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THERMOPHYSICAL AND MECHANICAL PROPERTIES OF ADVANCED CARBIDE AND NITRIDE FUELS

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THERMOPHYSICAL AND MECHANICAL PROPERTIES OF ADVANCED CARBIDE AND NITRIDE FUELS

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June 1976

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Lord Rayleigh (1874)

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INTRODUCTION

The increasing demand for electrical energy is already placing a burden on our nation's fuel resources. The continued addition of nuclear power plants to the existing power-generating systems will provide economical power into the 1980's; however, the successful introduction of breeder reactors into utility generating systems is necessary if an adequate supply of fuel and a reasonable cost of electricity are to be maintained. The first-generation breeder reactors, which will not be introduced on a commercial basis before the mid-1980's, are powered with mixed oxide fuels. Continuing breeder-reactor research has shown, however, that fuels other than oxides may provide improved performance, and alternative fuel systems are being considered for the long term. Among the most promising of these are the carbides and nitrides of uranium and plutonium. In addition to possessing neutronic properties more conducive to breeding, these compounds have thermal conductivities that are about five times that of the mixed oxide. The high thermal conductivities permit operation of fuel pins at higher linear power ratings and allow design flexibility to optimize breeding performance, fabrication cost, and fissile-material inventory. These attractive features have resulted in a renewed interest in the development of carbide and nitride fuels.

In support of the national effort to develop advanced carbide and nitride breeder-reactor fuels, this handbook of Thermophysical and Mechanical Properties of Advanced Carbide and Nitride Fuels is being compiled for use as a common, authoritative source of data. Because research in the area of thermophysical and mechanical properties is an on-going effort, this handbook must be continuously updated in order to provide readily usable data to all participants in the advanced carbide/nitride fuel program. A handbook that reflects a consensus of workers in the field has several advantages. Firstly, it provides a breadth and depth of information not available in a document compiled by a single organization. Overlapping requirements and data needs of various activities can be met in a single document which is continuously revised. Secondly, the handbook provides a consistent set of data for use throughout the national advanced carbide/nitride fuel program, a consideration that is especially important where only limited data exist. Finally, by the use of a single handbook, deficiencies in the thermophysical and mechanical properties data for advanced carbide and nitride fuels can be readily identified and corrected by additional experimental effort. In this manner, this handbook will provide a broad base of experience in fuel-properties data to support the national effort on the development of advanced carbide and nitride reactor fuels.

Initially, this handbook comprises thermophysical and mechanical properties data for UC, PuC, (U,Pu)C, UN, PuN, and (U,Pu)N. Data for the sesqui- and di-carbides and sesqui- and dinitrides as well as data for carbo-nitrides will be added later.

Each compound is listed in a separate section containing a list of recommended values (in SI units) for each property. References to literature data will accompany each recommended value so that the reader can easily consult the original work. For each compound, the properties are divided into five sections and arranged alphabetically within each section.

The section headings and properties in each section are given below.

A. Physical

Critical constants
Density
Emissivity
Lattice constants
Melting point
Surface tension
Thermal expansion

B. Thermodynamic

Compressibility
Enthalpy
Entropy
Free energy of formation
Heat capacity
Heat of formation
Heat of fusion
Heat of sublimation
Heat of vaporization
Vapor pressure

C. Mechanical

Creep
Elastic constants
Fraction stress
Hardness
Stress relaxation
Thermal shock
Yield stress
Young's modulus

D. Transport

Diffusion
Electrical conductivity
Grain growth
Seebeck coefficient
Thermal conductivity
Thermal diffusivity
Viscosity

E. Chemical

Compatibility with cladding
Kinetics
Phase equilibria

Work on this handbook began with the preparation of a bibliography of properties data (the first entry in the list given below) on carbides, nitrides, carbonitrides, oxycarbides, and oxynitrides of uranium, plutonium, and mixed

uranium-plutonium compounds. Literature references were sought in Nuclear Science Abstracts and Chemical Abstracts. The bibliography contained 743 entries and included literature through September 1974. Selected values for properties data have been updated since then by means of formal and informal contacts with researchers in the properties field. Work leading to the information contained in this handbook continued with the issuance of critical reviews of the chemical, mechanical and thermodynamic properties of UC, U_2C_3, PuC, Pu_2C_3, (U,Pu)C, $(U,Pu)_2C_3$, UN, U_2N_3, PuN, and (U,Pu)N. The critical reviews listed below represent the efforts of staff personnel from Argonne National Laboratory, Battelle Columbus Laboratories, and Los Alamos Scientific Laboratory. The critical reviews contain references, discussions and comparisons of experimental techniques and data, and the rationale and method of analysis used in establishing the recommended thermophysical and mechanical properties values that now appear in this handbook. The bibliography and critical reviews are as follows:

ANL/CEN/AF-100
Bibliography of Properties Data on Actinide Carbides and Nitrides
A. Sheth, S. D. Gabelnick, M. S. Foster, M. G. Chasanov, and C. E. Johnson (September 1974)

ANL-AFP-2
Equation of State for Advanced Fuels
A. Sheth and L. Leibowitz (October 1974)

ANL-AFP-3
Thermal Conductivity Values for Advanced Fuels
A. Sheth and L. Leibowitz (November 1974)

ANL-AFP-7
Elastic, Diffusional, and Mechanical Properties of Carbide and Nitride Nuclear Fuels
J. L. Routhbort and R. N. Singh (March 1975)

ANL-AFP-8
Review of the Thermodynamics of the U-C, Pu-C, and U-Pu-C Systems
M. Tetenbaum (ANL), A. Sheth (ANL), and W. Olson (LASL) (June 1975)

ANL-AFP-9
Chemical Compatibility Between Cladding Alloys and Advanced Fuels
D. C. Fee and C. E. Johnson (May 1975)

ANL-AFP-10
Phase Equilibria and Melting Point Data for Advanced Fuel Systems
D. C. Fee and C. E. Johnson (June 1975)

ANL-AFP-11
Equation of State and Transport Properties of Uranium and Plutonium Carbides in the Liquid Region
A. Sheth and L. Leibowitz (September 1975)

ANL-AFP-12
Equation of State and Transport Properties of Uranium and Plutonium Nitrides in the Liquid Region
A. Sheth and L. Leibowitz (October 1975)

BMI-X-659
Thermodynamic and Transport Characteristics of Actinide Nitride Fuels
C. A. Alexander, J. S. Ogden, M. P. Rausch (June 1975)

LA-6037-MS
Review of Thermal Expansion and Density of Uranium and Plutonium Carbides
J. F. Andrew and T. W. Latimer (July 1975)

LA-6096
Electrical and Thermal Transport Properties of Uranium and Plutonium Carbides: A Review of the Literature
H. D. Lewis and J. F. Kerrisk (March 1976)

The data-compilation effort is an on-going activity. The open literature is constantly being reviewed for relevant properties data and, as these data become available, revised pages will be issued for insertion into this handbook. To facilitate revision, each page of the handbook is dated when it is prepared for publication.

June 1976 Carl E. Johnson

A. Physical

A-1 CRITICAL CONSTANTS

Critical temperature (estimated) - 9750 K [A-1]

A-2 DENSITY

$^{238}UC_{1.0}$ 293 K $13.61 \pm 0.01 \times 10^3$ kg/m^3 [A-2]

$$\rho = 1.3726 \times 10^4 - 3.873 \times 10^{-1}\ T - 3.783 \times 10^{-5}\ T^2 \text{ kg/m}^3 \quad [A-2]$$

$$(290 < T < 2270 \text{ K})$$

$^{235}UC_{1.0}$ 293 K $13.45 \pm 0.01 \times 10^3$ kg/m^3 [A-2]

For liquid UC

$$\rho = \frac{12.57 \times 10^3 \text{ kg/m}^3}{1 + 9.98 \times 10^{-5}\ T} \text{ (estimated) } T \geq 2780 \text{ K} \quad [A-1]$$

A-3 EMISSIVITY

$$\varepsilon_{total} = 0.42 \pm 0.02 \ (1250 < T < 1980 \text{ K}) \quad [A-3]$$

at 0.65×10^{-6} m

$$\varepsilon = 0.539 - 2 \times 10^{-5}\ T \ (1150 < T < 1890 \text{ K}) \quad [A-3]$$

A-4 LATTICE PARAMETER - CRYSTAL STRUCTURE

$4.9605 \pm 0.0002 \times 10^{-10}$ m [A-4]

Face centered, NaCl type [A-4]

A-5 MELTING POINT

$UC_{1.00}$ 2780 ± 25 K [A-5]

A-6 SURFACE TENSION

A-7 THERMAL EXPANSION

$UC_{0.98}$ to $UC_{1.08}$ 99.3% T.D.

$$\frac{L_T - L_o}{L_o} = -2.86 \times 10^{-3} + 9.40 \times 10^{-6}\ T + 1.17 \times 10^{-9}\ T^2 \qquad [A-2]$$

$$(293 < T < 2273\ K)$$

References

[A-1] A. Sheth, Argonne National Laboratory, private communication (1975).

[A-2] R. Mendez-Peñalosa and R. E. Taylor, J. Amer. Ceram. Soc. *47*, 101 (1964).

[A-3] L. N. Grossman, J. Amer. Ceram. Soc. *46*, 264 (1963).

[A-4] F. B. Litton, LA-3799 (October 6, 1967).

[A-5] R. J. Ackermann, P. Potter, M. Rand, and E. K. Storms, IAEA Panel - Assessment of Thermodynamic Properties of U-C, Pu-C, and U-Pu-C Systems, Grenoble, France, May 6-8, 1974, to be published.

B. Thermodynamic

B-1 COMPRESSIBILITY

Isothermal compressibility, 296 K

$$7.1 \times 10^{-12}\ m^2/N \qquad [B-1]$$

B-2 ENTHALPY

$$H^\circ_T - H^\circ_{298} = -2.1648 \times 10^4 + 6.1618 \times 10^1\ T - 1.1185 \times 10^{-3}\ T^2 + 1.3934 \times 10^{-6}\ T^3 + \frac{9.9567}{T} \times 10^5\ J/mol \qquad [B-2]$$

$$(298 < T < 2418\ K)$$

Calculated values are listed in Table B-1.

For liquid UC

$$H^\circ_T - H^\circ_{298} = 5.1362 \times 10^4 + 4.9887 \times 10^1\ T + 3.8972 \times 10^{-3}\ T^2\ J/mol \qquad [B-3]$$

(estimated value) $(2780 < T < 7800\ K)$

B-3 ENTROPY

$$S^\circ_T = -2.9696 \times 10^2 + 61.618 \ln T - 2.2370 \times 10^{-3}\ T + 2.0901 \times 10^{-6}\ T^2 + \frac{4.9748}{T^2} \times 10^5\ J\ mol^{-1}\ K^{-1} \qquad [B-2]$$

$$(298 < T < 2418\ K)$$

Calculated values are listed in Table B-1.

B-4 FREE ENERGY OF FORMATION - $UC_{1.0}$

$$\Delta G^\circ_{f,298} = -98.87\ kJ/mol \qquad [B-2]$$

$$\Delta G^\circ_{f,T} = -96.002 - 9.652 \times 10^{-3}\ T\ kJ/mol \quad \sigma = \pm 0.54\ kJ/mol \qquad [B-2]$$

$$(300 < T < 1400\ K)$$

$$\Delta G^\circ_{f,T} = -109.51 + 6.514 \times 10^{-4}\ T\ kJ/mol \quad \sigma = \pm 0.08\ kJ/mol \qquad [B-2]$$

$$(1400 < T < 2800\ K)$$

Calculated values are listed in Table B-1.

TABLE B-1. Thermodynamic Properties of $UC_{1.0}$ [B-2]

T, K	$(H^\circ_T - H^\circ_{298})$ J/mol	C°_p J/mol, K	S°_T J/mol, K	$-(G^\circ_T - H^\circ_{298})/T$ J/mol, K	$-\Delta G^\circ_f$ kJ/mol	$-\Delta H^\circ_f$ kJ/mol
298	0	50.12	59.20	59.20	98.86	97.90
300	92	50.25	59.49	59.20	98.86	97.86
400	5397	55.19	74.72	61.25	99.45	96.35
500	11046	57.57	87.32	65.22	100.37	95.06
600	16878	58.99	97.94	69.83	101.55	94.18
700	22836	60.08	107.11	74.51	102.85	93.76
800	28886	60.96	115.23	79.11	104.14	93.72
900	35024	61.76	122.42	83.55	105.39	93.93
1000	41242	62.55	128.99	87.78	106.48	97.15
1100	47539	63.39	134.98	91.79	107.15	101.88
1200	53919	64.27	140.54	95.60	107.65	102.01
1300	60392	65.19	145.73	99.28	108.11	102.09
1400	66961	66.19	150.58	102.76	108.57	102.13
1500	73630	67.24	155.18	106.11	108.57	108.78
1600	80408	68.37	159.58	109.33	108.53	109.24
1700	87299	69.54	163.72	112.38	108.49	109.66
1800	94320	70.84	167.74	115.35	108.41	109.96
1900	101470	72.17	171.63	118.24	108.28	110.16
2000	108759	73.60	175.34	121.00	108.20	110.25
2100	116194	75.14	178.99	123.68	108.11	110.21
2200	123788	76.74	182.51	126.27	107.99	110.04
2300	131541	78.41	185.98	128.78	107.91	109.70
2400	139469	80.17	189.33	131.25	107.86	109.20
2500[a]	147478	82.01	192.63	133.64	107.82	108.53
2600[a]	155871	83.93	195.89	135.98	107.78	107.74
2700[a]	164360	85.90	199.12	138.24	107.82	106.73
2780[a]	171297	87.57	201.63	140.00	107.86	105.52

[a]Extrapolated [B-3]

B-5 HEAT CAPACITY

$$C_p^\circ = 61.618 - 2.2370 \times 10^{-3}\ T + 4.1803 \times 10^{-6}\ T^2 - \frac{9.9567}{T^2} \times 10^5\ \text{J mol}^{-1}\ \text{K}^{-1} \qquad [B-2]$$

$$(298 < T < 2418\ \text{K})$$

Calculated values are listed in Table B-1.

For liquid UC

$$C_p^\circ = 49.8866 + 7.7943 \times 10^{-3}\ T \quad \text{J mol}^{-1}\ \text{K}^{-1} \qquad [B-3]$$

(estimated value) $(2780 < T < 7800\ \text{K})$

B-6 HEAT OF FORMATION - $UC_{1.0}$

$$\Delta H^\circ_{f,298} = -97.91\ \text{kJ/mol} \qquad [B-2 - B-6]$$

Tabulated $\Delta H^\circ_{f,T}$ values (Table B-1) exhibit large scatter, but two temperature regions can be identified. The average ΔH°_f and standard deviation are provided.

$$\Delta H^\circ_{f,T} = 97.49\ \text{kJ/mol} \qquad \sigma = \pm 3.6\ \text{kJ/mol}$$

$$(300 < T < 1400\ \text{K})$$

$$\Delta H^\circ_{f,T} = 109.0\ \text{kJ/mol} \qquad \sigma = \pm 1.4\ \text{kJ/mol}$$

$$(1500 < T < 2800\ \text{K})$$

B-7 HEAT OF FUSION

48.87 kJ/mol (estimated value) [B-3]

B-8 HEAT OF SUBLIMATION

The heat of sublimation for $UC_{1.00}$ is 535 ± 25 kJ/mol (2000 < T < 2500 K) estimated from the total vapor pressure (see property B-10) using the relationship

$$\frac{d\ \ln P}{d(1/T)} = \frac{-\Delta H_{subl}}{R}$$

where R = gas constant

In this treatment, the vapor is <u>assumed</u> to be composed solely of UC(g). In experimental work to date, UC(g) has not been identified.

B-9 HEAT OF VAPORIZATION

514 ± 25 kJ/mol (2800 < T < 3500 K)

Estimated in the same manner as the heat of sublimation using the estimated total pressure of the gaseous species in the liquid region (property B-10). In this treatment, the vapor is assumed to be composed solely of UC(g). In experimental work to date, UC(g) has not been identified.

B-10 VAPOR PRESSURE

$UC_{1.00}$

$$\log P_U(\text{Pa}) = -\frac{2.80 \times 10^4}{T} + 10.51 \qquad [B\text{-}2,7,8]$$

$$(2000 < T < 2500 \text{ K})$$

$$\log P_{total}(\text{Pa}) = -\frac{2.80 \times 10^4}{T} + 10.53 \qquad [B\text{-}2,7,8]$$

$$(2000 < T < 2500 \text{ K})$$

$$1 \text{ Pa} = 1 \text{ Newton/m}^2$$

For information on the temperature dependency of vapor species over differing UC_x compositions, see Table 5, Ref. B-4.

For liquid UC, estimated partial pressures at 2800 < T < 9000 K are [B-3]

$$\log P_U(\text{Pa}) = 9.59 - (25400/T)$$

$$\log P_{UC_2}(\text{Pa}) = 11.46 - (36100/T)$$

$$\log P_{C_1}(\text{Pa}) = 12.54 - (37500/T)$$

$$\log P_{C_2}(\text{Pa}) = 13.30 - (43300/T)$$

$$\log P_{C_3}(\text{Pa}) = 12.41 - (41000/T)$$

$$\log P_{C_4}(\text{Pa}) = 13.57 - (53600/T)$$

$$\log P_T(\text{Pa}) = -19.0032 - (18132/T) + 7.5425 \log T$$

$$P_T = P_U + P_{UC_2} + P_{C_1} + P_{C_2} + P_{C_3} + P_{C_4}$$

References

[B-1] C. P. Kempter, J. Less Common Metals *10*, 294 (1966).

