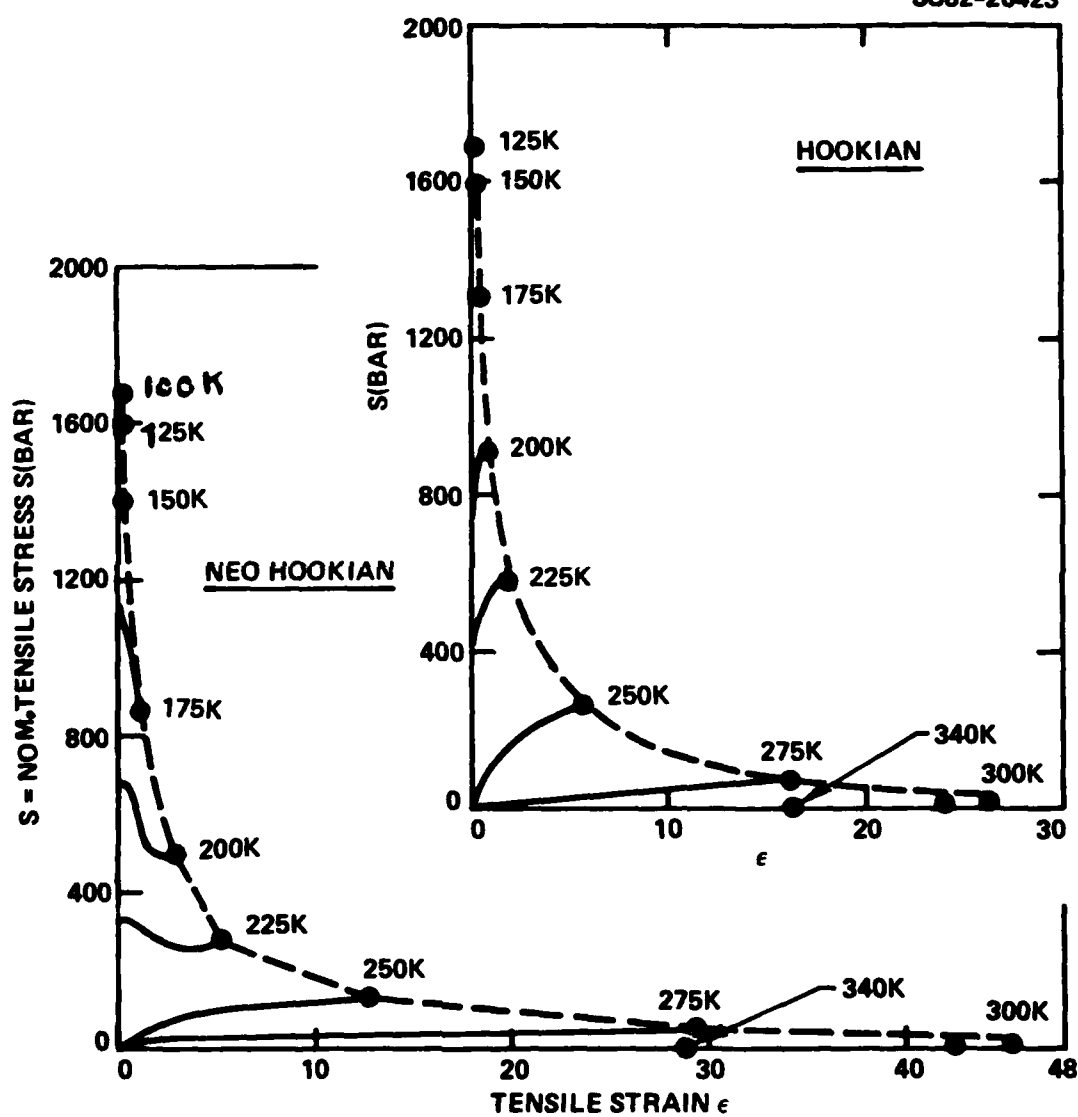


Fig. 6-6 Calculated tensile stress vs strain response for equimolar isoamyl-neopentyl acrylate copolymer ($M_n = 1.03E6$ g/mol, $T_g = 230K$).

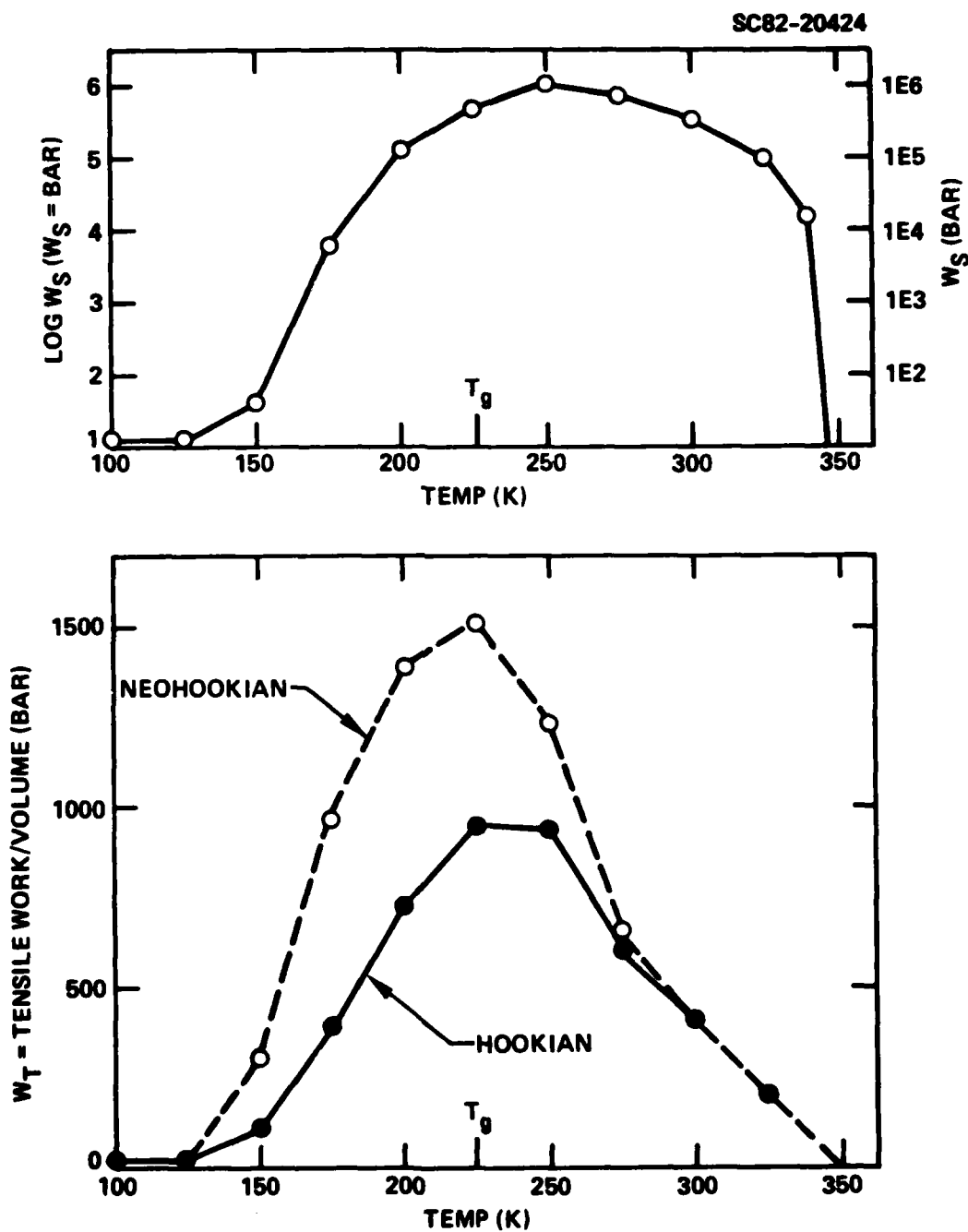


Fig. 6-7 Calculated shear (upper view) and tensile (lower view) works of deformation per unit volume.