[B-2] R. J. Ackermann, P. Potter, M. Rand, and E. K. Storms, IAEA Panel - Assessment of Thermodynamic Properties of U-C, Pu-C, and U-Pu-C Systems, Grenoble, France, May 6-8, 1974, to be published.

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[B-6] E. J. Huber and C. E. Holley, J. Chem. Thermodyn. *1*, 267 (1969).

[B-7] E. K. Storms, *Thermodynamics*, Vol. I, Vienna, p. 309, IAEA (1966).

[B-8] E. K. Storms, *The Refractory Carbides*, Chapter XI, Academic Press, New York, pp. 205-213 (1967).

C. Mechanical

C-1 CREEP

a. Steady State

$$\dot{\varepsilon} = A\, d^{-m}\, \sigma^{n} \exp(-Q/RT)$$

d = grain size
σ = stress
Q = apparent activation energy for creep
A,m,n = constants at constant structure
R = the gas constant
T = absolute temperature

The steady state compressive creep data are summarized in Table C-1 and Figs. C-1 and C-2.

b. Irradiation Induced

The irradiation-induced creep behavior of UC is shown in Table C-2.

C-2 ELASTIC CONSTANT

a. Elastic Stiffness Moduli at 298 K

	10^{11} Pa				
	C_{11}	C_{12}	C_{44}	C'	
$UC_{0.96}$	3.149	0.788	0.652	1.177	[C-21]
$UC_{1.03}$	3.180	0.791	0.646	1.178	[C-21]

Porosity Correction $M = M_o\ (1 + 0.55\ P)$

M_o = modulus
P = fraction porosity
C_{ij} = single crystal elastic constants
$C' = 1/2[C_{11} - C_{12}]$

b. Shear Modulus (P = 0)

$$G = 0.873 \times 10^{11}\ \text{Pa} \qquad [C\text{-}22]$$

c. Bulk Modulus (P = 0)

$$K = 1.768 \times 10^{11}\ \text{Pa} \qquad [C\text{-}22]$$

d. Poissons Ratio

$$\nu = 0.284\ (1 - 1.17\ P) \qquad [C\text{-}22]$$

TABLE C-1. A Summary of Steady-State Compressive Creep Properties of UC

Refs.	Temp., K	Grain Size, 10^{-6} m	Purity	Carbon, wt %	Stress Range, MNm^{-2}	n	Q, kJ/mol	Comments[a]	Possible Creep Mechanisms
$UC_{1\pm x}$									
C-1	1870-2270	Single Crystal	-	Stoichio-metric	1-20	5-6	288-384	$Q \approx \Delta H^C_{UC_{1.0}}$ (may be $\approx \Delta H^U_p$)	Weertman [C-2] or Nabarro [C-3] climb mechanism. Probably Nabarro because $Q < \Delta H^U_{UC_{1.0}}$.
C-4[b]	1770-2170	300-400	50 ppm Fe 15 ppm Ni 40 ppm Si	Slight excess of Uranium	4-20	5	158	Q is $< \Delta H^C_{UC_{1-x}}$	n value suggests dislocation models. Weertman model [C-2] with carbon mono-vacancy controls the climb if $D^U_{UC_{1-x}}$ is enhanced sufficiently along the grain boundaries $\Delta H^U_{gb} < \Delta H^C_{UC_{1-x}}$.
C-5[c]	1370-1570	30	0.02 wt % Ni	4.5	41	-	217	-	-
C-6[c]	1170-1470	15-120	300-1000 ppm Ni ~5% porosity	4.6-4.8	7-27	-	121-213	Activation energy increased as the stress increased.	-
C-7[b]	1170-1370	150	500 ppm Al 100 ppm Ni 50 ppm Fe 200 ppm O_2 100 ppm N_2	4.6-4.8	27-54	1.0	188	$Q \approx \Delta H^C_{UC_{1-x}}$ (monovacancy)	Diffusional creep controlled by the diffusion of carbon monovacancies. Grain-size dependence needed for con-firmation.
C-5[c]	1370-1570	30	0.05 wt % Si 0.05 wt % Fe 0.02 wt % Cr	4.9	41-54	2.3	184	$Q \approx \Delta H^C_{UC_{1+x}}$	Stress exponent suggests glide controlled by Peierls barrier or Langdon grain-boundary sliding [C-8].
C-9[b]	1470-1670	300	0.05 wt % Al 0.01 wt % Ti 0.005 wt % Fe 200 ppm O_2 100 ppm N_2	4.9	13-54	1.8	205	$Q \approx \Delta H^C_{UC_{1+x}}$	Langdon grain-boundary sliding [C-8] may be operative but Q has lower values than $\Delta H^U_{UC_{1+x}}$.

TABLE C-1. A Summary of Steady-State Compressive Creep Properties of UC (cont'd)

Refs.	Temp., K	Grain Size, 10^{-6} m	Purity	Carbon, wt %	Stress Range, MNm^{-2}	n	Q, kJ/mol	Comments[a]	Possible Creep Mechanisms
C-10[b]	1470-1870	∿100	50 ppm O_2 50 ppm N_2 100 ppm metals	5.2	20-68	3	376	Q ≈ extrinsic $\Delta H^U_{UC_{1+x}}$	Weertman solute drag mechanism [C-11] or Nabarro dislocation climb model [C-3].
C-6[c]	1270-1570	5-100	0-10^4 ppm Ni ∿5% porosity	4.8-4.97	-	2.13	-	Q varied with temperature from 334-1003 kJ/mol	-
C-12[c]	1270-1670	-	0.1 wt % O_2 0.06 wt % N_2 0-0.3 wt % Ni 300 ppm W 200 ppm Si	4.83-5.4	10-36	2.5	418	Q ≈ extrinsic $\Delta H^U_{UC_{1+x}}$	-
C-13[b]	1500-1870	-		5.2-5.6	10-68	1.8	284±96	Q ≈ $\Delta H^U_{gb}(UC_{0.9})$	-
						4.2	594±87	Q ≈ $\Delta H^U_p(UC_{1+x})$	The activation energy is lower than expected for the $UC_{1.1}$ and could be due to pipe diffusion. The n value suggests creep controlled by dislocation climb via diffusion in the core or the Nabarro model [C-3].
C-14[b]	1670-1970	200	613 ppm O_2 73 ppm N_2	4.88	7-30	6.0	443±32	Q ≈ ΔH^U_p or extrinsic $\Delta H^U_{UC_{1+x}}$	The activation energy is lower than expected for the $UC_{1.1}$ and could be due to pipe diffusion. The n value suggests creep controlled by dislocation climb via diffusion in the core or the Nabarro model [C-3].
C-14[b]	1670-1970	50	67 ppm O_2 407 ppm N_2	5.05	7-69	3-6	443		Stress exponent decreases as the temperature decreases, which appears anomalous. Phase transformation could be taking place.
C-14[b]	1670-2070	-	94 ppm O_2 70 ppm N_2 3.42 wt % Zr 3.78 wt % W	5.73	15-69	1.8	648	Q ≈ $\Delta H^U_{UC_{1.01}}$	n and Q suggest grain-boundary sliding, but grain-size dependence is unknown.

[a] H_p = pipe diffusion activation enthalpy.

[b] Arc-cast material.

[c] Sintered material.

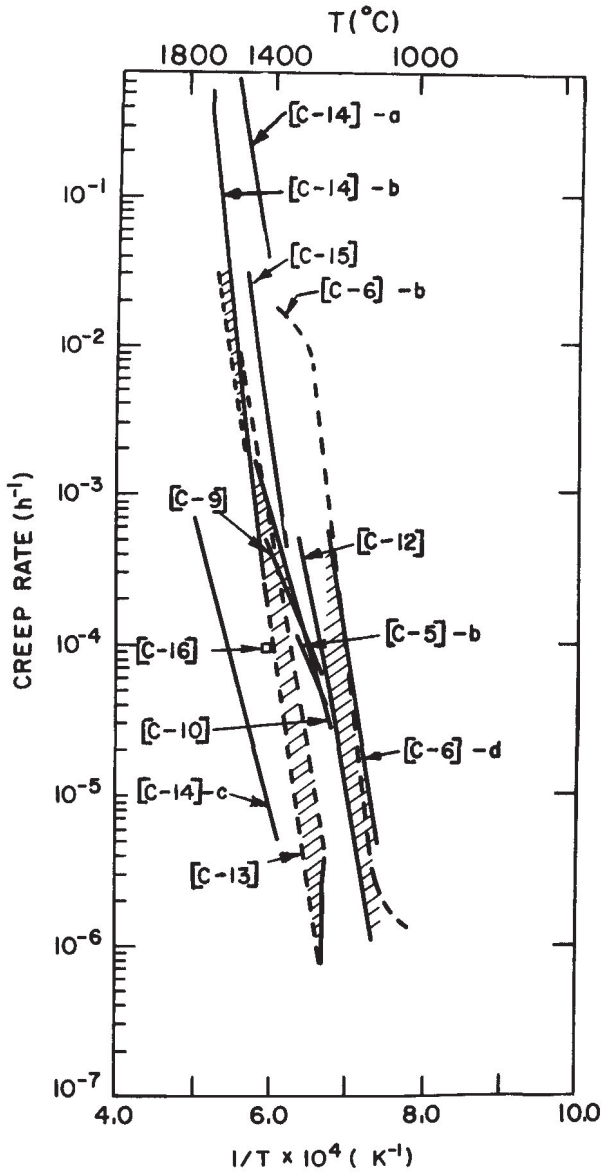

Fig. C-1

Summary of the steady-state creep rates of hyperstoichiometric UC and (U,Pu)C at a stress of 41 MNm^{-2}. The symbols represent the following sintered material: [C-5]-b, UC, 4.9 wt % C; [C-6]-b, UC, 4.8-4.97 wt % C; [C-6]-d, $(U_{0.85}Pu_{0.15})C$, 4.9 wt % C, at a stress of 20 MNm^{-2}; [C-12], UC, 4.83 wt % C; [C-15], $(U_{0.79}Pu_{0.21})C$, 5.1 wt % C; and the following arc-cast material; [C-13], UC, 5.2-5.6 wt % C; [C-14]-a, UC, 4.88 wt % C; [C-14]-b, UC, 5.05 wt % C; [C-14]-c, $(U_{0.9}Zr_{0.1})C+W$, 5.73 wt % C; [C-9], UC, 4.9 wt % C; [C-10], UC, 5.2 wt % C; and [C-16], UC, 5.2 wt % C, at a tensile stress of 34 MNm^{-2}.

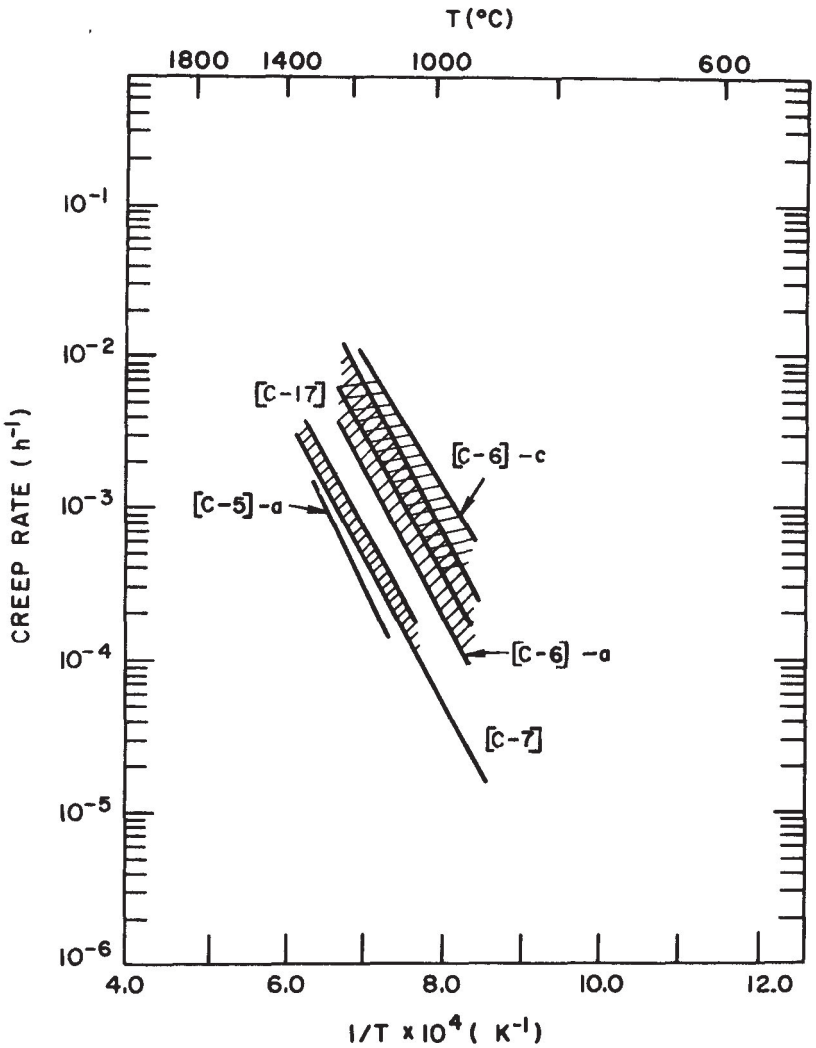

Fig. C-2

Summary of the steady-state creep rates of hypo-stoichiometric UC and (U,Pu)C at a stress of 41 MNm^{-2}. The symbols represent the following sintered material: [C-5]-a, UC, 4.5 wt % C; [C-6]-a, UC, 4.6-4.8 wt % C; [C-6]-c, $(U_{0.85}Pu_{0.15})C$, 4.6-4.8 wt % C, at a stress of 20 MNm^{-2}; [C-17], UC, 4.4-4.6 wt % C; and arc-cast material; [C-7], UC, 4.6-4.8 wt % C.

TABLE C-2. Radiation-Induced Creep Behavior of UC

Investigators	Material	$\dot{\varepsilon}_R$ [a] s^{-1}	Experimental Conditions
Clough [C-18]	UC	1×10^{-9}	4.85 wt % C, 95.5% TD, 30×10^{-6} m grain size, effective specimen temp. 1070 K, 6×10^{18} fissions/m^3-s, stress 25.5 MNm^{-2}. Irradiation creep measured in tension, unirradiated in compression.
Clough [C-19]	UC	3×10^{-11} to 8×10^{-10}	4.8 wt % C, 97% TD, 45×10^{-6} m grain size, effective specimen temp. 720 K, 1×10^{19} fissions/m^3-s, stress 13-53 MNm^{-2}. Irradiation creep measured in three-point bending.
Brucklacher *et al.* [C-20]	UC	2×10^{-10} to 1×10^{-9}	4.9 wt % C, 85% TD, effective specimen temp. 970 K, 3.4×10^{20} fissions/m^3-s, stress 24 MNm^{-2}. Irradiation creep measured in compression.

[a] $\dot{\varepsilon}_R$ = Radiation-induced creep rate.

C-3 FRACTURE STRESS

The stress-strain behavior is shown in Fig. C-3.

C-4 HARDNESS

	Hardness, 10^6 kg/m^2		
	25°	1000°C	
$UC_{0.91}$	720	120	[C-24]
$UC_{1.05}$	640	100	[C-24]

For diamond point hardness (DPH), 10 DPH = 10 x 10^6 kg/m^2

C-5 STRESS RELAXATION

Polycrystalline, nearly stoichiometric UC

$$\sigma_o - \sigma_t = \frac{RT}{V^*} \ln(1 + t/t_o) \qquad [C-4]$$

$$(1773 < T < 2173 \text{ K})$$

σ_o = initial stress
σ_t = stress at time t
V^* = apparent activation volume
R = gas constant
T = absolute temperature
t_o = delay time

The apparent activation volume is inversely proportional to stress and does not change with temperature (over the range 1773-2173 K) at a constant stress.

C-6 THERMAL SHOCK RESISTANCE

Thermal shock rupture moduli 380 MN m^{-2} [C-25,26]

C-7 YIELD STRESS

Polycrystalline, nearly stoichiometric UC

$$\dot{\varepsilon} = K \sigma^5 \exp(-157000 \text{ J/RT}) \qquad [C-4]$$

$$(1770\text{-}1970 \text{ K})$$

The compositional and temperature dependence of flow stress for UC is summarized in Fig. C-4. The strain-rate dependence of flow stress is shown in Fig. C-5.

FIGURE REDACTED FOR COPYRIGHT

Fig. C-3. Curves Showing the Effects of Temperature and Strain Rate on the Stress-Strain Behavior of Uranium Carbide [C-23]

lot C_1 - 4.91% C
lot C_2 - 4.87% C

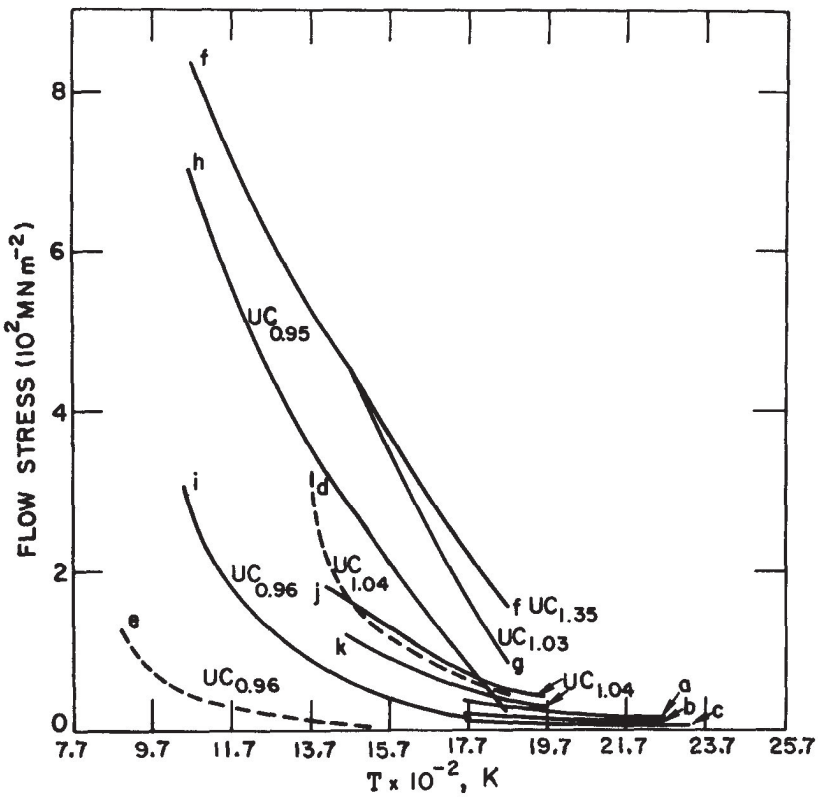

Fig. C-4

Variation of flow stress (at 0.06% strain) as a function of temperature for UC_{1+x} and UC_{1-x}. The letters represent the following: a, b, and c [C-4], single crystals at $\varepsilon = 0.0006$ and $\dot{\varepsilon} = 7 \times 10^{-6}\ s^{-1}$; d and e [C-2], polycrystalline proportional limit at $\dot{\varepsilon} = 3 \times 10^{-6}\ s^{-1}$; f, g, h, and i [C-28], polycrystals at $\varepsilon = 0.002$ and $\dot{\varepsilon} = 6.5 \times 10^{-4}\ s^{-1}$; and j and k [C-23], polycrystals at $\varepsilon = 0.004$ and $\dot{\varepsilon} = 4 \times 10^{-4}\ s^{-1}$ and $4 \times 10^{-5}\ s^{-1}$, respectively.

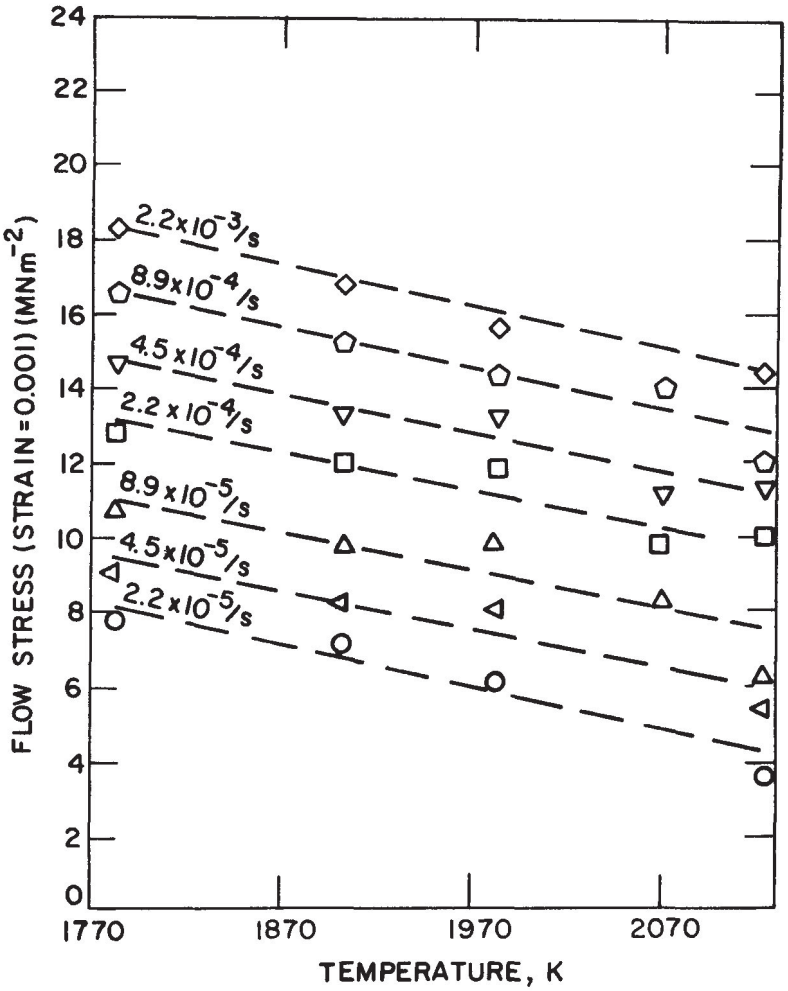

Fig. C-5. Variation of Flow Stress as a Function of Temperature and Strain Rate for Nearly Stoichiometric UC (from Ref. C-4)

C-8 YOUNG'S MODULUS

$$E = 2.25\ (1 - 2.3\ P) \times 10^{11}\ \text{Pa} \quad (298\ \text{K}) \qquad [C\text{-}22]$$

$$P = \text{volume fraction porosity}$$

$$1\ \text{Pa} = 1\ \text{Newton/m}^2$$

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D. Transport

D-1 DIFFUSION

a. Self Diffusion - U in $UC_{1.00}$

$$D_V^U = 6.9 \times 10^{-4} \exp(-589000\ J/RT)\ m^2/sec \qquad [D-1]$$

$$(1970 < T < 2780\ K)$$

b. Grain Boundary Diffusion - U in $UC_{1.00}$

$$D_{gb}^U = 1.8 \times 10^{-5} \exp(-311000\ J/RT)\ m^2/sec \qquad [D-2]$$

$$(1800 < T < 2600\ K)$$

c. Surface Diffusion - U in $UC_{0.97}$

$$D_{sd}^U = 5.6 \times 10^{-12} \exp(-131000\ J/RT)\ m^2/sec \qquad [D-3]$$

$$(1400 < T < 1800\ K)$$

d. Self Diffusion - C in $UC_{1.00}$

Large scatter in results, no recommended value

$$D_V^C = D_o \exp(-\Delta H/RT)\ m^2/sec$$

Temp, K	ΔH kJ/mol	D_o 10^{-4} m^2/sec	
1460-2620	266 ± 6	0.30	[D-4]
1770-2170	351 ± 25	75	[D-5]

e. Diffusion of Xenon in UC

Temp, K	D_o, m^2/sec	ΔH kJ/mol	Neutron Dose, nvt	
1270-1670	2.1×10^{-9}	356	$\sim 1.8 \times 10^{16}$	[D-6]
1070-1570	10^{-11} to 10^{-7}	188	10^{17}	[D-7]
1270-2270	$(1.17 \pm 0.16) \times 10^{-10}$	230 ± 5	$\leq 3 \times 10^{15}$	[D-8]
1270-1870	0.3×10^{-4}	351 ± 21	$< 6 \times 10^{15}$	[D-9]

D-2 ELECTRICAL RESISTIVITY

$UC_{1.00}$ 100% T.D.

$$\rho_o = -8.88 \times 10^{-8} + 1.73 \times 10^{-9}\ T - 2.688 \times 10^{-13}\ T^2\ \Omega\ m \qquad [D\text{-}10]$$

$$(298 < T < 1873\ K)$$

$$\rho_o = \rho(1 - P)^{1.38}$$

ρ_o = resistivity at 100% T.D.
ρ = resistivity of low density material
P = volume fraction porosity

D-3 GRAIN GROWTH

D-4 SEEBECK COEFFICIENT

10^{-6} V K^{-1}			
298 K	770 K	1270 K	
25	48	38	[D-11]
50	39	32	[D-12]

D-5 THERMAL CONDUCTIVITY

$UC_{1.0}$ 100% T.D.

$$\lambda_{TD} = 22.8 - 5.01 \times 10^{-3}\ T + 3.61 \times 10^{-6}\ T^2\ W\ m^{-1}\ K^{-1} \qquad [D\text{-}13]$$

$$(323 < T < 973\ K)$$

$$\lambda_{TD} = 19.8 + 1.48 \times 10^{-3}\ T\ W\ m^{-1}\ K^{-1} \qquad [D\text{-}13]$$

$$(973 < T < 2573\ K)$$

$$\lambda = (1 - P)\lambda_{TD}$$

λ = conductivity of low density material
λ_{TD} = conductivity of 100% theoretical density material
P = volume fraction porosity

For liquid UC

$$\lambda_{TD} = 20.5 \text{ W/m} \cdot \text{K} \qquad [D-14]$$

(estimated value) ($T \geq 2780$ K)

D-6 THERMAL DIFFUSIVITY

$$\alpha = \frac{\lambda}{\rho C_p}$$

α = thermal diffusivity
λ = thermal conductivity (property D-5)
ρ = density (property A-2)
C_p = heat capacity (property B-5)

D-7 VISCOSITY

$$\mu = 8 \times 10^{-3} \text{ Pa-sec (estimated value)} \qquad [D-14]$$

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E. Chemical

E-1 COMPATIBILITY

Hypostoichiometric

Contains free U metal which reacts rapidly with cladding [E-1 - E-5]

Hyperstoichiometric

Contains U_2C_3, leads to greater carburization of the cladding [E-4,6-8]

Carburization

Increases with increasing carbon content [E-9]

Increases with use of sodium as a bonding agent [E-4,7,10,11,14]

Fission Products

Do not appear to migrate to the cladding and do not participate in cladding attack [E-12 - E-14]

Temperature

Carburization depth increases with increasing temperature

For SS 316, only advanced alloy tested (the advanced alloys are 316 SS-20% CW, 330 SS, A286, M813, PE-16, Inconel 706, Inconel 718, Incoloy 901, and HT-9), depth of carburization from sodium-bonded UC (4.89% C) was 25 x 10^{-6} m at 970 K and 425 x 10^{-6} m at 1070 K in tests of three month duration. [E-15] At 1170 K, the rate of carburization is extremely rapid even for gas bonding [E-14]

For further details, see ANL-AFP-9.

E-2 KINETICS

E-3 PHASE EQUILIBRIUM

See Fig. E-1, phase diagram of the U-C system. [E-16]

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FIGURE REDACTED FOR COPYRIGHT

Fig. E-1. Phase Diagram of the U-C System [E-16]

A. Physical

A-1 CRITICAL CONSTANTS

$PuC_{0.88}$ Critical temperature (estimated) - 6550 K [A-1]

A-2 DENSITY

$PuC_{0.90}$ 295 K $13.49 \pm 0.01 \times 10^3$ kg/m^3 [A-2]

$$\rho = 1.358 \times 10^4 - 2.59 \times 10^{-1} T - 1.17 \times 10^{-4} T^2 \text{ kg/m}^3 \quad [A-2]$$

$$(298 < T < 1173 \text{ K})$$

For liquid $PuC_{0.88}$

$$\rho = \frac{11.69 \times 10^3 \text{ kg/m}^3}{1 + 7.77 \times 10^{-5} T} \text{ (estimated) } T \geq 1875 \text{ K} \quad [A-1]$$

A-3 EMISSIVITY - $PuC_{0.88}$

$$\varepsilon_{total} = 0.42 \pm 0.02 \ (1250 < T < 1980 \text{ K}) \quad [A-3]$$

at 0.65×10^{-6} m

$$\varepsilon = 0.539 - 2 \times 10^{-5} T \ (1150 < T < 1890 \text{ K}) \quad [A-3]$$

A-4 LATTICE PARAMETER - CRYSTAL STRUCTURE

$PuC_{0.90}$ $4.9734 \pm 0.0005 \times 10^{-10}$ m (298K) [A-4 - A-7]

Face centered, NaCl type [A-4 - A-7]

A-5 MELTING POINT

$PuC_{0.87}$ 1875 ± 25 K [A-8]

A-6 SURFACE TENSION

A-7 THERMAL EXPANSION

$PuC_{0.85}$, unknown density

$$\frac{L_T - L_o}{L_o} = -2.44 \times 10^{-3} + 6.66 \times 10^{-6}\ T + 3.00 \times 10^{-9}\ T^2 \qquad [A-2]$$

$$(298 < T < 1173\ K)$$

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B. Thermodynamic

B-1 COMPRESSIBILITY

B-2 ENTHALPY - $PuC_{0.88}$

$$H^\circ_T - H^\circ_{298} = -2.3968 \times 10^4 + 77.8517\ T - 3.9085 \times 10^{-2}\ T^2 + 2.07 \times 10^{-5}\ T^3 + \frac{1.1 \times 10^6}{T}\ \text{J/mol} \qquad [B\text{-}1]$$

$$(298 < T < 1875\ \text{K})$$

Calculated values are listed in Table B-1.

For liquid $PuC_{0.88}$

$$H^\circ_T - H^\circ_{298} = 4.917 \times 10^4 + 49.8867\ T + 3.3823 \times 10^{-3}\ T^2\ \text{J/mol} \qquad [B\text{-}2]$$

(estimated value) $(1875 < T < 5200\ \text{K})$

B-3 ENTROPY - $PuC_{0.88}$

$$S^\circ_T = -3.5597 \times 10^2 + 77.8517 \ln T - 7.817 \times 10^{-2}\ T + 3.1049 \times 10^{-5}\ T^2 + \frac{5.5003 \times 10^5}{T^2}\ \text{J mol}^{-1}\ \text{K}^{-1} \qquad [B\text{-}1]$$

$$(298 < T < 1875\ \text{K})$$

Calculated values are listed in Table B-1.

B-4 FREE ENERGY OF FORMATION - $PuC_{0.88}$

$$\Delta G^\circ_{f,298} = -47.70\ \text{kJ/mol} \qquad [B\text{-}1]$$

$$\Delta G^\circ_{f,T} = -45.5102 - 2.9298 \times 10^{-2}\ T + 2.7309 \times 10^{-5}\ T^2 - 8.6215 \times 10^{-9}\ T^3\ \text{kJ/mol} \qquad [B\text{-}1]$$

Average error = ±0.06 kJ/mol

$$(300 \le T \le 1800\ \text{K})$$

Calculated values are listed in Table B-1.

Table B-1. Thermodynamic Properties of $PuC_{0.88}$

T, K	$(H^\circ_T-H^\circ_{298})$ J/mol	C°_p J/(mol)(K)	S°_T J/(mol)(K)	$-(G^\circ_T-H^\circ_{298})/T$ J/(mol)(K)	$-\Delta G^\circ_f$ kJ/mol	$-\Delta H^\circ_f$ kJ/mol
298	0	47.70	72.72	72.72	47.70	47.70
300	88	47.78	73.01	72.72	52.09	47.70
400	4987	49.62	87.11	74.60	53.51	50.59
500	9966	49.92	98.20	78.28	54.31	50.79
600	14970	50.29	107.3	82.38	55.02	51.59
700	20041	51.30	115.1	86.48	55.52	51.80
800	25267	53.30	122.1	90.5	55.90	53.60
900	30748	56.40	128.6	94.39	56.19	56.40
1000	36593	60.71	134.7	98.12	56.19	56.40
1100	42924	66.11	140.7	101.7	56.19	56.32
1200	49852	72.72	146.8	105.2	56.19	55.52
1300	57505	80.50	152.9	108.6	56.40	54.10
1400	66003	89.62	159.2	112.0	56.61	51.88
1500	75463	99.79	165.7	115.4	57.11	48.79
1600[a]	86010	111.3	172.5	118.7	57.70	44.60
1700[a]	97768	124.1	179.6	122.1	58.79	39.20
1800[a]	110859	138.0	187.1	125.5	60.08	32.51

[a]Extrapolated

B-5 HEAT CAPACITY - $PuC_{0.88}$

$$C_p^\circ = 77.8517 - 7.817 \times 10^{-2}\ T + 6.2099 \times 10^{-5}\ T^2 - \frac{1.1 \times 10^6}{T^2}\ \text{J mol}^{-1}\ \text{K}^{-1} \qquad [B-1]$$

$$(298 < T < 1875\ \text{K})$$

Calculated values are listed in Table B-1.

For liquid $PuC_{0.88}$

$$C_p^\circ = 49.8867 + 6.7647 \times 10^{-3}\ T \quad \text{J mol}^{-1}\ \text{K}^{-1} \qquad [B-2]$$

(estimated value) $(1875 \leq T \leq 5200\ \text{K})$

B-6 HEAT OF FORMATION - $PuC_{0.88}$

$$\Delta H^\circ_{f,298} = -47.70\ \text{kJ/mol} \qquad [B-1]$$

From the tabulated values of $\Delta H^\circ_{f,T}$ (Table B-1), two temperature regions can be identified. They are:

$$\Delta H^\circ_{f,T} = -24.2843 - 1.3519 \times 10^{-1}\ T + 2.2845 \times 10^{-4}\ T^2 - 1.3112 \times 10^{-7}\ T^3 \quad \text{kJ/mol} \qquad [B-1]$$

Average error = ±0.21 kJ/mol

$$(300 \leq T \leq 900\ \text{K})$$

$$\Delta H^\circ_{f,T} = -54.1179 + 1.6614 \times 10^{-2}\ T - 3.9357 \times 10^{-5}\ T^2 + 2.0439 \times 10^{-8}\ T^3 \quad \text{kJ/mol} \qquad [B-1]$$

Average error = ±0.025 kJ/mol

$$(1000 \leq T \leq 1800\ \text{K})$$

B-7 HEAT OF FUSION - $PuC_{0.88}$

32.97 kJ/mol (estimated value) [B-2]

B-8 HEAT OF SUBLIMATION

The heat of sublimation for $PuC_{0.88}$ is 331 ± 15 kJ/mol (1200 < T < 1800 K) estimated from the total vapor pressure (see property B-10) using the relationship

$$\frac{d \ln P}{d(1/T)} = \frac{-\Delta H_{subl}}{R}$$

where R = gas constant

(Cont'd on following page)

In this treatment, the vapor is assumed to be composed solely of PuC(g). In experimental work to date, PuC(g) has not been identified.