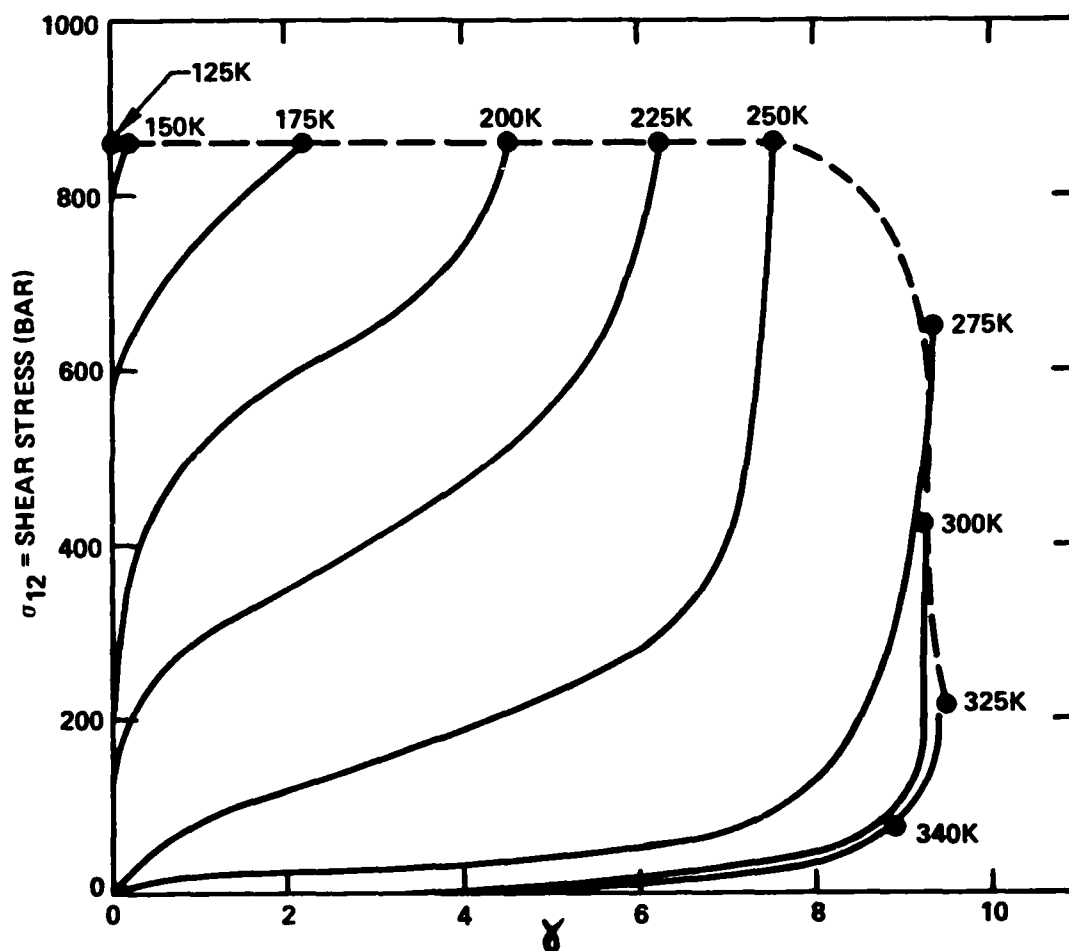


Fig. 6-8 Calculated shear stress vs strain response for equimolar isoamyl-neopentyl acrylate copolymer ($M_n = 1.03E6$ g/mol, $T_g = 230K$) with light crosslinking ($M_c = 3.42E4$ g/mol).



SC82-20428

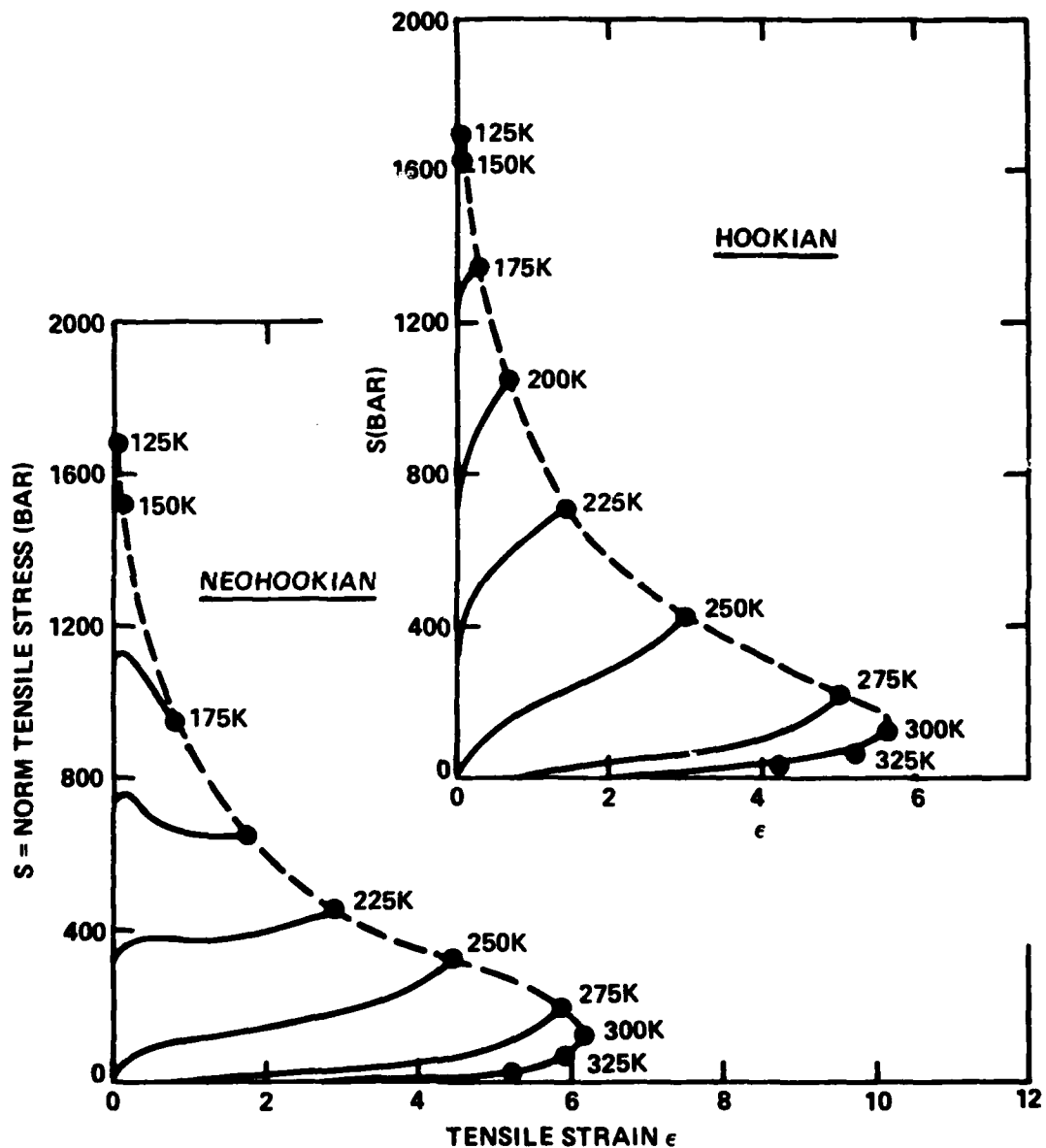


Fig. 6-9

Calculated tensile stress vs strain response for equimolar isoamyl-neopentyl copolymer ($M_n = 1.06E6$ g/mol, $T_g = 230K$) and light crosslinking ($M_c = 3.42E4$ g/mol).