B-9 HEAT OF VAPORIZATION - $PuC_{0.88}$

299 ± 15 kJ/mol (1900 ≤ T ≤ 2500 K)

Estimated in the same manner as the heat of sublimation using the estimated total pressure of the gaseous species in the liquid region (property B-10). In this treatment, the vapor is assumed to be composed solely of PuC(g). In experimental work to date, PuC(g) has not been identified.

B-10 VAPOR PRESSURE

$PuC_{0.88}$

$$\log P_{Pu}(Pa) = 8.65 - \frac{17300}{T} \qquad [B-3]$$

$$(1000 < T < 1800 \text{ K})$$

$$\log P_{T}(Pa) = 8.65 - \frac{17300}{T} \qquad [B-3]$$

$$(1000 < T < 1800 \text{ K})$$

For information on the temperature dependency of less important carbon vapor species, see Table 9, Ref. B-3.

For liquid $PuC_{0.88}$, estimated partial pressures at 1900 < T < 8000 K are

$$\log P_{Pu}(Pa) = 7.97 - (15600/T) \qquad [B-2]$$

$$\log P_{C_1}(Pa) = 12.72 - (38300/T)$$

$$\log P_{C_2}(Pa) = 14.17 - (44900/T)$$

$$\log P_{C_3}(Pa) = 13.85 - (43400/T)$$

$$\log P_{T}(Pa) = -60.0338 + (4484.9/T) + 17.505 \log T$$

$$P_T = P_{Pu} + P_{C_1} + P_{C_2} + P_{C_3}$$

$$1 \text{ Pa} = 1 \text{ Newton/m}^2$$

References

[B-1] R. J. Ackermann, P. Potter, M. Rand, and E. K. Storms, IAEA Panel - Assessment of Thermodynamic Properties of U-C, Pu-C, and U-Pu-C Systems, Grenoble, France, May 6-8, 1974, to be published.

[B-2] A. Sheth, Argonne National Laboratory, private communication (1975).

[B-3] M. Tetenbaum, A. Sheth, and W. Olson, ANL-AFP-8 (1975).

C. Mechanical

C-1 CREEP

a. Steady State

b. Irradiation Induced

C-2 ELASTIC CONSTANT

a. Elastic Stiffness Moduli

b. Shear Modulus

c. Bulk Modulus

d. Poisson's Ratio

C-3 FRACTURE STRESS

C-4 HARDNESS

	Hardness, 10^6 kg/m^2		
	300 K	1273 K	
$PuC_{0.93}$	810	40	[C-1]

For diamond point hardness (DPH), 10 DPH = 10 x 10^6 kg/m^2

C-5 STRESS RELAXATION

C-6 THERMAL SHOCK RESISTANCE

C-7 YIELD STRESS

C-8 YOUNG'S MODULUS

References

[C-1] M. Tokar, J. Amer. Ceram. Soc. *56*, 173 (1973).

D. Transport

D-1 DIFFUSION

D-2 ELECTRICAL RESISTIVITY

$PuC_{0.85}$ 100% T.D.

$$\rho_o = 2.68 \times 10^{-6} - 4.645 \times 10^{-10}\ T + 3.23 \times 10^{-13}\ T^2 \quad \Omega\ m \qquad [D-1]$$

$$(300 < T < 1025\ K)$$

$PuC_{1.0}$ unknown density ($PuC_{1.x} + Pu_2C_3$)

$$\rho_o = 2.86 \times 10^{-6} - 3.77 \times 10^{-10} T + 3.869 \times 10^{-13} T^2 \quad \Omega\ m \qquad [D-2]$$

$$(375 < T < 1075\ K)$$

$$\rho_o = \rho(1-P)^{1.38}$$

ρ_o = resistivity at 100% T.D.
ρ = resistivity of low density material
P = volume fraction porosity

D-3 GRAIN GROWTH

D-4 SEEBECK COEFFICIENT

10^{-6} V K^{-1}		
298 K	773 K	
5	8	[D-1]
8	15	[D-3]

D-5 THERMAL CONDUCTIVITY

$PuC_{0.99}$ 100% T.D.

$$\lambda_{TD} = 9.45 - 1.06 \times 10^{-2}\ T + 1.20 \times 10^{-5}\ T^2 \quad W\ m^{-1}\ K^{-1} \quad [D-4,D-5]$$

$$(373 < T < 1573\ K)$$

$$\lambda = \lambda_{TD} \left(\frac{1-P}{1+P}\right)$$

λ_{TD} = conductivity of 100% theoretical density material
λ = conductivity of low density material
P = volume fraction porosity

For liquid PuC

$$\lambda_{TD} = 27.2 \quad W\ m^{-1}\ K^{-1}$$

(estimated value) ($T \geq 1875$ K) [D-6]

D-6 THERMAL DIFFUSIVITY

$$\alpha = \frac{\lambda}{\rho C_p}$$

α = thermal diffusivity
λ = thermal conductivity (property D-5)
ρ = density (property A-2)
C_p = heat capacity (property B-5)

D-7 VISCOSITY - $PuC_{0.88}$

$$\mu = 4 \times 10^{-3}\ \text{Pa-sec (estimated value)} \quad [D-6]$$

$$(T \geq 1875\ K)$$

References

[D-1] O. L. Kruger and J. B. Moser, J. Chem. Phys. *46*, 891 (1967).

[D-2] J. A. Leary, R. L. Thomas, A. E. Ogard and G. C. Wonn, *Carbides in Nuclear Energy*, L. E. Russell, Ed., Macmillan, Vol. I, p. 365, (1964). [LADC-5924 (1963)]

[D-3] P. Costa and R. Lallement, Phys. Lett. *7*, 21 (1963).

[D-4] J. B. Moser and O. L. Kruger, *Proc. 7th Conf. on Thermal Conductivity*, NBS, Spec. Publ. *302*, 461 (1968).

[D-5] H. D. Lewis and J. F. Kerrisk, LA-6096 (1976).

[D-6] A. Sheth, Argonne National Laboratory, private communication (1975).

E. Chemical

E-1 COMPATIBILITY

No data are available concerning the compatibility of PuC with current advanced alloys (namely, 316 SS-20% CW, 330 SS, A286, M813, PE-16, Inconel 706, Inconel 718, Incoloy 901, and HT-9). Compatibility behavior similar to UC is expected.

E-2 KINETICS

E-3 PHASE EQUILIBRIUM

See Fig. E-1, phase diagram of the PuC system. [E-1]

References

[E-1] R. J. Ackermann, P. Potter, M. Rand, and E. K. Storms, IAEA Panel - Assessment of Thermodynamic Properties of U-C, Pu-C, and U-Pu-C Systems, Grenoble, France, May 6-8, 1974, to be published.

FIGURE REDACTED FOR COPYRIGHT

Fig. E-1. Phase Diagram of the PuC System [E-1]

A. Physical

A-1 CRITICAL CONSTANTS - $(U_{0.80}Pu_{0.20})C$

Critical temperature (estimated) - 9653 K [A-1]

A-2 DENSITY - $(U_{0.80}Pu_{0.20})C_{0.99}$

0.7% ^{235}U, 99.3% ^{238}U 88-94% ^{239}Pu, 6-12% ^{240}Pu	298 K	$13.58 \pm 0.01 \times 10^3$ kg/m^3	[A-2]
93% ^{235}U, 7% ^{238}U 88-94% ^{239}Pu, 6-12% ^{240}Pu	298 K	$13.46 \pm 0.01 \times 10^3$ kg/m^3	[A-2]

$(^{235}U_{0.80}Pu_{0.20})C_{0.99}$

$$\rho = 1.360 \times 10^4 - 4.34 \times 10^{-1} T - 2.84 \times 10^{-5} T^2 \text{ kg/m}^3 \quad [A-3]$$

$$(298 < T < 1673 \text{ K})$$

For liquid $(U_{0.80}Pu_{0.20})C$

$$\rho = \frac{12.39 \times 10^3 \text{ kg/m}^3}{1 + 9.84 \times 10^{-5} T} \text{ (estimated)} \quad [A-1]$$

$$T \geq 2758 \text{ K}$$

A-3 EMISSIVITY - $(U_{0.80}Pu_{0.20})C$

$$\varepsilon_{total} = 0.42 \pm 0.02 \ (1250 < T < 1980 \text{ K}) \quad [A-4]$$

at 0.65×10^{-6} m

$$\varepsilon = 0.539 - 2 \times 10^{-5} T \ (1150 < T < 1890 \text{ K}) \quad [A-4]$$

A-4 LATTICE PARAMETER - CRYSTAL STRUCTURE

$(U_{0.80}Pu_{0.20})C_{0.99}$	4.9639×10^{-10} m	(298K)	[A-2]

Face centered, NaCl type

A-5 MELTING POINT

	Temp., K		
	Solidus	Liquidus	
$(U_{0.81}Pu_{0.19})C_{0.95}$	2523 ± 25	2758 ± 25	[A-5]
$(U_{0.81}Pu_{0.19})C_{0.99}$	2575 ± 25	2758 ± 25	[A-5]

A-6 SURFACE TENSION

A-7 THERMAL EXPANSION

$(U_{0.80}Pu_{0.20})C$

$$\frac{L_T - L_o}{L_o} = -3.22 \times 10^{-3} + 9.71 \times 10^{-6}\ T + 1.40 \times 10^{-9}\ T^2 \qquad [A-2, A-3]$$

$$(290 < T < 1700\ K)$$

References

[A-1] A. Sheth, Argonne National Laboratory, private communication (1975).

[A-2] J. F. Andrew and T. W. Latimer, LA-6037-MS (1975).

[A-3] D. Stahl and A. Strasser, *Carbides in Nuclear Energy*, L. E. Russell, Ed., Macmillan, London, Vol. I, p. 373 (1964).

[A-4] L. N. Grossman, J. Amer. Ceram. Soc. *46*, 264 (1963).

[A-5] J. G. Reavis, K. A. Johnson, and J. A. Leary, *Plutonium 1970*, The Metallurgical Society, AIMMPE, New York, p. 791.

B. Thermodynamic

B-1 COMPRESSIBILITY

B-2 ENTHALPY - $(U_{0.80}Pu_{0.20})C$

$$H^\circ_T - H^\circ_{298} = -2.0029 \times 10^4 + 58.0823\ T + 5.976 \times 10^{-4}\ T^2 + 9.5671 \times 10^{-7}\ T^3 + \frac{7.8730 \times 10^5}{T}\ \text{J/mol} \qquad [B-1]$$

$$(298 < T < 1800\ \text{K})$$

Calculated values are listed in Table B-1.

For liquid $(U_{0.80}Pu_{0.20})C$

$$H^\circ_T - H^\circ_{298} = 4.3794 \times 10^4 + 49.8867\ T + 3.8612 \times 10^{-3}\ T^2\ \text{J/mol} \qquad [B-2]$$

(estimated value) $(2758 < T < 7800\ \text{K})$

B-3 ENTROPY - $(U_{0.80}Pu_{0.20})C$

$$S^\circ_T = -2.7381 \times 10^2 + 58.0823 \ln T + 1.1952 \times 10^{-3}\ T + 1.4351 \times 10^{-6}\ T^2 + \frac{3.9365 \times 10^5}{T^2}\ \text{J mol}^{-1}\ \text{K}^{-1} \qquad [B-1]$$

$$(298 < T < 1800\ \text{K})$$

Calculated values are listed in Table B-1.

B-4 FREE ENERGY OF FORMATION - $(U_{0.80}Pu_{0.20})C$

$$\Delta G^\circ_{f,298} = -88.62\ \text{kJ/mol} \qquad [B-1]$$

$$\Delta G^\circ_{f,T} = -85.4858 - 1.2638 \times 10^{-2}\ T + 8.3124 \times 10^{-7}\ T^2 + 1.2138 \times 10^{-9}\ T^3\ \text{kJ/mol} \qquad [B-1]$$

Average error = ±0.18 kJ/mol

$$(300 \leq T \leq 1800\ \text{K})$$

Calculated values are listed in Table B-1.

Table B-1. Thermodynamic Properties of $(U_{0.80}Pu_{0.20})C$

T, K	$(H^\circ_T-H^\circ_{298})$ J/mol	C°_p J/(mol)(K)	S°_T J/(mol)(K)	$-(G^\circ_T-H^\circ_{298})/T$ J/(mol)(K)	$-\Delta G^\circ_f$ kJ/mol	$-\Delta H^\circ_f$ kJ/mol
298	0	49.62	61.92	61.92	88.62	87.86
300	100	49.96	62.34	62.01	89.50	87.82
400	5330	54.10	77.36	64.02	90.25	87.20
500	10857	56.23	89.66	67.95	91.17	86.19
600	16556	57.66	100.1	72.47	92.22	85.69
700	22376	58.70	109.0	77.07	93.35	85.35
800	28292	59.66	116.9	81.59	94.48	85.69
900	34300	60.50	124.0	85.90	95.56	86.44
1000	40397	61.38	130.4	90.04	96.44	88.99
1100	46572	62.22	136.3	93.97	96.94	92.76
1200	52840	63.10	141.8	97.74	97.36	92.72
1300	59195	64.02	146.9	101.3	97.78	92.51
1400	65647	64.98	151.6	104.8	98.16	92.09
1500	72195	65.98	156.2	108.0	98.28	96.78
1600	78843	67.03	160.5	111.2	98.37	96.32
1700	85600	68.16	164.6	114.2	98.53	95.56
1800	92471	69.29	168.5	117.1	98.74	94.48

B-5 HEAT CAPACITY - $(U_{0.80}Pu_{0.20})C$

$$C_p^\circ = 58.0823 + 1.1952 \times 10^{-3}\ T + 2.8701 \times 10^{-6}\ T^2 - \frac{7.8730 \times 10^5}{T}\ J\ mol^{-1}\ K^{-1} \qquad [B-1]$$

$$(298 < T < 1800\ K)$$

Calculated values are listed in Table B-1.

For liquid $(U_{0.8}Pu_{0.2})C$

$$C_p^\circ = 49.8867 + 7.7224 \times 10^{-3}\ T \quad J\ mol^{-1}\ K^{-1} \qquad [B-2]$$

(estimated value) $(2758 < T < 7800\ K)$

B-6 HEAT OF FORMATION - $(U_{0.80}Pu_{0.20})C$

$$\Delta H^\circ_{f,298} = -87.86\ kJ/mol \qquad [B-1]$$

Tabulated values of $\Delta H^\circ_{f,T}$ (Table B-1) exhibit large scatter, but two temperature regions can be identified. The average ΔH°_f and error bands are:

$$\Delta H^\circ_{f,T} = -85.67\ kJ/mol, \quad \text{Average error} = \pm 1.0\ kJ/mol \qquad [B-1]$$

$$(300 < T < 1000\ K)$$

$$\Delta H^\circ_{f,T} = -94.15\ kJ/mol, \quad \text{Average error} = \pm 1.63\ kJ/mol \qquad [B-1]$$

$$(1100 < T < 1800\ K)$$

B-7 HEAT OF FUSION - $(U_{0.80}Pu_{0.20})C$

45.69 kJ/mol (estimated value) [B-2]

B-8 HEAT OF SUBLIMATION

The heat of sublimation for $(U_{0.80}Pu_{0.20})C$ is 365 ± 20 kJ/mol (1500 < T < 2500 K) estimated from the total vapor pressure (see property B-10) using the relationship

$$\frac{d\ \ln P}{d(1/T)} = \frac{-\Delta H_{subl}}{R}$$

where R = gas constant

In this treatment, the vapor is <u>assumed</u> to be composed solely of UC(g) and PuC(g). In experimental work to date, UC(g) and PuC(g) have not been identified.

B-9 HEAT OF VAPORIZATION - $(U_{0.80}Pu_{0.20})C$

331 ± 20 kJ/mol ($2800 \leq T \leq 3000$ K)

Estimated in the same manner as the heat of sublimation using the estimated total pressure of the gaseous species in the liquid region (property B-10). In this treatment, the vapor is assumed to be composed solely of UC(g) and PuC(g). In experimental work to date, UC(g) and PuC(g) have not been identified.

B-10 VAPOR PRESSURE - $(U_{0.80}Pu_{0.20})C$

$$\log P_{Pu}(Pa) = 8.64 - (19100/T) \quad (1500 < T < 2500 \text{ K}) \qquad [B-1]$$

$$\log P_{U}(Pa) = 10.93 - (30900/T) \quad (1500 < T < 2500 \text{ K})$$

$$\log P_{C_T}(Pa) = 13.55 - (38500/T) \quad (1500 < T < 2500 \text{ K})$$

where $P_{C_T} = P_{C_1} + P_{C_2} + P_{C_3}$

For information on the temperature dependency of individual carbon vapor species and $UC_2(g)$ species, see Table 12, Ref. B-1.