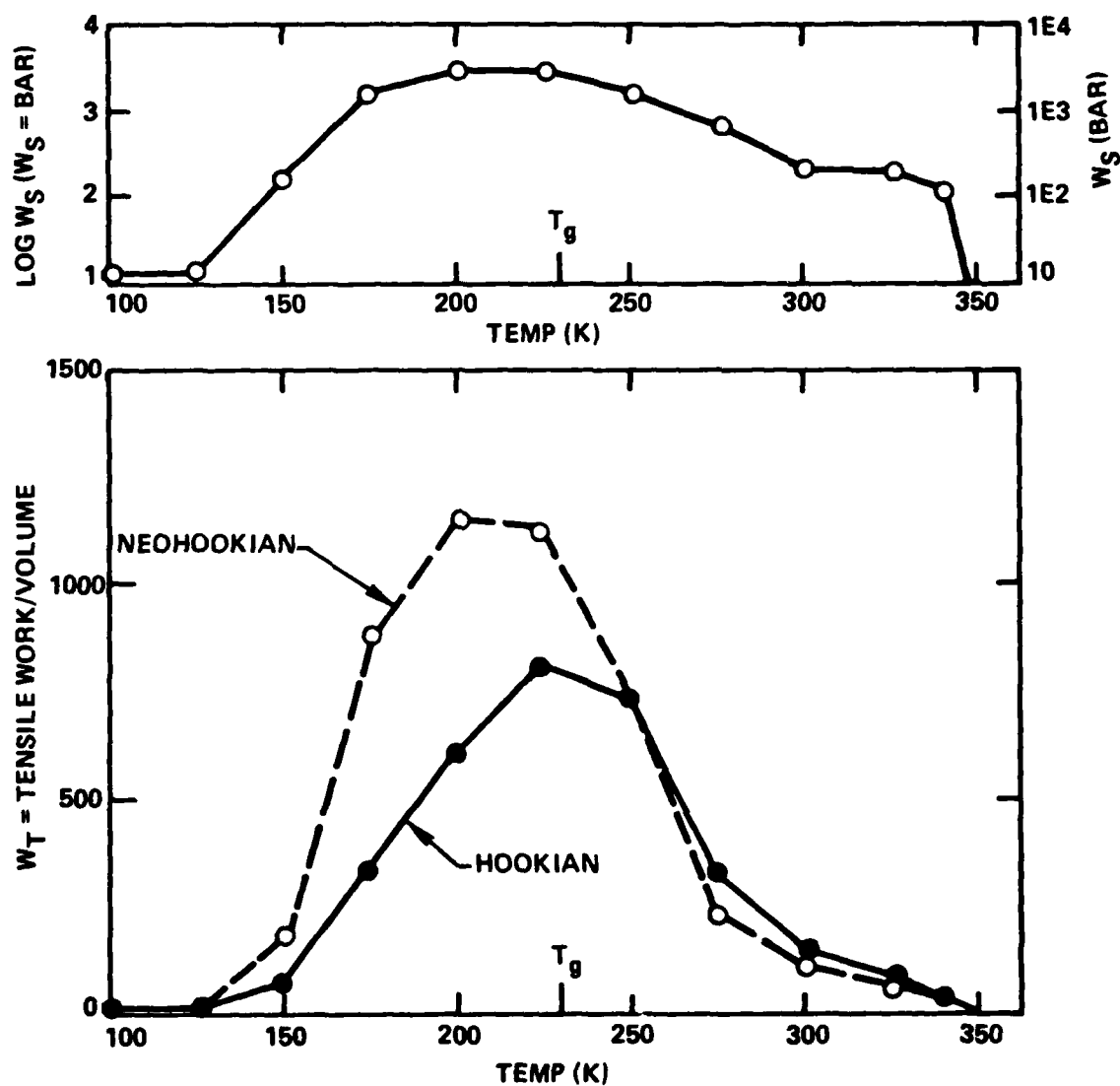


Fig. 6-10 Calculated shear (upper view) and tensile (lower view) works of deformation per unit volume.



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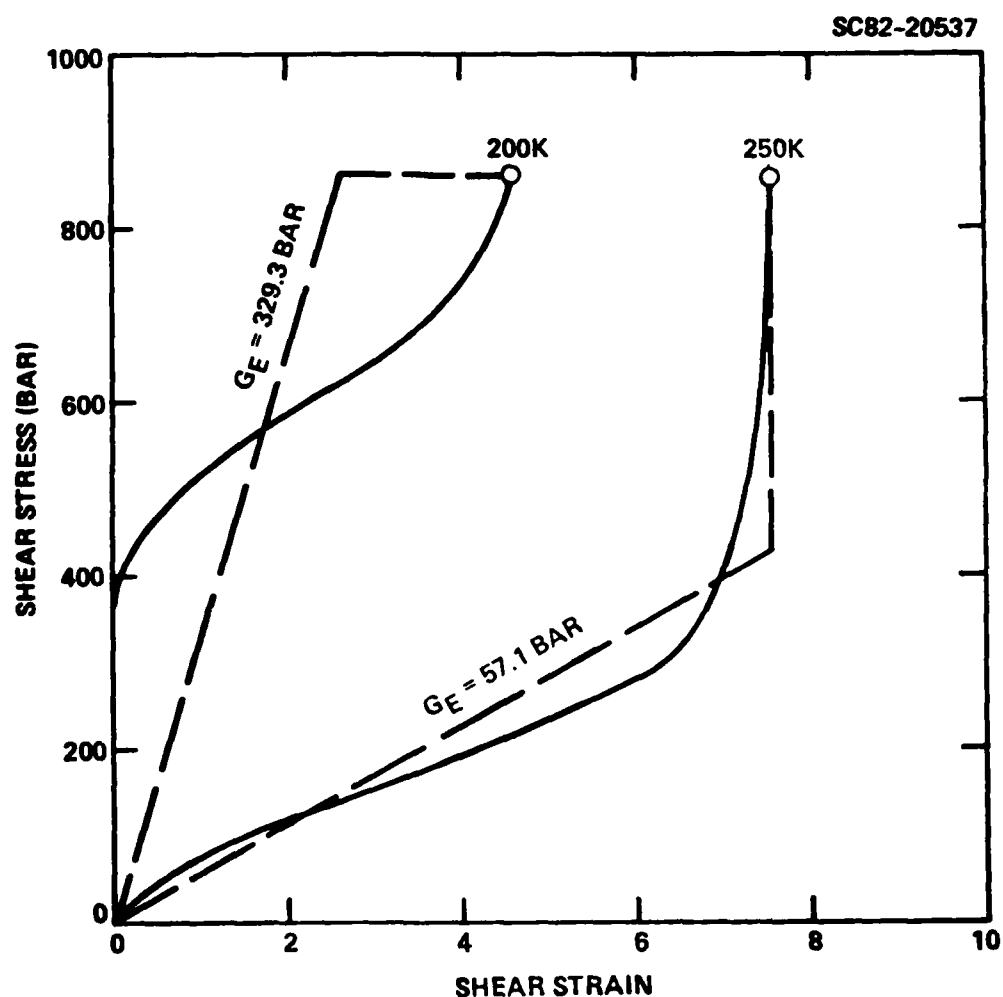


Fig. 6-11

Calculated shear stress vs strain (solid curves) response (see Fig. 6-8) and elastic-plastic analogs (dashed curves) for lightly crosslinked equimolar isoamyl-neopentyl acrylate copolymer.