For liquid $(U_{0.80}Pu_{0.20})C$, estimated partial pressures at $2800 < T < 9000$ K are

$$\log P_{Pu}(Pa) = 7.78 - (16700/T) \qquad [B-2]$$

$$\log P_{U}(Pa) = 10.06 - (28500/T)$$

$$\log P_{C_1}(Pa) = 12.27 - (35500/T)$$

$$\log P_{C_2}(Pa) = 13.02 - (39400/T)$$

$$\log P_{C_3}(Pa) = 11.99 - (35200/T)$$

$$\log P_{C_4}(Pa) = 11.71 - (42700/T)$$

$$\log P_{UC_2}(Pa) = 11.59 - (35000/T)$$

$$\log P_{T}(Pa) = -33.8352 - (6157.4/T) + 10.985 \log T$$

$$P_T = P_{Pu} + P_U + P_{C_1} + P_{C_2} + P_{C_3} + P_{C_4} + P_{UC_2}$$

$$1 \text{ Pa} = 1 \text{ Newton/m}^2$$

References

[B-1] M. Tetenbaum, A. Sheth, and W. Olson, ANL-AFP-8 (1975).

[B-2] A. Sheth, Argonne National Laboratory, private communication (1975).

C. Mechanical

C-1 CREEP

a. Steady State

$$\dot{\varepsilon} = A\, d^{-m}\, \sigma^{n} \exp(-Q/RT)$$

d = grain size
σ = stress
Q = apparent activation energy for creep
A,m,n = constants at constant structure
R = the gas constant
T = absolute temperature

The steady-state compressive creep data are summarized in Table C-1 and Fig. C-1.

b. Irradiation Induced

The irradiation-induced creep behavior of (U,Pu)C has not been studied.

C-2 ELASTIC CONSTANT

a. Young's Modulus (E)

The porosity and temperature dependence of E can be described as

$$E = 2.02\ (1 - 1.54P)\ [1 - 0.92 \times 10^{-4}\ (T - 298)] \times 10^{11}\ \text{Pa} \qquad [C\text{-}5,6]$$

P = volume fraction porosity

b. Shear Modulus (G)

$$G = 0.78\ (1 - 1.54P)\ [1 - 0.92 \times 10^{-4}\ (T - 298)]/$$
$$[1 - 0.44 \times 10^{-4}\ (T - 298)] \times 10^{11}\ \text{Pa} \qquad [C\text{-}5,6]$$

c. Bulk Modulus (K)

Bulk modulus can be calculated from E and G by

$$K = EG/[3(3G-E)]$$

d. Poisson's Ratio

Poisson's ratio can also be calculated from E and G by

$$\nu = (E/2G)-1$$

TABLE C-1. A Summary of Steady-state Compressive Creep Properties of (U,Pu)C from Ref. [C-1]

References	Temp., K	Grain size, 10^{-6} m	Purity	Carbon (wt %)	Stress range, MN/m^2	n	Q, KJ/mole	Comments
C-2[a]	1273-1423	8-40	13.1-13.3 Pu/U 5% porosity	4.6-4.8	3-25	0.35-1.8	∿188	Diffusion studies not complete
C-3[a]	1356-1453	20-50	14.1 Pu/U 4% porosity	4.9	∿25	-	∿418	
C-4[a]	1573-1773	20-30	21 Pu/U 8% porosity	4.9	13.6-41	2.4	527	

[a]Sintered material.

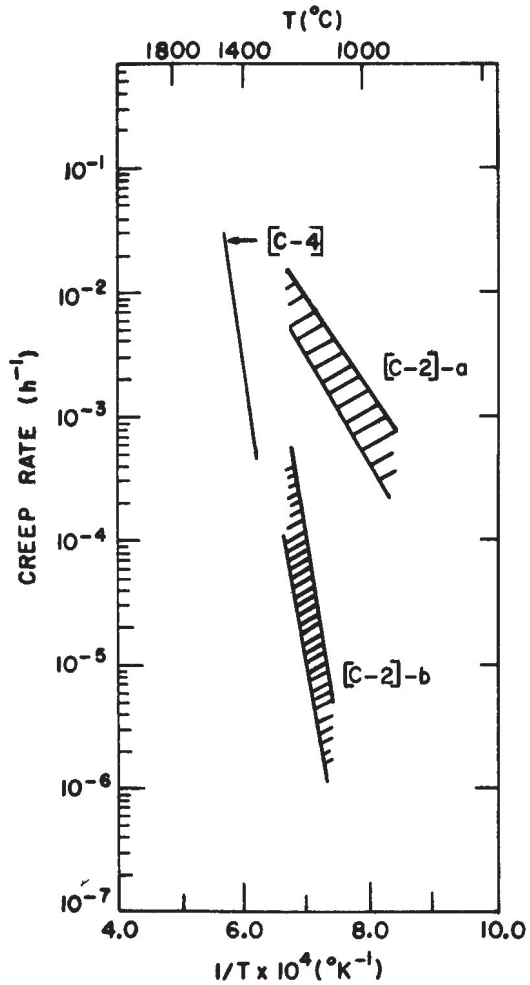

Fig. C-1. Summary of the Steady-state Creep Rates of Hypo-stoichiometric and Hyper-stoichiometric (U,Pu)C. The symbols represent the following sintered material: [C-2]-a, $(U_{0.85}Pu_{0.15})C$, 4.6-4.8 wt% C, 20 MN/m^2; [C-2]-b, $(U_{0.85}Pu_{0.15})C$, 4.9 wt% C, 20 MN/m^2; [C-4], $(U_{0.79}Pu_{0.21})C$, 5.1 wt% C, 41 MN/m^2.

C-3 FRACTURE STRESS

C-4 HARDNESS

	Hardness, 10^6 kg/m^2		
	300 K	1273 K	
$(U_{0.8}Pu_{0.2})C_{0.95}$	720	130	[C-4]
$(U_{0.3}Pu_{0.7})C_{0.93}$	680	100	[C-4]

For diamond point hardness (DPH), 10 DPH = 10 x 10^6 kg/m^2

C-5 STRESS RELAXATION

C-6 THERMAL SHOCK RESISTANCE

C-7 YIELD STRESS

C-8 YOUNG'S MODULUS

$$E = 2.02\ (1 - 1.54P) \times 10^{11}\ \text{Pa}\ (298\ \text{K})$$ [C-5,6]

P = volume fraction porosity

1 Pa = 1 Newton/m^2

References

[C-1] J. L. Routbort and R. N. Singh, ANL-AFP-7 (1975).

[C-2] N. M. Killey, E. King, and H. J. Hedger, J. Brit. Nucl. Energy Soc. *10*, 65-72 (1971).

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D. Transport

D-1 DIFFUSION

D-2 ELECTRICAL RESISTIVITY

$(U_{0.80}Pu_{0.20})C$ 100% T.D.

$$\rho = 3.98 \times 10^{-7} + 1.42 \times 10^{-9}\ T \quad \Omega\ m \qquad [D\text{-}1]$$

$$(373 < T < 1073\ K)$$

$(U_{0.85}Pu_{0.15})C$ 100% T.D.

$$\rho = 3.87 \times 10^{-7} + 1.22 \times 10^{-9}\ T \quad \Omega\ m \qquad [D\text{-}2)$$

D-3 GRAIN GROWTH

D-4 SEEBECK COEFFICIENT

D-5 THERMAL CONDUCTIVITY

$(U_{0,80}Pu_{0,20})C$ 100% T.D.

$$\lambda_{TD} = 19.67 - 1.01 \times 10^{-2}\ T + 8.14 \times 10^{-6}\ T^2 \quad W\ m^{-1}\ K^{-1} \quad [D\text{-}3]$$

$$(323 < T \leq 773\ K)$$

$$\lambda_{TD} = 10.28 + 9.73 \times 10^{-3}\ T - 1.88 \times 10^{-6}\ T^2 \quad W\ m^{-1}\ K^{-1} \quad [D\text{-}3]$$

$$(773 < T < 2573\ K)$$

λ = conductivity of low density material
λ_{TD} = conductivity of 100% Theoretical density material
P = volume fraction porosity

For densities less than 95% theoretical density

$$\lambda = \left(\frac{1 - P}{1 + P}\right) \lambda_{TD}$$

For liquid $(U_{0.80}Pu_{0.20})C$

$$\lambda_{TD} = 19.66\ W\ m^{-1}\ K^{-1} \quad [D\text{-}4]$$

(estimated value) $(T \geq 2758\ K)$

D-6 THERMAL DIFFUSIVITY

$$\alpha = \frac{\lambda}{\rho C_p}$$

α = thermal diffusivity
λ = thermal conductivity (property D-5)
ρ = density (property A-2)
C_p = heat capacity (property B-5)

D-7 VISCOSITY - $(U_{0.80}Pu_{0.20})C$

$$\mu = 7 \times 10^{-3}\ \text{Pa-sec (estimated value)} \quad [D\text{-}4]$$

$$(T \geq 2758\ K)$$

References

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E. Chemical

E-1 COMPATIBILITY

Hypostoichiometric

Contains free uranium and plutonium metal which react rapidly with cladding [E-1,E-2]

Hyperstoichiometric

Contains $(U,Pu)_2C_3$, leads to greater carburization of the cladding [E-2 - E-5]

Carburization

Increases with increasing carbon content [E-6]

Increases with use of sodium as a bonding agent [E-6,E-7]

Fission Products

Do not appear to migrate to the cladding and do not participate in cladding attack [E-8 - E-10]

Temperature

Carburization depth increases with increasing temperature. Upper operational limits have been established for 316 SS (1170 K) and PE-16 [E-11]
(1020 K), the only advanced alloys (316 SS - [E-12]
20% CW, 330 SS, A286, M813, PE-16, Inconel 706, Inconel 718, Incoloy 901, and HT-9) tested.

For further details, see ANL-AFP-9.

E-2 KINETICS

E-3 PHASE EQUILIBRIA

See Fig. E-1, phase diagram of the (U,Pu)C system. [E-13]

FIGURE REDACTED FOR COPYRIGHT

Fig. E-1. Tentative Isothermal Section in the System U-Pu-C at 1873 K [E-13]

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A. Physical

A-1 CRITICAL CONSTANTS — $UN_{1.00}$

Critical temperature (estimated) - 10620 K [A-1]

A-2 DENSITY

$UN_{1.00}$ 14.32×10^3 kg/m^3 298 K [A-2]

$$\rho = 1.443 \times 10^4 - 3.43 \times 10^{-1}\ T - 3.78 \times 10^{-5}\ T^2 \text{ kg/m}^3 \quad [A-2-A-4]$$

$$(298 < T < 1873 \text{ K})$$

For liquid $UN_{1.00}$

$$\rho = \frac{14.24 \times 10^3 \text{ kg/m}^3}{1 + 8.08 \times 10^{-5}\ T} \quad \text{(estimated)} \quad T > 3035 \text{ K} \quad [A-1]$$

A-3 EMISSIVITY — $UN_{1.00}$

$$\varepsilon_{Total} = 0.65 \quad [A-5]$$

(estimated value)

A-4 LATTICE PARAMETER-CRYSTAL STRUCTURE

$UN_{1.00}$ $4.8895 \pm 0.0005 \times 10^{-10}$ m (298 K) [A-6]

Face centered cubic, NaCl type [A-6]

A-5 MELTING POINT — $UN_{1.00}$

3106 ± 40 K	N_2 pressure $\geq 2.2 \times 10^5$ Pa	[A-7-A-9]
3035 ± 40 K	N_2 pressure $= 1.0 \times 10^5$ Pa	[A-7-A-9]

A-6 SURFACE TENSION

A-7 THERMAL EXPANSION

$UN_{1.00}$, 97.7% theoretical density

$$\frac{L_T - L_o}{L_o} = -2.49 \times 10^{-3} + 7.80 \times 10^{-6}\ T + 1.11 \times 10^{-9}\ T^2 \qquad [A-3]$$

$$(293 < T < 1873\ K)$$

References

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B. Thermodynamic

B-1 COMPRESSIBILITY

B-2 ENTHALPY

$$H_T^\circ - H_{298}^\circ = -1.6436 \times 10^4 + 48.8733\ T + 5.5605 \times 10^{-3}\ T^2 + \frac{4.1053}{T} \times 10^5\ \text{J/mol} \qquad [B\text{-}1]$$

$$(298 < T < 2500\ \text{K})$$

Calculated values are listed in Table B-1.

For liquid UN

$$H_T^\circ - H_{298}^\circ = 5.5415 \times 10^4 + 49.8867\ T + 3.2326 \times 10^{-3}\ T^2\ \text{J/mol} \qquad [B\text{-}2]$$

(estimated value) $(3035 < T < 8500\ \text{K})$

B-3 ENTROPY

$$S_T^\circ = -2.2136 \times 10^2 + 48.8733 \ln T + 11.1211 \times 10^{-3}\ T + \frac{2.0527}{T^2} \times 10^5\ \text{J mol}^{-1}\ \text{K}^{-1}$$

$$(298 < T < 2500\ \text{K})$$

$$S_{298.15}^\circ = 62.7243\ \text{J mol}^{-1}\ \text{K}^{-1} \qquad [B\text{-}3]$$

Calculated values are listed in Table B-1.

B-4 FREE ENERGY OF FORMATION

$$\Delta G_{f,T}^\circ = -2.9114 \times 10^5 + 66.838\ T + 1.1554 \times 10^{-2}\ T^2 - 2.1086 \times 10^{-6}\ T^3,\ \text{kJ/mol} \quad \sigma = \pm 0.20\ \text{kJ/mol} \qquad [B\text{-}4]$$

$$(298 \le T \le 3000\ \text{K})$$

Calculated values are listed in Table B-1.

Table B-1. Thermodynamic Properties of UN

Temp, K	$(H_T^\circ - H_{298}^\circ)$, J/mol	C_p°, J/(mol)(K)	S_T°, J/(mol)(K)	$-\Delta G_f^\circ$, kJ/mol	$-\Delta H_f^\circ$, kJ/mol
298	0	47.56	62.70	270.91	295.81
300	95	47.65	63.02	270.75	295.81
400	5029	50.76	77.19	262.50	295.06
500	10212	52.79	88.75	254.47	294.26
600	15574	54.41	98.52	246.56	293.67
700	21086	55.82	107.0	238.74	293.38
800	26735	57.13	114.6	230.91	293.30
900	32510	58.37	121.4	223.13	293.38
1000	38408	59.58	127.6	215.14	296.40
1100	44426	60.77	133.3	206.77	300.83
1200	50561	61.93	138.6	198.24	300.58
1300	56812	63.09	143.6	189.74	300.24
1400	63178	64.23	148.4	181.25	299.74
1500	69659	65.37	152.8	172.34	306.56
1600	76253	66.51	157.1	163.39	306.31
1700	82960	67.64	161.2	154.47	305.89
1800	89780	68.77	165.0	145.56	305.35
1900	96713	69.89	168.8	136.73	304.60
2000	103758	71.01	172.4	127.91	303.67
2100	110915	72.13	175.9	119.16	302.59
2200	118185	73.25	179.3	110.46	301.25
2300	125566	74.37	182.6	101.80	299.74
2400	133059	75.49	185.8	93.22	298.03
2500	140665	76.61	188.9	84.73	296.06
2600[a]	148381	77.73	191.9	76.32	293.84
2700[a]	156210	78.84	194.8	67.99	291.37
2800[a]	164150	79.96	197.7	59.79	288.70
2900[a]	172202	81.08	200.6	51.67	285.73
3000[a]	180365	82.19	203.3	43.64	282.46

[a]Extrapolated [B-7]

B-5 HEAT CAPACITY

$$C_p^\circ = 48.8733 + 11.1211 \times 10^{-3}\ T - \frac{4.1053}{T^2} \times 10^5\ J\ mol^{-1}\ K^{-1} \qquad [B-1]$$

$$(298 < T < 2500\ K)$$

Calculated values are listed in Table B-1.