SC82-24025

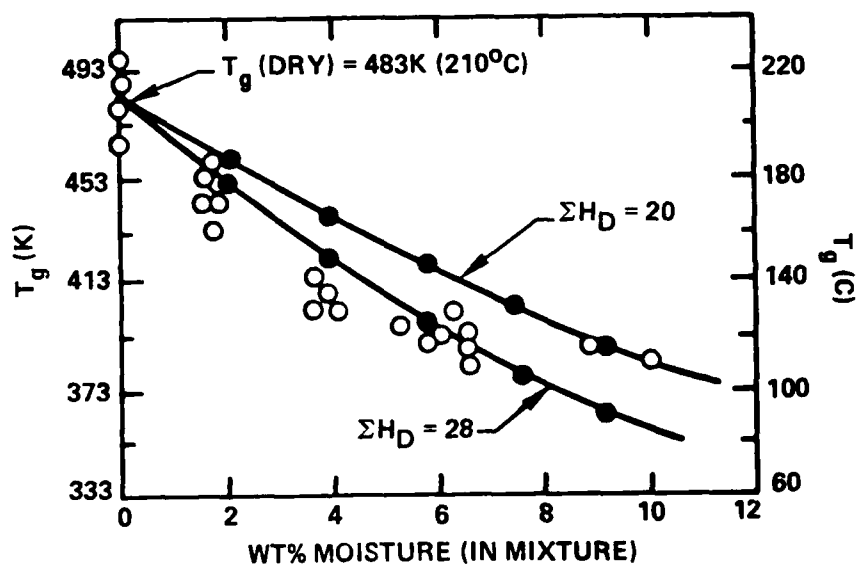


Fig. 6-12 Calculated (X) and experiment (•) effects of moisture on T_g of six cured epoxy resins (3501-5, 3501-6, 5208, 934, 3502, and NMD 2373); (for data see Ref. 6, 36).



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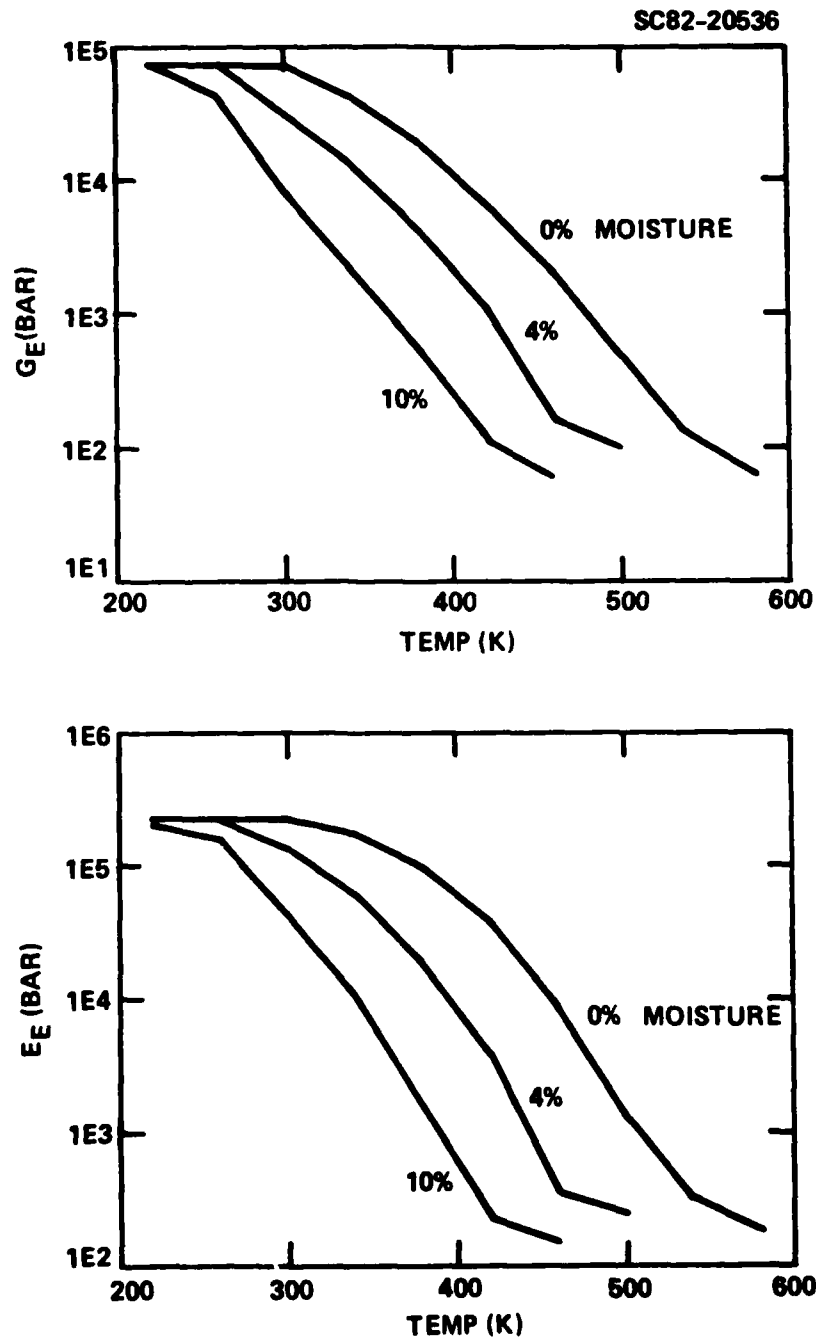


Fig. 6-13 Calculated engineering shear modulus (upper) and tensile modulus (lower curves) for cured epoxy with varied wt% moisture.