For liquid UN

$$C_p^\circ = 49.8867 + 6.4651 \times 10^{-3}\ T\ \ J\ mol^{-1}\ K^{-1} \qquad [B-2]$$

(estimated values) $(3035 < T < 8500\ K)$

B-6 HEAT OF FORMATION

$$\Delta H^\circ_{f,298} = -295.81\ \ kJ/mol \qquad [B-4]$$

From the tabulated values of $\Delta H^\circ_{f,T}$ (Table B-1), it is not possible to identify clear trends, but one can approximate those values as:

$$\Delta H^\circ_{f,T} = -294.56\ kJ/mol \quad \sigma = \pm 1.55\ kJ/mol \qquad [B-4]$$

$$(300 < T < 1000\ K)$$

$$\Delta H^\circ_{f,T} = -302.53\ kJ/mol \quad \sigma = \pm 4.27\ kJ/mol \qquad [B-4]$$

$$(1100 < T < 2400\ K)$$

$$\Delta H^\circ_{f,T} = -289.69\ kJ/mol \quad \sigma = \pm 6.8\ kJ/mol$$

$$(2500 < T < 3000\ K) \qquad [B-4]$$

B-7 HEAT OF FUSION

53.35 kJ/mol (estimated value) [B-2]

B-8 HEAT OF SUBLIMATION

$$\Delta H_{subl} = 733.25\ kJ/mol \quad (2400 < T < 2600\ K) \qquad [B-5]$$

B-9 HEAT OF VAPORIZATION

678 ± 15 kJ/mol (estimated value)

Estimated from the partial pressure of UN (g) over UN (c) in the liquid region (property B-10). In doing so, use was made of the relation:

$$\frac{d \ln P}{d(1/T)} = \frac{-\Delta H_{vap}}{R}$$

where R = gas constant

B-10 VAPOR PRESSURE

Vaporization of UN can be considered incongruent vaporization by preferential loss of nitrogen to form a two-phase system comprising nitrogen-saturated liquid uranium and uranium-saturated non-stoichiometric uranium mononitride. Since the study of the phase equilibrium of UN is not yet complete and until additional data becomes available it is recommended that the two-phase region data of Gingerich [B-6] be used. Equations for partial pressure of U and N_2 are as follows:

$$\log P_U(\text{Pa}) = 10.83 - (26800/T) \qquad \text{[B-6]}$$

$$(1910 < T < 2230 \text{ K}) \qquad \text{[B-6]}$$

$$\log P_{N_2}(\text{Pa}) = 13.91 - (30500/T \qquad \text{[B-6]}$$

$$(1910 < T < 2230 \text{ K})$$

Alexander and co-workers [B-7] estimated the partial pressure of UN species as:

$$\log P_{UN}(\text{Pa}) = 13.40 - (38200/T) \qquad \text{[B-7]}$$

Adding all the partial pressures, one computes the total pressure P_T, which is given by:

$$P_T = P_U + P_{N_2} + P_{UN}$$

$$\log P_T(\text{Pa}) = 11.4408 - (29695/T) + 0.6386 \log T \qquad \text{[B-2]}$$

For liquid UN

In the absence of low-temperature data for single-phase UN, the data from the two-phase study of Gingerich [B-6] were extrapolated to the liquid region, and represent an upper limit. Since, with increasing temperature the N/U atom ratio shifts towards lower values, substoichiometric UN will have lower vapor pressures than

that calculated by extrapolation. In the absence of any information on how and to what extent this substoichiometry affects the results, it is recommended that the following data (the extrapolation to the liquid region) should be used with care.

The estimated partial pressures at 3100 K < T < 8000 K are:

$$\log P_U(\mathrm{Pa}) = 9.92 - (24100/T) \qquad [B-2]$$

$$\log P_{N_2}(\mathrm{Pa}) = 12.08 - (24900/T)$$

$$\log P_{UN}(\mathrm{Pa}) = 12.48 - (35400/T)$$

$$\log P_T(\mathrm{Pa}) = 10.0025 - (24048/T) + 0.51735 \log T$$

$$P_T = P_U + P_{N_2} + P_{UN}$$

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C. Mechanical

C-1 CREEP

a. Steady State

$$\dot{\varepsilon} = A\, d^{-m}\, \sigma^{n} \exp(-Q/RT)$$

d = grain size
σ = stress
Q = apparent activation energy for creep
A,m,n = constants at constant structure
R = the gas constant
T = absolute temperature

The steady-state compressive creep data are summarized in Table C-1 and Fig. C-1.

b. Irradiation Induced

The irradiation-induced creep behavior of UN is shown in Table C-2.

C-2 ELASTIC CONSTANTS

a. Elastic Stiffness Moduli at 298 K

	10^{11} Pa				
	C_{11}	C_{12}	C_{44}	C'	
$UN_{1.006}$	4.121	0.837	0.763	1.645	[C-10]

Porosity correction $M = M_o\ (1 - 0.55P)$

M_o = modulus at zero porsity
P = fraction porosity
Cij = single crystal elastic constants
$C' = \frac{1}{2}\,[C_{11} - C_{12}]$

b. Shear Modulus (G)

$$G = \frac{(1-2.22P)(1.06 - 9.5 \times 10^{-5}\ T)}{(1.03 - 4.4 \times 10^{-5}\ T)} \times 10^{11}\ \text{Pa} \qquad [C\text{-}11,12,13]$$

$(298 < T < 3035\ K)$

P = volume fraction porosity

TABLE C-1. A Summary of Steady-state Creep Properties of UN from Ref. [C-1]

References	Temperature, K	Atmosphere Pa	Grain size, 10^{-6} m	Fabrication technique	Purity	Stress range, MNm^{-2}	n	Q, KJ/mole	Comments	Possible creep mechanisms
[C-2]	1373-1623	1.33×10^{-4}	30	Sintered, 95% dense	1100 ppm C 2600 ppm O_2 0.05 wt% Si 0.05 wt% Fe 0.02 wt% Ni 0.02 wt% Cr	41-54	4.15	251-259	Compressive creep. Q may $\rightarrow D_{UN}^{N}$. N/U not constant.	The stress exponent suggests glide controlled by climb creep or Weertman [C-3] mechanism.
[C-4]	1773-2073	p_{N_2} = 2.66×10^4	140	Isostatic hot-pressing, 100% dense	400 ppm O_2 100 ppm C 50 ppm Ca 30 ppm Fe 20 ppm Si	14-34	6±1	314±42	Compressive creep. N/U not constant. n decreases as temperature decreases.	High n could suggest athermal stress contributions and dislocation creep mechanism. Anomalous temperature dependence of n suggests that compositional changes may be occurring.
[C-5]	1673-1973	p_{N_2} = 10.13 p_{N_2} = 4.05×10^2	25	-	130 ppm O_2 400 ppm C 100 ppm others	17-34	~3	-	Tensile creep. Limited study.	Creep mechanism cannot be determined.
[C-6]	1583-1773	1.33×10^{-3}	15	Sintered, 91% dense	0.21 wt% O_2 10-180 ppm Si 4-33 ppm Al 4-39 ppm Ni	10-41	-	-	Compressive creep. Creep rate varies with the ratio N/(C+N) in UC+UN solid solutions. N/U not constant.	

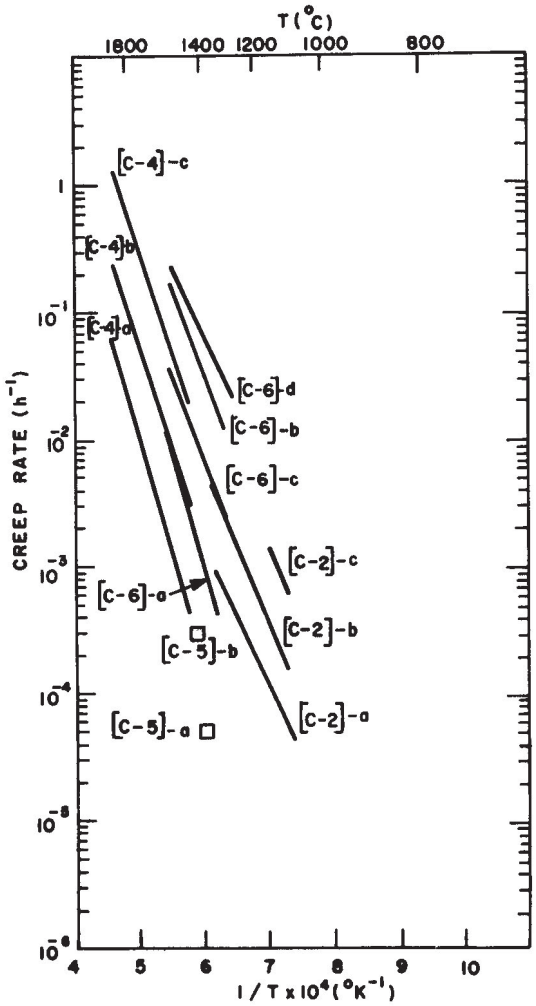

Fig. C-1. Summary of the Steady-state Creep Rates for UN. The symbols represent the material, stress in MNm^{-2}, and oxygen level (where known) as follows: [C-2]-a, UN, 41, 2600 ppm; [C-2]-b, UN, 54.4, 2600 ppm; [C-2]-c, UN, 41, 400 ppm; [C-4]-a, UN, 20.4, 400 ppm; [C-4]-b, UN, 27, 400 ppm; [C-4]-c, UN, 34, 400 ppm; [C-6]-a, UC, 41, 0.11 wt%; [C-6]-b, UN, 41, 0.21 wt%; [C-6]-c, $UC_{0.28}N_{0.72}$, 41, 0.21 wt%; [C-6]-d, $UC_{0.78}N_{0.22}$, 41, 0.22 wt%; and the following tensile creep data: [C-5]-a, UN, 17; and [C-5]-b, UN, 34.

TABLE C-2. Radiation-induced Creep Behavior of UN

Investigators	Material	$\dot{\varepsilon}_R$[a] S^{-1}	Experimental conditions
Brucklacher et al. [C-7]	UN	2.2×10^{-10} to 1.4×10^{-9}	Stoichiometric, 95% TD, 20×10^{-6} m grain size, effective specimen temperature 973 K, 3.4×10^{20} fissions/m^3-s, stress 24 MNm^{-2}. Irradiation creep measured in compression.
Brucklacher and Dienst [C-8]	UN	$4.2\text{-}5.5 \times 10^{-10}$	83-87% TD, $6\text{-}10 \times 10^{-6}$ m grain size, 6 vol % UO_2, effective temperature 1023 K, 3.6×10^{19} fissions/m^3-s, stress 40 MNm^{-2}. Irradiation creep measured in compression.
Brucklacher [C-9]	UN	1.4×10^{-10}	93% TD, for T <1173 K, enhancement; for T >1173 K, little enhancement.

[a] $\dot{\varepsilon}_R$ = radiation-induced creep rate.

c. Bulk Modulus (P = 0)

$$K = 1.842 \times 10^{11} \text{ Pa} \quad (298 \text{ K}) \qquad [C\text{-}12]$$

also

$$K = EG/[3(3G - E)]$$

d. Poisson's Ratio (P = 0)

$$\nu = 0.263 \quad (298 \text{ K}) \qquad [C\text{-}12]$$

also

$$\nu = (E/2G)-1$$

E = Young's Modulus (Property C-8)

C-3 FRACTURE STRESS

C-4 HARDNESS

	Hardness, 10^6 kg/m^2		
	300 K	1273 K	
UN	450	50	[C-14]

For diamond point hardness (DPH), 10 DPH = 10×10^6 kg/m^2

C-5 STRESS RELAXATION

C-6 THERMAL SHOCK RESISTANCE

C-7 YIELD STRESS

C-8 YOUNG'S MODULUS

$$E = (1-2.27P)(2.69 - 2.56 \times 10^{-4}\ T) \times 10^{11} \text{ Pa} \qquad [C\text{-}11,12,13]$$

$$(298 < T < 3035 \text{ K})$$

P = volume fraction porosity

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D. Transport

D-1 DIFFUSION

a) Self Diffusion* U in UN (measured at 3.73×10^4 Pa N_2)

$$D_V^U = 4.01 \times 10^{-8} \, (P_{N_2}/3.73 \times 10^4) \exp(-565000 \text{ J/RT}) \text{ m}^2/\text{sec} \qquad [D\text{-}1]$$

$$(1973 < T < 2173 \text{ K})$$

*see also refs D-2, D-3

D-2 ELECTRICAL RESISTIVITY

$$\rho_o = 1.33 \times 10^{-6} + 5.52 \times 10^{-10} \, T - 1.35 \times 10^{-13} \, T^2 \; \Omega \text{ m} \qquad [D\text{-}4\text{-}D\text{-}6]$$

$$(200 < T < 1500 \text{ K})$$

$\rho_o = \rho \, (1 - P)/(1 + .5P)$

ρ_o = resistivity at 100% T.D.

ρ = resistivity of low density material

P = volume fraction porosity

D-3 GRAIN GROWTH

D-4 SEEBECK COEFFICIENT

$$S = -3.48 \times 10^{-10} + 2.88 \times 10^{-7} \, T - 1.81 \times 10^{-6} \, T^2 \quad \text{V K}^{-1} \qquad [D\text{-}4]$$

$$(60 < T < 400 \text{ K})$$

D-5 THERMAL CONDUCTIVITY

$UN_{1.0}$ 100% T.D.

$$\lambda_{TD} = 4.63 + 2.32 \times 10^{-2}\ T - 5.96 \times 10^{-6}\ T^2\ W\ m^{-1}\ K^{-1}$$ [D-4,D-7,D-8]

$$(400 < T < 2100\ K)$$

$$\lambda_{TD} = \lambda\ (1 + .5P)/(1 - P)$$

λ_{TD} = conductivity of 100% theoretically dense material

λ = conductivity of low density material

P = volume fraction porosity

For liquid UN

$$\lambda_{TD} = 24.3\ \ W\ m^{-1}\ K^{-1}$$ [D-9]

(estimated value) ($T \geqslant 3035$ K)

D-6 THERMAL DIFFUSIVITY

$$\alpha = \frac{\lambda}{\rho C_p}$$

α = thermal diffusivity

λ = thermal conductivity (property D-5)

ρ = density (property A-2)

C_p = heat capacity (property B-5)

D-7 VISCOSITY

$$\mu = 4 \times 10^{-3}\ \text{Pa-sec}$$ [D-9]

(estimated value) ($T \geqslant 3035$ K)

References

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[D-7] A. B. G. Washington, TRG 2236 (1973).

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[D-9] A. Sheth, Argonne National Laboratory, private communication (1976).

E. Chemical

E-1 COMPATIBILITY

Hypostoichiometric

Contains free U metal which reacts rapidly with cladding [E-1]

Hyperstoichiometric

Contains U_2N_3, leads to greater nitriding of the cladding [E-2 - E-5]

Nitriding

In general, no difference in nitriding is observed between helium *vs.* sodium bonding. [E-6 - E-8]
However, increased nitriding with a sodium bond has been reported. [E-3]

Fission Products

Do not appear to migrate to the cladding and do not appear to participate in cladding attack [E-1,E-9]

Temperature

No large temperature dependence of nitriding in tests up to 1270 K [E-1 - E-13]

No difference in nitriding between SS 316 and NIMONIC PE-16, the only advanced alloys tested. [E-5]
(The advanced alloys are 316 SS-20% CW, 330 SS, A286, M813, PE-16, Inconel 706, Inconel 718, Incoloy 901, and HT-9.)

For further details, see ANL-AFP-9.

E-2 KINETICS

E-3 PHASE EQUILIBRIUM

See Fig. E-1 and E-2, phase diagrams of the U-N system. [E-14-E-17] Figure E-2 illustrates how lowering the nitrogen over pressure lowers the decomposition (melting) temperature of UN (lower curve in Fig. E-2) and U_2N_3 (upper curve in Fig. E-2) given by the reaction

$$UN_{(c)} = U(\ell) + 1/2\ N_{2(g)} \text{ and}$$

$$U_2N_{3+x}(c) = 2UN_{(c)} + 1/2\ (1+x)N_2(g)$$

For example, the decomposition temperature of UN is lowered from 3106 K to 2500 K when the nitrogen over pressure is reduced from 2.5×10^5 Pa to 1×10^2 Pa. For a discussion of the effects of low level oxygen content in the U-N-O system, see Reference E-18 and E-19.