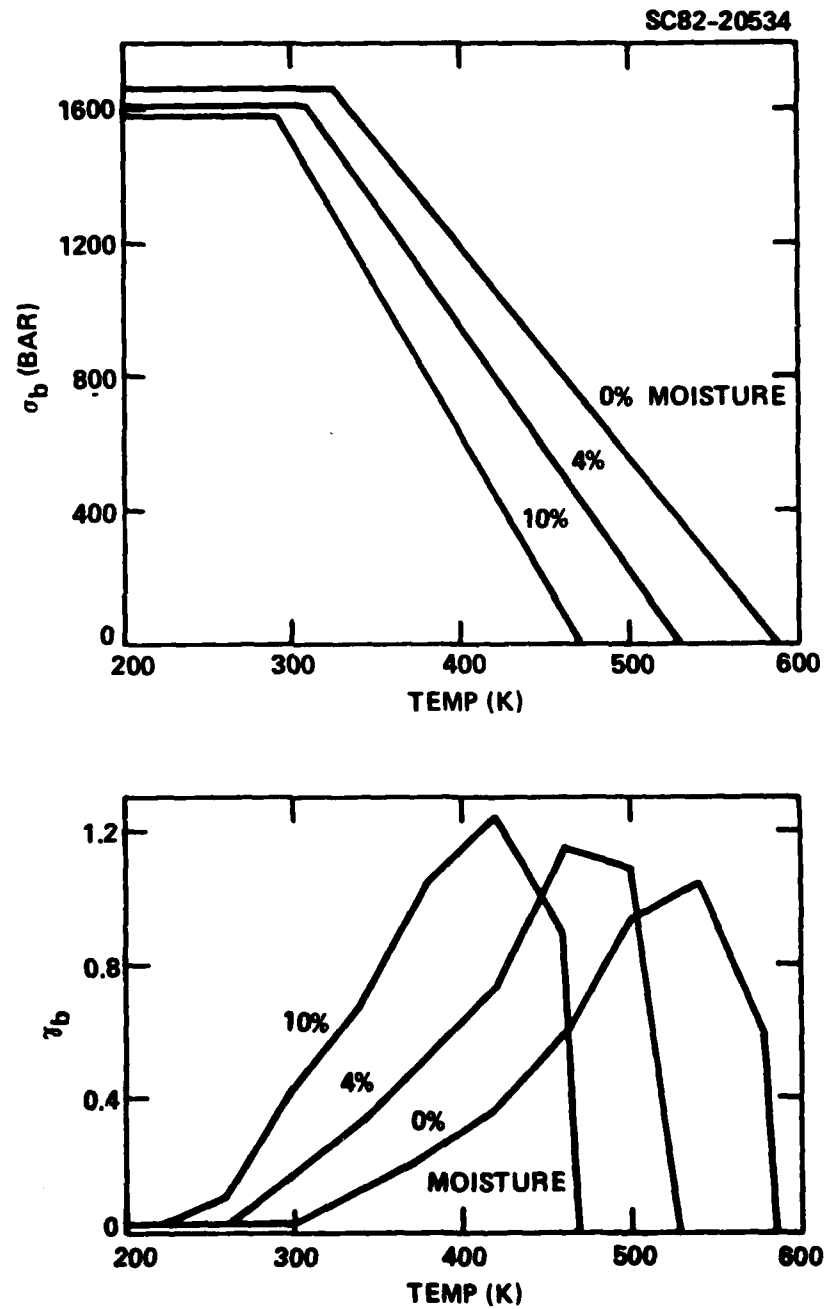


Fig. 6-14 Calculated shear strength (upper) and shear extensibility (lower curves) for cured epoxy with varied wt% moisture.

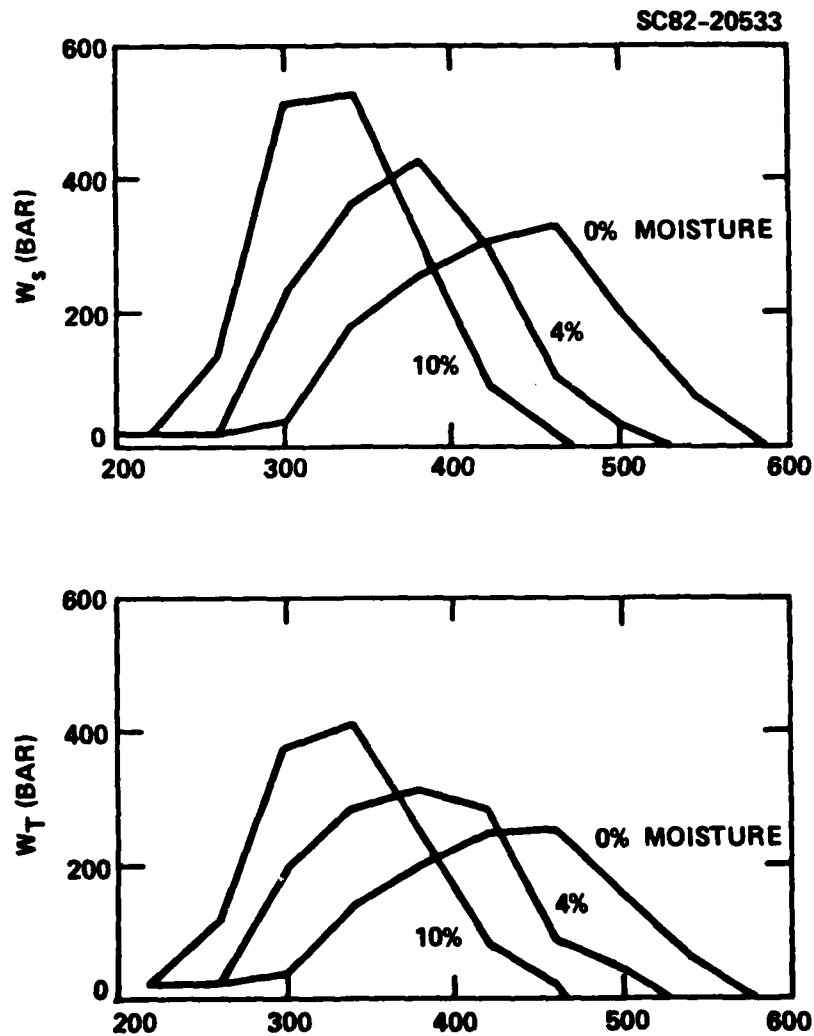


Fig. 6-15 Calculated specific fracture energy in shear (upper) and tension (lower curves) for cured epoxy with varied wt% moisture.

SC82-20532

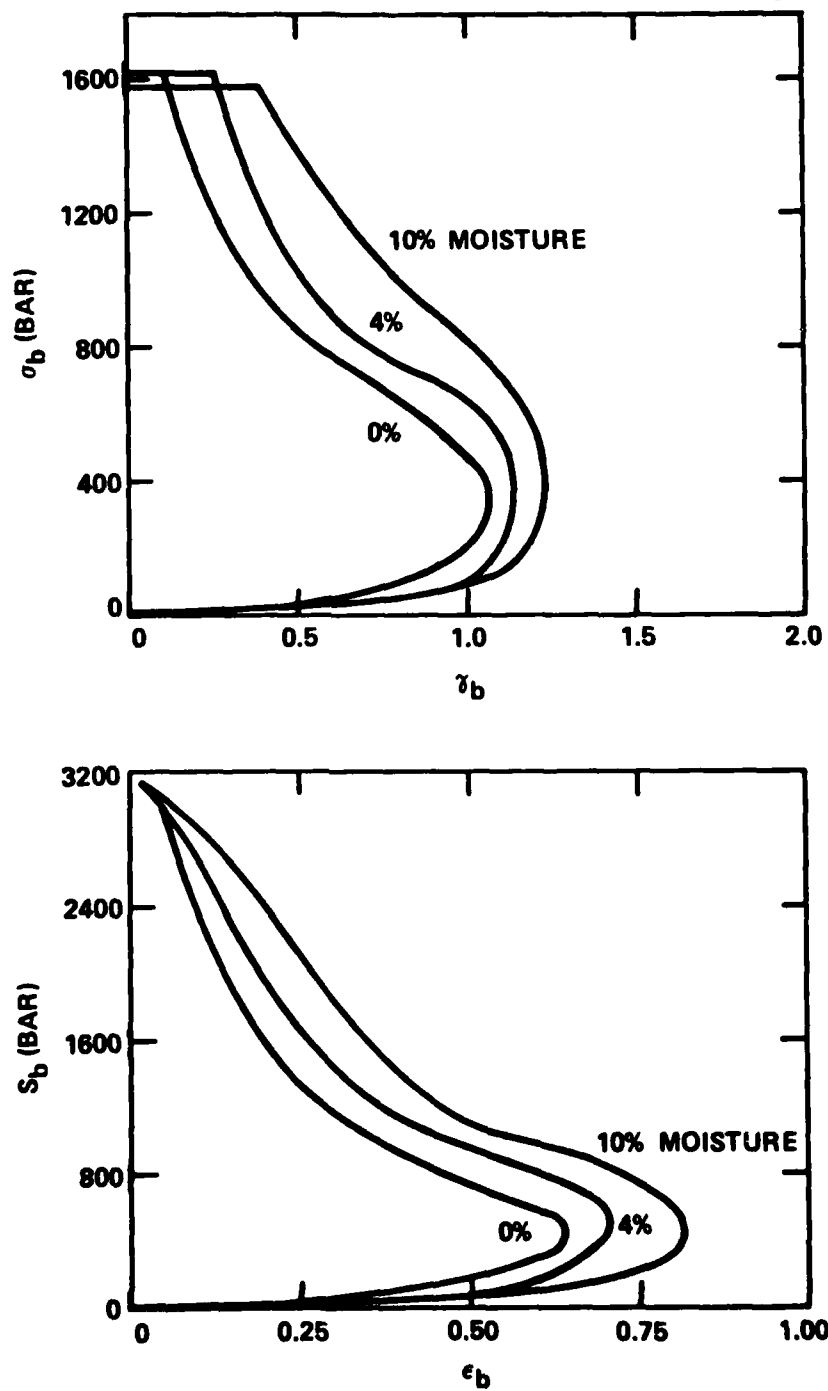


Fig. 6-16 Calculated failure envelopes in shear (upper) and tension (lower curves) for cured epoxy with varied wt% moisture.



SC83-20656

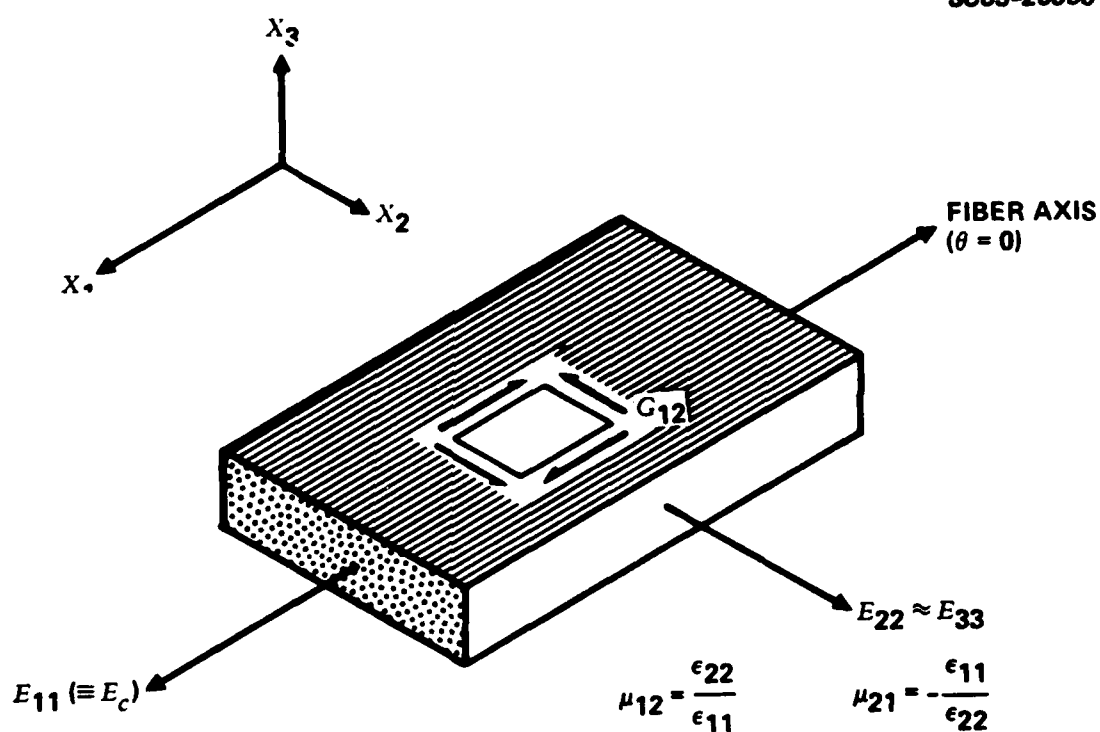


Fig. 6-17 Unidirectional reinforced composite.

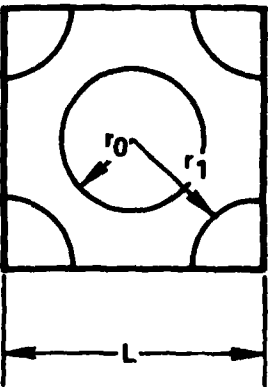
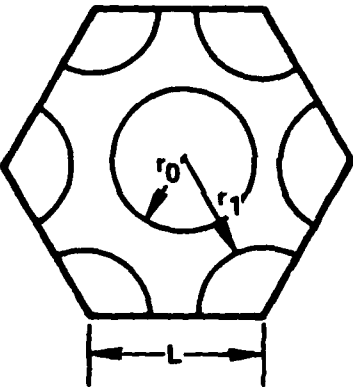
LATTICE TYPE	SQUARE	HEXAGONAL
UNIT GEOMETRY		
FIBERS/UNIT CELL	2.0	3.0
FIBER VOLUME FRACTION (ν)	$2\pi(r_0/L)^2$	$1.1548\pi(r_0/L)^2$
UNIT CELL AREA (A)	$2\pi r_0^2/\nu$	$3\pi r_0^2/\nu$
$a = (r_1 - r_0)$	$r_0[(\pi/\nu)^{1/2} - 2]$	$r_0[1.074(\pi/\nu)^{1/2} - 2]$
ν AT $(r_1 - r_0) = 0$	0.785	0.906

Fig. 6-18 Packing geometries for regular uniaxial fiber arrays.



SC83-20658

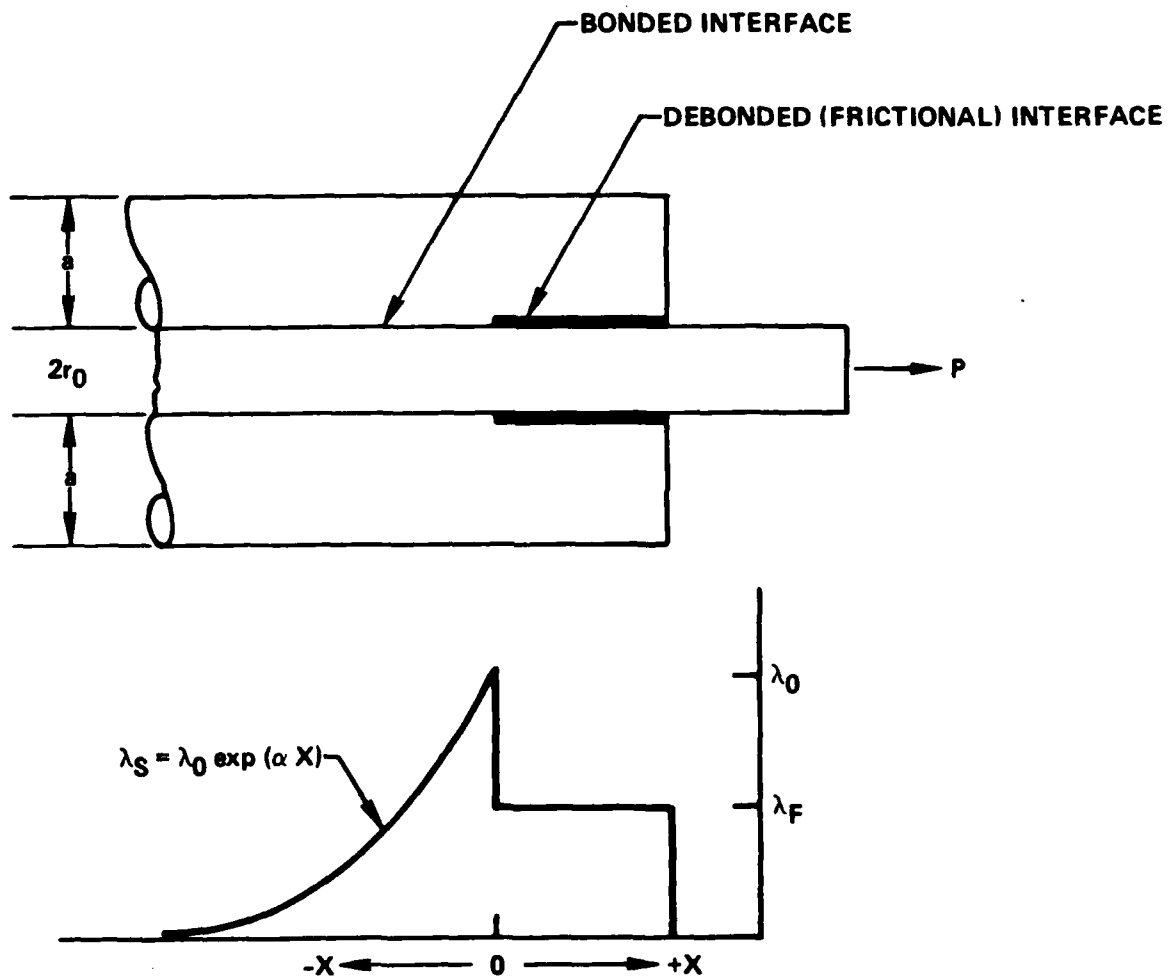


Fig. 6-19 Frictional (λ_F) and bonded (λ_S) interfacial shear stresses during fiber pull-out.