The UN phase has a stoichiometry range of 0.995 to 0.997 in the N/U ratio at 1473 K and 0.995 to 1.000 in the N/U ratio between 1773 and 2373 K. [E-17,E-20]

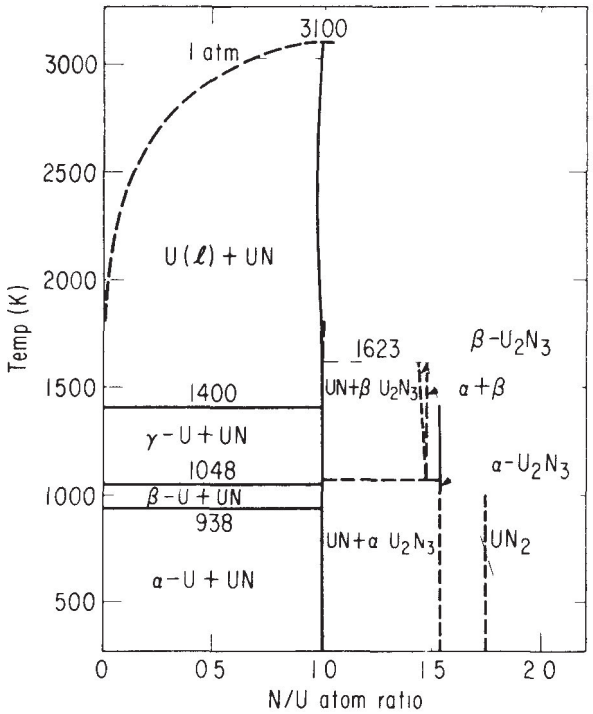

Fig. E-1. Phase Diagram of the U-N System [E-14]

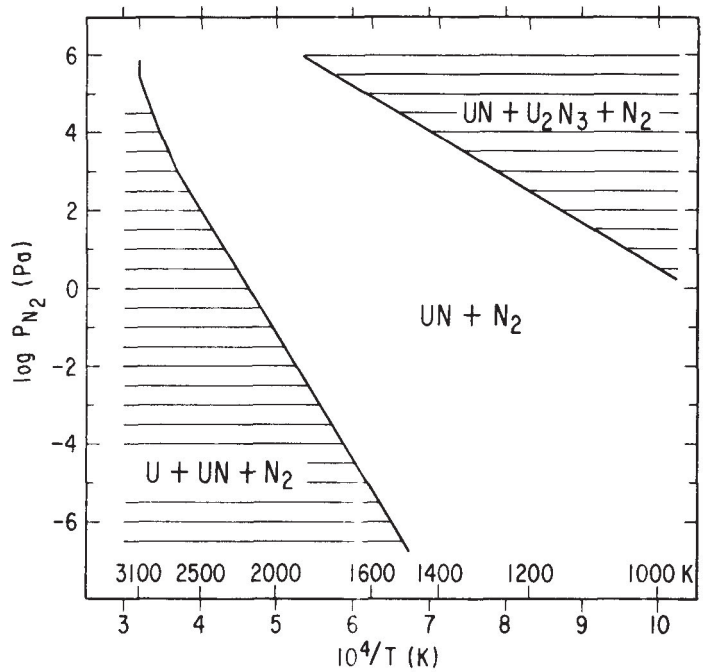

Fig. E-2. Uranium-Nitrogen Phase Diagram [E-14-E-17]

References

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A. Physical

A-1 CRITICAL CONSTANTS — $PuN_{1.00}$

Critical Temperature (estimated) - 9950 K [A-1]

A-2 DENSITY

$PuN_{0.99}$ 298 K $14.24 \pm 0.01 \times 10^3$ kg/m^3 [A-2,A-3]

$$\rho = 1.436 \times 10^4 - 3.74 \times 10^1\ T - 1.22 \times 10^{-4}\ T^2 \quad kg/m^3 \qquad [A-2-A-6]$$

$$(298 < T < 2500\ K)$$

For liquid $PuN_{1.00}$

$$\rho = \frac{16.15 \times 10^3\ kg/m^3}{1 + 1.75 \times 10^{-4}\ T} \quad \text{(estimated)} \qquad [A-1]$$

$$T \geq 2843\ K$$

A-3 EMISSIVITY — $PuN_{1.00}$

$$\varepsilon_{total} = 0.65 \qquad [A-5]$$

(estimated value)

A-4 LATTICE PARAMETER - CRYSTAL STRUCTURE

$PuN_{0.99}$ $4.9055 \pm 0.0003 \times 10^{-10}m$ (298 K) [A-2,A-3]

Face centered cubic, NaCl type [A-2,A-3]

A-5 MELTING POINT

$PuN_{0.95}$ - $PuN_{1.00}$ 2843 ± 30 K [A-7,A-8]

at 1×10^5 Pa Nitrogen pressure

A-6 SURFACE TENSION

A-7 THERMAL EXPANSION

$PuN_{1.00}$, 88% theoretical density

$$\frac{L_T - L_o}{L_o} = -2.64 \times 10^{-3} + 7.70 \times 10^{-6}\ T + 3.70 \times 10^{-9}\ T^2 \qquad [A-4,A-5]$$

$$(298 < T < 2500\ K)$$

References

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B. Thermodynamic

B-1 COMPRESSIBILITY

B-2 ENTHALPY

$$H^\circ_T - H^\circ_{298} = -1.5302 \times 10^4 + 49.7896\ T + 5.23 \times 10^{-3}\ T^2 \quad \text{J/mol} \quad [B\text{-}1]$$

(estimated value) $(298 < T < 2000\ K)$

Calculated values are listed in Table B-1.

For liquid PuN

$$H^\circ_T - H^\circ_{298} = 2.9476 \times 10^4 + 49.8867\ T + 5.8367 \times 10^{-3}\ T^2 \quad \text{J/mol} \quad [B\text{-}2]$$

(estimated value) $(2843 < T < 8000\ K)$

B-3 ENTROPY

$$S^\circ_T = -2.183 \times 10^2 + 49.7896 \ln T + 10.46 \times 10^{-3}\ T \quad \text{J mol}^{-1}\ \text{K}^{-1}$$

$(298 < T < 2000\ K)$

$$S^\circ_{298.15} = 68.5\ \text{J mol}^{-1}\ \text{K}^{-1} \quad [B\text{-}1]$$

Calculated values are listed in Table B-1.

B-4 FREE ENERGY OF FORMATION

$$\Delta G^\circ_{f,T} = -3.1666 \times 10^2 + 8.7538 \times 10^{-2}\ T + 1.3070 \times 10^{-5}\ T^2$$
$$- 7.073 \times 10^{-9}\ T^3 + 1.0175 \times 10^{-12}\ T^4 \quad \text{kJ/mol} \quad [B\text{-}3]$$

$$\sigma = \pm\ 0.025\ \text{kJ/mol}$$

$(298 < T < 2843\ K)$

Calculated values are listed in Table B-1.

Table B-1. Thermodynamic Properties of PuN

Temp, K	$(H_T^\circ - H_{298}^\circ)$, J/mol	C_p°, J/(mol)(K)	S_T°, J/(mol)(K)	$-\Delta G_f^\circ$, kJ/mol	$-\Delta H_f^\circ$, kJ/mol
298	0	52.91	68.47	289.47	316.73
300	106	52.93	68.83	289.28	316.72
400	5451	53.97	84.20	280.17	319.39
500	10900	55.02	96.35	270.42	319.20
600	16455	56.07	106.5	261.16	318.90
700	22113	57.11	115.2	251.12	318.05
800	27877	58.16	122.9	241.49	319.16
900	33745	59.20	129.8	231.85	317.95
1000	39718	60.25	136.1	222.07	319.63
1100	45795	61.30	141.9	212.14	318.38
1200	51977	62.34	147.3	202.79	317.08
1300	58263	63.39	152.3	193.32	315.75
1400	64654	64.43	157.0	183.94	313.97
1500	71150	65.48	161.5	174.69	312.98
1600	77750	66.53	165.8	165.51	311.53
1700	84455	67.57	169.8	156.42	310.05
1800	91264	68.62	173.7	147.43	308.53
1900	98179	69.66	177.5	138.52	306.96
2000	105197	70.71	181.1	129.75	305.37
2100[a]	112320	71.76	184.5	120.96	303.73
2200[a]	119548	72.80	187.9	112.30	302.06
2300[a]	126881	73.85	191.2	103.70	300.35
2400[a]	134318	74.89	194.3	95.19	298.61
2500[a]	141859	75.94	197.4	86.74	296.85
2600[a]	149506	76.99	200.4	78.38	294.91
2700[a]	157257	78.03	203.3	70.10	292.98
2800[a]	165112	79.08	206.2	61.88	291.11

[a]Extrapolated [B-1]

B-5 HEAT CAPACITY

$$C_p^\circ = 49.7896 + 10.46 \times 10^{-3}\ T \quad J\ mol^{-1}\ K^{-1} \qquad [B-1]$$

$$(298 < T < 2000\ K)$$

Calculated values are listed in Table B-1.

For liquid PuN

$$C_p^\circ = 49.8867 + 1.1673 \times 10^{-2}\ T \quad J\ mol^{-1}\ K^{-1} \qquad [B-2]$$

(estimated value) $(2843 < T < 8000\ K)$

B-6 HEAT OF FORMATION

$$\Delta H^\circ_{f,298} = -316.73\ kJ/mol \qquad [B-3]$$

From the tabulated values of $\Delta H^\circ_{f,T}$ (Table B-1), two temperature regions can be identified:

$$\Delta H^\circ_{f,T} = -318.41 \pm 1.46 \quad kJ/mol \qquad [B-3]$$

$$(300 < T < 1100\ K)$$

$$\Delta H^\circ_{f,T} = -3.3956 \times 10^2 + 2.5065 \times 10^{-2}\ T - 7.28 \times 10^{-6}\ T^2 + 1.639 \times 10^{-9}\ T^3\ kJ/mol\ \sigma = \pm 0.2\ kJ/mol \qquad [B-3]$$

$$(1200 < T < 2843\ K)$$

B-7 HEAT OF FUSION

49.96 kJ/mol (estimated value) [B-2]

B-8 HEAT OF SUBLIMATION

The heat of sublimation for PuN is 586 ± 12 kJ/mol (1600 < T < 2800 K) estimated from the partial pressure of PuN (g) over PuN (c) in the solid region (see property B-10) using the relationship:

$$\frac{d\ \ln P}{d(1/T)} = \frac{-\Delta H_{subl}}{R}$$

where R = gas constant

B-9 HEAT OF VAPORIZATION

536 ± 12 kJ/mol (estimated value)

Estimated from the partial pressure of PuN (g) over PuN (c) in the liquid region (property B-10) in the same manner as the heat of sublimation.

B-10 VAPOR PRESSURE

Plutonium nitride can vaporize congruently requiring that the number of moles of plutonium vaporizing per unit time be exactly twice the molar rate of nitrogen vaporizing. Recommended equations for the partial pressures of plutonium and nitrogen are:

$$\log P_{Pu}(Pa) = 10.99 - (21056/T) \qquad [B-4]$$

$$\log P_{N_2}(Pa) = 10.22 - (20967/T) \qquad [B-4]$$

$$(1400 < T < 2400\ K)$$

Alexander and co-workers [B-1] estimated the partial pressure of PuN species as:

$$\log P_{PuN}(Pa) = 13.30 - (30600/T) \qquad [B-1]$$

Partial pressures of Pu_2 species is given by:

$$\log P_{Pu_2}(Pa) = 12.28 - (30300/T) \qquad [B-2]$$

Adding all the partial pressures, one obtains the total pressure, P_T which is given by:

$$P_T = P_{Pu} + P_{N_2} + P_{PuN} + P_{Pu_2}$$

$$\log P_T(Pa) = 7.7598 - (20329/T) + 0.89151 \log T \qquad [B-2]$$

For liquid PuN, estimated partial pressures at 2900 < T < 8000 K are:

$$\log P_{Pu}(Pa) = 10.08 - (18400/T) \qquad [B-2]$$

$$\log P_{N_2}(Pa) = 8.39 - (15700/T)$$

$$\log P_{PuN}(Pa) = 12.39 - (28000/T)$$

$$\log Pu_2(Pa) = 10.45 - (25100/T)$$

$$\log P_T(Pa) = -4.7131 - (15234/T) + 3.984 \log T$$

$$P_T = P_{Pu} + P_{PuN} + P_{Pu_2} + P_{N_2}$$

B-5 HEAT CAPACITY

$$C_p^\circ = 49.7896 + 10.46 \times 10^{-3}\ T \quad J\ mol^{-1}\ K^{-1} \qquad [B-1]$$

$$(298 < T < 2000\ K)$$

Calculated values are listed in Table B-1.

For liquid PuN

$$C_p^\circ = 49.8867 + 1.1673 \times 10^{-2}\ T \quad J\ mol^{-1}\ K^{-1} \qquad [B-2]$$

(estimated value) $(2843 < T < 8000\ K)$

B-6 HEAT OF FORMATION

$$\Delta H^\circ_{f,298} = -316.73\ kJ/mol \qquad [B-3]$$

From the tabulated values of $\Delta H^\circ_{f,T}$ (Table B-1), two temperature regions can be identified:

$$\Delta H^\circ_{f,T} = -318.41 \pm 1.46 \quad kJ/mol \qquad [B-3]$$

$$(300 < T < 1100\ K)$$

$$\Delta H^\circ_{f,T} = -3.3956 \times 10^2 + 2.5065 \times 10^{-2}\ T - 7.28 \times 10^{-6}\ T^2 + 1.639 \times 10^{-9}\ T^3\ kJ/mol\ \sigma = \pm 0.2\ kJ/mol \qquad [B-3]$$

$$(1200 < T < 2843\ K)$$

B-7 HEAT OF FUSION

49.96 kJ/mol (estimated value) [B-2]

B-8 HEAT OF SUBLIMATION

The heat of sublimation for PuN is 586 ± 12 kJ/mol (1600 < T < 2800 K) estimated from the partial pressure of PuN (g) over PuN (c) in the solid region (see property B-10) using the relationship:

$$\frac{d\ \ln P}{d(1/T)} = \frac{-\Delta H_{subl}}{R}$$

where R = gas constant

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B-9 HEAT OF VAPORIZATION

536 ± 12 kJ/mol (estimated value)

Estimated from the partial pressure of PuN (g) over PuN (c) in the liquid region (property B-10) in the same manner as the heat of sublimation.

B-10 VAPOR PRESSURE

Plutonium nitride can vaporize congruently requiring that the number of moles of plutonium vaporizing per unit time be exactly twice the molar rate of nitrogen vaporizing. Recommended equations for the partial pressures of plutonium and nitrogen are:

$$\log P_{Pu}(pa) = 10.99 - (21056/T) \qquad [B-4]$$

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$$(1400 < T < 2400 \text{ K})$$

Alexander and co-workers [B-1] estimated the partial pressure of PuN species as:

$$\log P_{PuN}(pa) = 13.30 - (30600/T) \qquad [B-1]$$

Partial pressures of Pu_2 species is given by:

$$\log P_{Pu_2}(pa) = 12.28 - (30300/T) \qquad [B-2]$$

Adding all the partial pressures, one obtains the total pressure, P_T which is given by:

$$P_T = P_{Pu} + P_{N_2} + P_{PuN} + P_{Pu_2}$$

$$\log P_T(pa) = 7.7598 - (20329/T) + 0.89151 \log T \qquad [B-2]$$

For liquid PuN, estimated partial pressures at 2900 < T < 8000 K are:

$$\log P_{Pu}(pa) = 10.08 - (18400/T) \qquad [B-2]$$

$$\log P_{N_2}(pa) = 8.39 - (15700/T)$$

$$\log P_{PuN}(pa) = 12.39 - (28000/T)$$

$$\log Pu_2(pa) = 10.45 - (25100/T)$$

$$\log P_T(pa) = -4.7131 - (15234/T) + 3.984 \log T$$

$$P_T = P_{Pu} + P_{PuN} + P_{Pu_2} + P_{N_2}$$

DO NOT FILM

References

[B-1] C. A. Alexander, *et al.*, BMI-X-659 (1975).

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[B-3] F. L. Oetting, Chem. Rev. *67*, 261 (1967).

[B-4] A. Sheth and L. Leibowitz, ANL-AFP-2, (October 1974).

C. Mechanical

C-1 CREEP

a. Steady State

b. Irradiation Induced

C-2 ELASTIC CONSTANT

a. Elastic Stiffness Moduli at 298 K

b. Shear Modulus

c. Bulk Modulus

d. Poisson's Ratio

C-3 FRACTURE STRESS

C-4 HARDNESS

	Hardness, 10^6 kg/m^2		
	300 K	1273 K	
PuN	320	75	[C-1]

For diamond point hardness (DPH), 10 DPH = 10 x 10^6 kg/m^2

C-5 STRESS RELAXATION

C-6 THERMAL SHOCK RESISTANCE

C-7 YIELD STRESS

C-8 YOUNG'S MODULUS

References

[C-1] M. Tokar, A. W. Nutt, and J. A. Leary, LA-4452 (1972).

D. Transport

D-1 DIFFUSION

D-2 ELECTRICAL RESISTIVITY

D-3 GRAIN GROWTH

D-4 SEEBECK COEFFICIENT

D-5 THERMAL CONDUCTIVITY

$$\lambda_{TD} = 3.38 + 1.85 \times 10^{-2}\ T - 9.49 \times 10^{-6}\ T^2\ W\ m^{-1}\ K^{-1} \qquad [D-1]$$

$$(480 < T < 1100\ K)$$

$\lambda_{TD} = \lambda\ (1 + P)/(1-P)$

λ_{TD} = conductivity of 100% theoretically dense material

λ = conductivity of low density material

P = volume fraction porosity

For liquid PuN

$$\lambda_{TD} = 15.5\ \ W\ m^{-1}\ K^{-1} \qquad [D-2]$$

(estimated value) ($T \geqslant 2843$ K)

D-6 THERMAL DIFFUSIVITY

$$\alpha = \frac{\lambda}{\rho C_p}$$

α = thermal diffusivity

λ = thermal conductivity (property D-5)

ρ = density (property A-2)

C_p = heat capacity (property B-5)

D-7 VISCOSITY

$$\mu = 4 \times 10^{-3}\ \ \text{Pa-sec} \qquad [D-2]$$

(estimated value) ($T \geqslant 2843$ K)

References

[D-1] D. L. Keller, *Annual Report*, BMI-1845, p. A-60 (1968).

[D-2] A. Sheth, Argonne National Laboratory, private communication (1976).

E. Chemical

E-1 COMPATIBILITY

Hypostoichiometric

Contains free Pu metal which reacts rapidly with the cladding [E-1]

Nitriding

In general, no difference in nitriding is observed between helium *vs.* sodium bonding [E-2,E-3]

Temperature

No large temperature dependence of nitriding in tests up to 1270 K [E-1,2,4,5]

No difference in nitriding between SS 316 and NIMONIC PE-16, the only advanced alloys tested. (The advanced alloys are 316 SS-20% CW, 330 SS, A286, M813, PE-16, Incoloy 706, Inconel 718, Incoloy 901, and HT-9.) [E-5]

For further details, see ANL-AFP-9.

E-2 KINETICS

E-3 PHASE EQUILIBRIUM

See Fig. E-1, phase diagram of the Pu-N system. [E-6]

The PuN phase has a stoichiometry range of 0.04 in the N/Pu ratio. [E-7]

FIGURE REDACTED FOR COPYRIGHT

Fig. E-1. Phase Diagram of the Pu-N System [E-6]

References

[E-1] W. M. Pardue, V. W. Storhok, and R. A. Smith, *Plutonium 1965*, Chapman and Hall, London, p. 721.

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[E-7] C. A. Alexander, J. S. Ogden and M. P. Rausch, BMI-X-659 (1975).