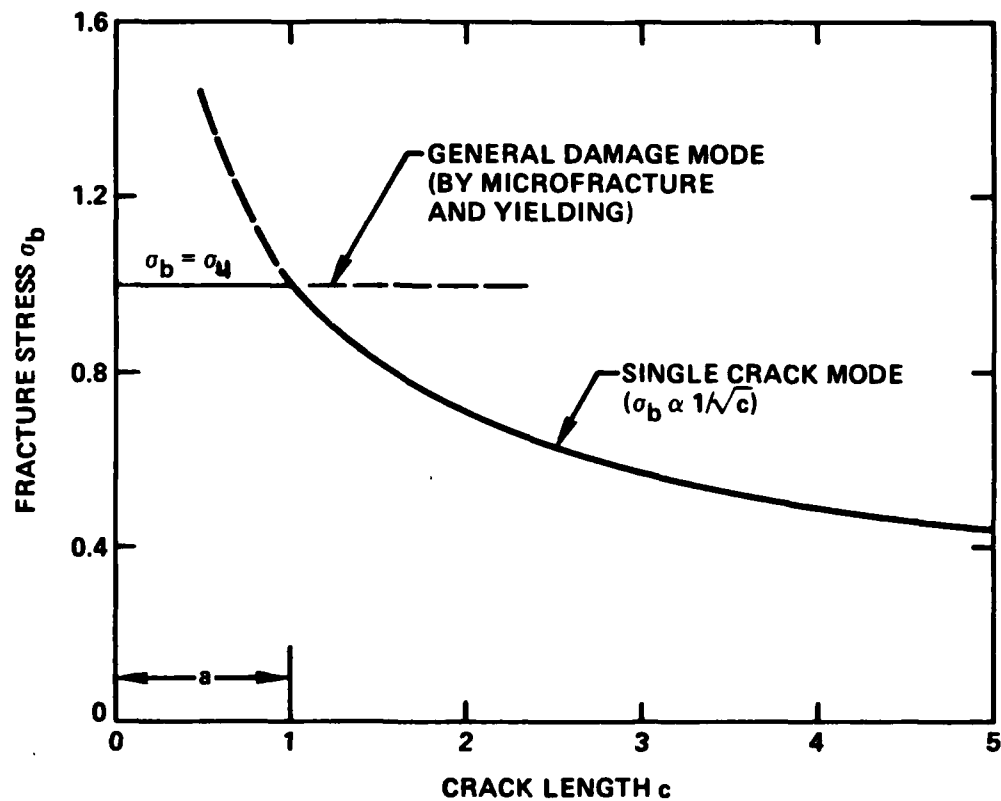


Fig. 6-20 Schematic showing the observed variation in failure mode and fracture stress σ_b with crack length c in damage tolerant composites.



SC83-20659

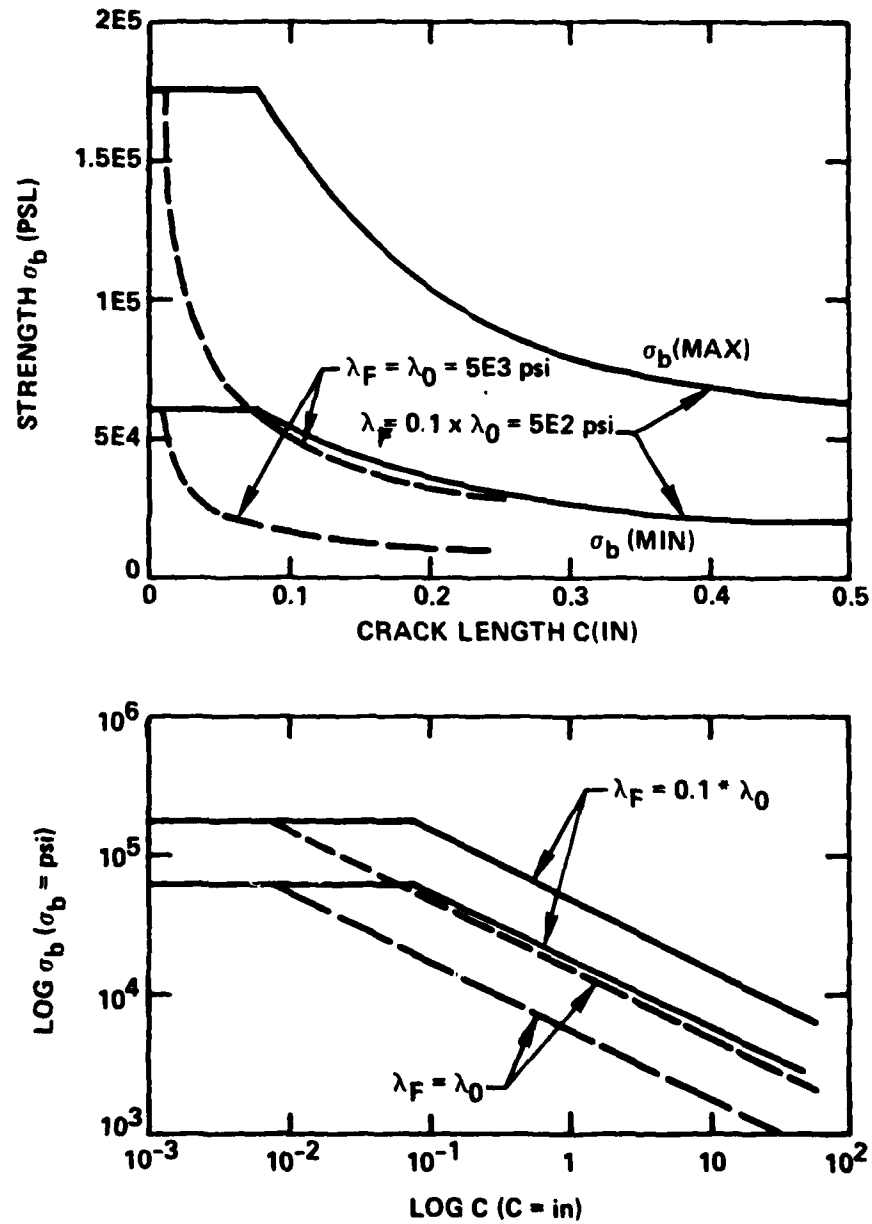


Fig. 6-21 Calculated curves of composite strength maximum σ_b (max) and minimum σ_b (min) vs crack length c.