A. Physical

A-1 CRITICAL CONSTANTS — $(U_{0.80}Pu_{0.20})N_{1.00}$

Critical temperature (estimated) - 10690 K [A-1]

A-2 DENSITY — $(U_{0.80}Pu_{0.20})N_{1.00}$

0.7% ^{235}U, 99.3% ^{238}U
88-94% ^{239}Pu, 6-12% ^{240}Pu 298 K $14.31 \pm 0.01 \times 10^3$ kg/m^3 [A-2-A-4]

93% ^{235}U, 7% ^{238}U
88-94% ^{239}Pu, 6-12% ^{240}Pu 298 K $14.18 \pm 0.01 \times 10^3$ kg/m^3 [A-2-A-4]

$(^{235}U_{0.80}\ ^{239}Pu_{0.20})N_{1.00}$ [A-2-A-6]

$$\rho = 1.428 \times 10^4 - 3.04 \times 10^{-1}\ T - 5.91 \times 10^{-5}\ T^2\ \text{kg/m}^3$$

$$(298 < T < 1800\ \text{K})$$

For liquid $(U_{0.80}Pu_{0.20})N$

$$\rho = \frac{14.36 \times 10^3\ \text{kg/m}^3}{1 + 8.65 \times 10^{-5}\ T} \quad \text{(estimated)} \quad T \geq 3053\ \text{K}$$ [A-1]

A-3 EMISSIVITY — $(U_{0.80},Pu_{0.20})N_{1.00}$

$$\varepsilon_{Total} = 0.65$$ [A-7]

(estimated value)

A-4 LATTICE PARAMETER - CRYSTAL STRUCTURE

$(U_{0.80}Pu_{0.20})N_{1.00}$ $4.8916 \pm 0.0012 \times 10^{-10}$m (298 K) [A-2-A-4]

Face centered cubic, NaCl type [A-2-A-4]

A-5 MELTING POINT

$(U_{0.8}Pu_{0.2})N_{0.99\pm0.01}$ 3053 ± 20 K [A-8]

at 1×10^5 Pa nitrogen pressure

A-6 SURFACE TENSION

A-7 THERMAL EXPANSION

$(U_{0.8}Pu_{0.2})N$, unknown density

$$\frac{L_T - L_o}{L_o} = -2.26 \times 10^{-3} + 6.95 \times 10^{-6}\ T + 1.63 \times 10^{-9}\ T^2 \qquad [A\text{-}5]$$

$$(298 < T < 1800\ K)$$

References

A-1 A. Sheth, Argonne National Laboratory, private communication (1975).

A-2 V. J. Tennery and E. S. Bomar, J. Am. Ceram. Soc. *54*, 247 (1971).

A-3 LA-3431-MS (1965), p. 44.

A-4 F. Anselin, J. Nucl. Mater. *10*, 301 (1963).

A-5 C. A. Alexander, J. S. Ogden, and W. M. Pardue, *Plutonium 1970*, The Metallurgical Society, AIMMPE, New York, Vol. I, p. 95.

A-6 For method, see J. F. Andrew and T. W. Latimer, LA-6037-MS (1975).

A-7 C. A. Alexander, J. S. Ogden and M. P. Rausch, BMI-X-659 (1975).

A-8 E. T. Weber, BNWL-843, Section 6.1 (1968).

B. Thermodynamic

B-1 COMPRESSIBILITY

B-2 ENTHALPY — $(U_{0.8}Pu_{0.2})N$

$$H_T^\circ - H_{298}^\circ = -1.3999 \times 10^4 + 45.3546\ T + 5.4392 \times 10^{-3}\ T^2\ \text{J/mol} \qquad [B-1]$$

$$(298 < T < 1800\ \text{K})$$

Calculated values are listed in Table B-1.

For liquid $(U_{0.8}Pu_{0.2})N$

$$H_T^\circ - H_{298}^\circ = 4.3735 \times 10^4 + 49.8867\ T + 3.4123 \times 10^{-3}\ T^2\ \text{J/mol} \qquad [B-2]$$

(estimated value) $(3053 < T < 8600\ \text{K})$

B-3 ENTROPY

B-4 FREE ENERGY OF FORMATION

B-5 HEAT CAPACITY — $(U_{0.8}Pu_{0.2})N$

$$C_p^\circ = 45.3546 + 10.8784 \times 10^{-3}\ T \quad \text{J mol}^{-1}\ \text{K}^{-1} \qquad [B-1]$$

$$(298 < T < 1800\ \text{K})$$

Calculated values are listed in Table B-1.

For liquid $(U_{0.8}Pu_{0.2})N$

$$C_p^\circ = 49.8867 + 6.8245 \times 10^{-3}\ T \quad \text{J mol}^{-1}\ \text{K}^{-1} \qquad [B-2]$$

$$(298 < T < 1800\ \text{K})$$

(estimated value) $(3053 < T < 8000\ \text{K})$

Table B-1. Thermodynamic Properties of $(U_{0.8}Pu_{0.2})N$

Temp, K	$(H^\circ_T - H^\circ_{298})$, J/mol	C°_p, J/(mol)(K)
298	0	48.60
300	97	48.62
400	5013	49.71
500	10038	50.79
600	15172	51.88
700	20414	52.97
800	25766	54.06
900	31226	55.14
1000	36795	56.23
1100	42472	57.32
1200	48259	58.41
1300	54154	59.50
1400	60158	60.58
1500	66271	61.67
1600	72493	62.76
1700	78823	63.85
1800	85262	64.94
1900[a]	91810	66.02
2000[a]	98467	67.11
2100[a]	105233	68.20
2200[a]	112107	69.29
2300[a]	119090	70.37
2400[a]	126182	71.46
2500[a]	133382	72.55
2600[a]	140692	73.64
2700[a]	148110	74.73
2800[a]	155637	75.81
2900[a]	163273	76.90
3000[a]	171018	77.99

[a]Extrapolated [B-1]

B-6 HEAT OF FORMATION — $(U_{0.8}Pu_{0.2})N$

$$\Delta H^{\circ}_{f,298} = 297.49 \text{ kJ/mol (estimated value)} \quad [B-3]$$

B-7 HEAT OF FUSION — $(U_{0.8}Pu_{0.2})N$

52.68 kJ/mol (estimated value) [B-2]

B-8 HEAT OF SUBLIMATION — $(U_{0.8}Pu_{0.2})N$

Gaseous species such as UN (g) and PuN (g) have not been identified above $(U_{0.8}Pu_{0.2})N$ condensed phase; however, for a hypothetical case assuming an ideal solution behavior, the estimated value for the heat of sublimation is given by:

704 kJ/mol (estimated value)

B-9 HEAT OF VAPORIZATION — $(U_{0.8}Pu_{0.2})N$

649 kJ/mol (estimated value)

Estimated in the same manner as heat of sublimation.

B-10 VAPOR PRESSURE — $(U_{0.8}Pu_{0.2})N$

$$\log P_U(\text{Pa}) = 12.67 - (30416/T) \quad [B-4]$$

$$\log P_{Pu}(\text{Pa}) = 10.26 - (20893/T) \quad [B-4]$$

$$\log P_{N_2}(\text{Pa}) = 9.58 - (21089/T) \quad [B-4]$$

$$(1400 < T < 2400 \text{ K})$$

Above equations were derived from the experimental values reported by Potter [B-5], and Keller. [B-6]

For liquid $(U_{0.8}Pu_{0.2})N$

Estimation for total pressure over $(U_{0.8}Pu_{0.2})N$ was made assuming an ideal solution of UN and PuN. The total pressure, P_T, in the temperature range $3100 < T < 8000$ K is represented by:

$$\log P_T(\text{Pa}) = 8.013 - (22886/T) + 0.98591 \log T \quad [B-2]$$

References

[B-1] C. A. Alexander, *et al.*, BMI-X-659 (1975).

[B-2] A. Sheth, Argonne National Laboratory, private communication (1975).

[B-3] C. A. Alexander, and J. S. Ogden, BMI-1848 (1968).

[B-4] A. Sheth, and L. Leibowitz, ANL-AFP-2 (1974).

[B-5] P. E. Potter, J. Nucl. Mater. *47*, 7 (1973).

[B-6] D. L. Keller, BMI-1845, pp. A-60 (1968).

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B-8 HEAT OF SUBLIMATION — $(U_{0.8}Pu_{0.2})N$

Gaseous species such as UN (g) and PuN (g) have not been identified above $(U_{0.8}Pu_{0.2})N$ condensed phase; however, for a hypothetical case assuming an ideal solution behavior, the estimated value for the heat of sublimation is given by:

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B-9 HEAT OF VAPORIZATION — $(U_{0.8}Pu_{0.2})N$

649 kJ/mol (estimated value)

Estimated in the same manner as heat of sublimation.

B-10 VAPOR PRESSURE — $(U_{0.8}Pu_{0.2})N$

$$\log P_U(pa) = 12.67 - (30416/T) \quad [B-4]$$

$$\log P_{Pu}(pa) = 10.26 - (20893/T) \quad [B-4]$$

$$\log P_{N_2}(pa) = 9.58 - (21089/T) \quad [B-4]$$

$$(1400 < T < 2400 \text{ K})$$

Above equations were derived from the experimental values reported by Potter [B-5], and Keller. [B-6]

For liquid $(U_{0.8}Pu_{0.2})N$

Estimation for total pressure over $(U_{0.8}Pu_{0.2})N$ was made assuming an ideal solution of UN and PuN. The total pressure, P_T, in the temperature range $3100 < T < 8000$ K is represented by:

$$\log P_T(pa) = 8.013 - (22886/T) + 0.98591 \log T \quad [B-2]$$

References

[B-1] C. A. Alexander, *et al.*, BMI-X-659 (1975).

[B-2] A. Sheth, Argonne National Laboratory, private communication (1975).

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[B-4] A. Sheth, and L. Leibowitz, ANL-AFP-2 (1974).

[B-5] P. E. Potter, J. Nucl. Mater. *47*, 7 (1973).

[B-6] D. L. Keller, BMI-1845, pp. A-60 (1968).

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C. Mechanical

C-1 CREEP

C-2 ELASTIC CONSTANTS

a. Poisson's Ratio (P = 0)

$$\nu = 0.275 \quad (298\ K) \qquad [C-1]$$

b. Shear Modulus (P = 0)

$$G = E/2\ (1 + \nu) = 1.02 \times 10^{11}\ Pa \quad (298\ K) \qquad [C-2]$$

c. Bulk Modulus (P = 0)

$$K = E/3\ (1 - 2\nu) = 1.925 \times 10^{11}\ Pa \quad (298\ K) \qquad [C-3]$$

P = volume fraction porosity

E = Young's Modulus (Property C-8)

C-3 FRACTURE STRESS

C-4 HARDNESS

	Hardness, 10^6 kg/m^2		
	300 K	1273 K	
$(U_{0.7}Pu_{0.3})N$	500	160	[C-3]

For diamond point hardness (DPH), 10 DPH = 10×10^6 kg/m^2

C-5 STRESS RELAXATION

C-6 THERMAL SHOCK RESISTANCE

C-7 YIELD STRESS

C-8 YOUNG'S MODULUS

$$E = 2.6\ (1 - 2.22P) \times 10^{11}\ \text{Pa}\ (298\ \text{K}) \qquad [C\text{-}2, C\text{-}3]$$

$$P = \text{volume fraction porosity}$$

$$1\ \text{Pa} = 1\ \text{Newton/m}^2$$

References

[C-1] A. Padel, A. Groff, and C. H. deNovion, J. Nucl. Mater. *36*, 297 (1970).

[C-2] R. N. Singh, Argonne National Laboratory, private communication.

[C-3] P. M. French and D. J. Hodkin, in *Plutonium 1965*, publisher: Chapman and Hall, London, 697 (1967).

D. Transport

D-1 DIFFUSION

D-2 ELECTRICAL RESISTIVITY

$(U_{0.8}Pu_{0.2})N$ 100% T.D.

$$\rho = 3.5 \times 10^{-6}\ \Omega\ m \qquad [D\text{-}1]$$

(estimated value) ($T \lesssim 400$ K)

D-3 GRAIN GROWTH

D-4 SEEBECK COEFFICIENT

D-5 THERMAL CONDUCTIVITY

$(U_{0.80}Pu_{0.20})N$ 93% T.D.

$$\lambda = 8.95 + 8.29 \times 10^{-3}\ T - 1.29 \times 10^{-6}\ T^2 \quad W\ m^{-1}\ K^{-1} \qquad [D\text{-}2]$$

($400 < T < 1900$ K)

$\lambda_{TD} = \lambda\ (1 + P)/(1 - P)$

λ_{TD} = conductivity of 100% theoretically dense material

λ = conductivity of low density material

P = volume fraction porosity

For liquid $(U_{0.80}Pu_{0.20})N$

$$\lambda_{TD} = 20.5 \quad W\ m^{-1}\ K^{-1} \qquad [D\text{-}3]$$

(estimated value) ($T \gtrsim 3053$ K)

D-6 THERMAL DIFFUSIVITY

$$\alpha = \frac{\lambda}{\rho C_p}$$

α = thermal diffusivity

λ = thermal conductivity (property D-5)

ρ = density (property A-2)

C_p = heat capacity (property B-5)

D-7 VISCOSITY

$(U_{0.80}Pu_{0.20})N$

$$\mu = 4 \times 10^{-3} \text{ Pa-sec} \qquad [D-3]$$

(estimated value) ($T \geqslant 3053$ K)

References

[D-1] C. A. Alexander, J. S. Ogden and M. P. Rausch, BMI-X-659 (1975).

[D-2] C. A. Alexander, J. S. Ogden and W. M. Pardue, Nucl. Met. Soc. AIME *17*, 95 (1970).

[D-3] A. Sheth, Argonne National Laboratory, private communication (1976).

E. Chemical

E-1 COMPATIBILITY

Hypostoichiometric

Contains free U and Pu metal which reacts rapidly with cladding [E-1 - E-5]

Hyperstoichiometric

Contains U_2N_3, leads to greater nitriding of the cladding [E-2,E-5]

Nitriding

In general, no difference in nitriding is observed between helium *vs.* sodium bonding. [E-1,2,3,5,6,7]

Fission Products

Do not appear to migrate to the cladding and do not participate in cladding attack [E-1,3,5,7]

Concurrently, in general there is no redistribution of uranium and plutonium in irradiated fuel. However, plutonium redistribution during thermal irradiation has been reported. [E-1]

Temperature

No large temperature dependence of nitriding in tests up to 1270 K for SS 316, the only advanced alloy tested. (The advanced alloys are 316-SS-20% CW, 330 SS, A286, M813, PE-16, Inconel 706, Inconel 718, Incoloy 901, and HT-9.) [E-1,3,7]

For further details, see ANL-AFP-9.

E-2 KINETICS

E-3 PHASE EQUILIBRIUM

See Fig. E-1, phase diagram of the U-Pu-N system. [E-8,E-9]

References

[E-1] D. L. Keller, BMI-1837 (1968).

[E-2] D. L. Keller, BMI-1845 (1968).

[E-3] W. M. Pardue, A. A. Bauer, and D. L. Keller, *Proc. Inter. Symp. on Ceramic Nuclear Fuels*, American Ceramic Society, p. 166 (1969).

[E-4] J. C. Hebeisen, D. P. Moak, and W. H. Pfeifer, BMI-1895 (1971).

[E-5] A. A. Bauer, Reactor Technology *15*, 87 (1972).

[E-6] W. M. Pardue, F. A. Rough, and R. A. Smith, Nuclear Metallurgy *13*, 369 (1968).

[E-7] J. C. Hebeisen, D. P. Moak, and J. H. Saling, Trans. Amer. Nucl. Soc. *12*, 595 (1969).

[E-8] H. Holleck, *Thermodynamics of Nuclear Materials*, Symposium Proceedings, Vienna, October 21-25, 1974, Vol. II, p. 213, IAEA (1975).

[E-9] P. E. Potter, J. Nucl. Mater. *47*, 7 (1973).

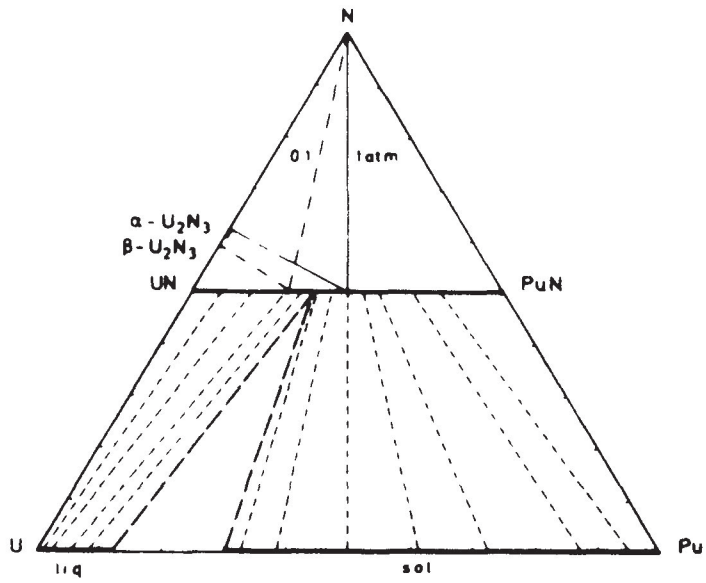

Fig. E-1. Calculated Isothermal Sections in the U-Pu-N System at 1270 K [E-8,E-9]