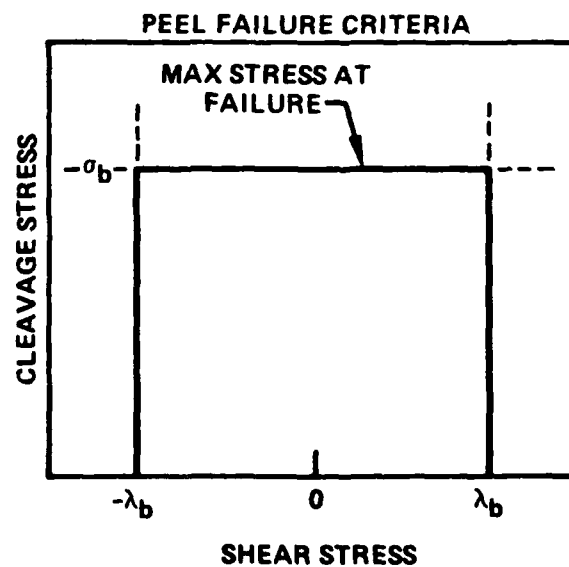
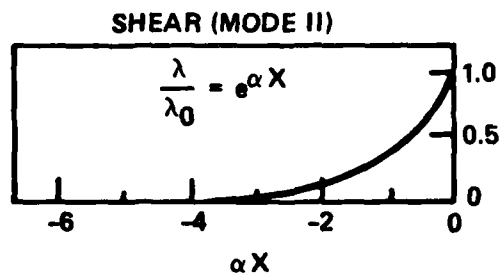
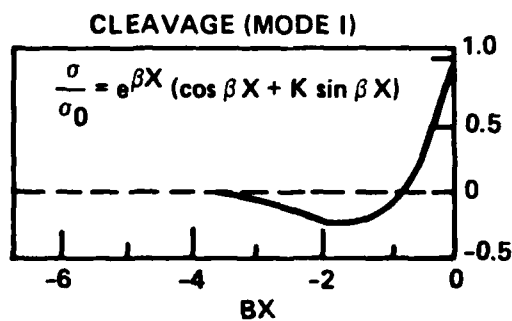
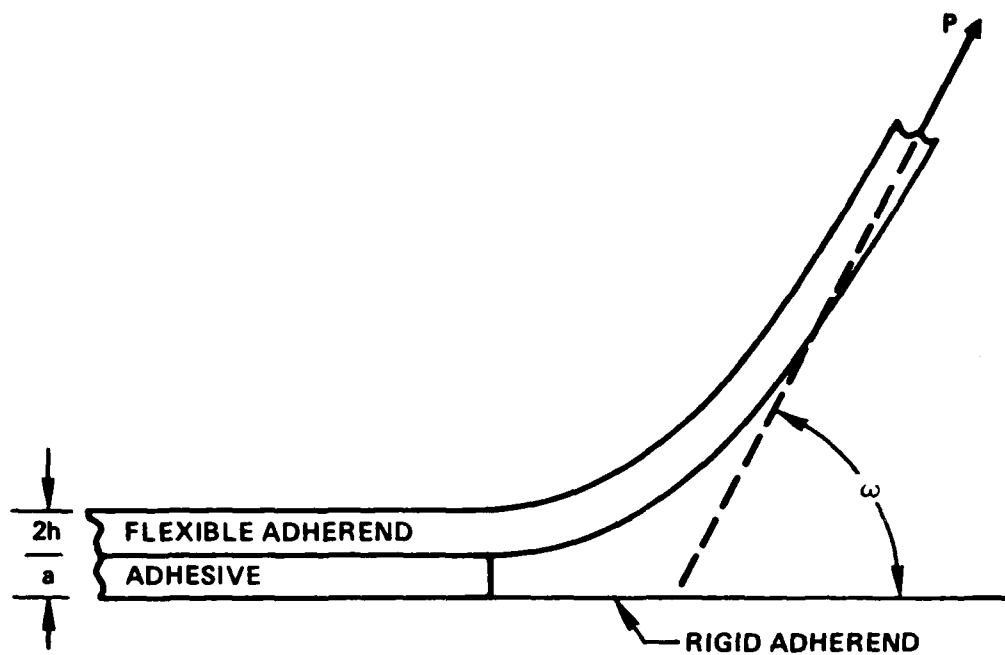


Fig. 6-22 Peel mechanics (upper and left views) and failure criteria.

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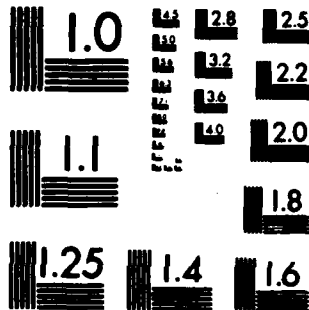
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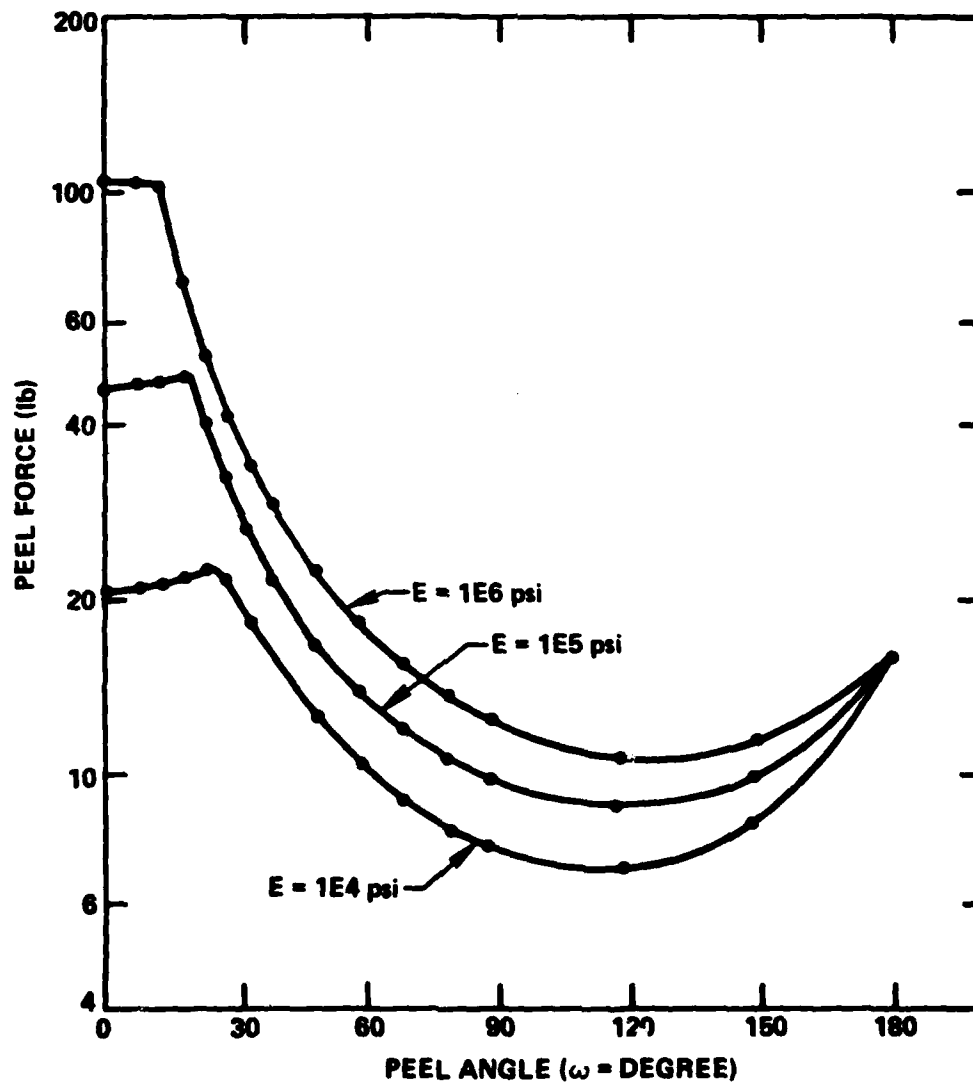


Fig. 6-23 Calculated curves of peel force P vs peel angle ω for three values of flexible adherend tensile modulus E.