

HANDBOOK OF REFRACTORY CARBIDES AND NITRIDES

**Properties, Characteristics,
Processing and Applications**

by

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1

Introduction

1.0 HISTORICAL PERSPECTIVE OF REFRACTORY CARBIDES

Refractory carbides have found a wide range of industrial applications and have become a subject of great interest to the metallurgist. Many of the applications are recent, but some have been known for over one hundred years. The first carbide extracted from steel and used in the nineteenth century. In 1891, the carbide, trademarked *Carborundum*, was synthesized by Moissan in an electric arc-furnace. Titanium carbide was identified by chemical analysis in 1907. The interest in this material will be presented in this chapter.

The industrial importance of refractory carbides is growing rapidly, not only because of their strength and resistance to wear, but also because of their use in tools and abrasives, but also in the field of opto-electronics. Some of the applications of refractory carbides are discussed in this chapter.

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Interstitial Nitrides: Properties and General Characteristics

1.0 GENERAL PROPERTIES OF INTERSTITIAL NITRIDES

This chapter is a review of the properties and general characteristics of the interstitial nitrides formed by the metals of Group IV (titanium, zirconium, and hafnium) and Group V (vanadium, niobium, and tantalum). As mentioned in Ch. 10, these six nitrides are the only refractory transition-metal nitrides. They have similar properties and characteristics and, of the six, titanium nitride has the greatest importance from an application standpoint.

These nitrides are produced mostly in the form of coatings or powders. The fabrication processes and the applications for each nitride are summarized in Secs. 6-11 and reviewed in more detail in Chs. 14, 15, and 16.

2.0 PHYSICAL AND THERMAL PROPERTIES OF INTERSTITIAL NITRIDES

In this section and the next three, the properties of the interstitial nitrides of Group IV and V are examined and compared with those of the

parent metals and the corresponding carbides. The values given are those for composition as close to stoichiometry as possible.^{[1]-[11]} Like the interstitial carbides, interstitial nitrides are essentially non-stoichiometric compounds which accounts in part for the variations in the property values reported in the literature. The values given here should be considered typical.

The properties of interstitial nitrides have not been studied as extensively as those of the interstitial carbides and many gaps remain, particularly in determining the effects of composition and impurities, the thermodynamic functions, and the mechanical properties.

2.1 Composition and Stoichiometry

Unlike the interstitial monocarbides, MC_x , where C is never >1 , the interstitial mononitrides, MN_x , can have a composition where $x >1$. In substoichiometric compositions ($x < 1$), the sublattice of nitrogen is predominantly deficient while at hyperstoichiometric compositions ($x > 1$), the metal lattice is predominantly deficient. The lattice parameter is at a maximum at stoichiometry. Even at stoichiometry, a substantial fraction of both nitrogen and metal sites are usually vacant.

2.2 Density and Melting Point

The density and melting point of interstitial nitrides are shown in Table 11.1 and compared with the values for corresponding carbides and host metals.

As could be expected, the density increases considerably with the increasing atomic number of the metal. The melting point of the nitrides is lower in every case than that of the corresponding carbides but, with the exception of NbN, higher than the parent metals. At a nitrogen pressure of 1 MPa, the nitrides of Group IV melt without decomposition but those of Group V decompose (see Table 10.6, Ch. 10 for a comparison of bond energies).

Table 11.1: Density and Melting Point of Interstitial Nitrides and Other Refractory Compounds

Material	Density (g/cm ³)	Melting Point °C
TiN	5.40	2950
ZrN	7.32	2980
HfN	13.8	3387
VN	6.0	2177*
NbN	7.3	near 2400*
TaN	14.3	3093*
TiC	4.91	3067
ZrC	6.59	3420
HfC	12.67	3928
VC	5.65	2830
NbC	7.79	3600
TaC	14.5	3950
Ti	4.54	1660
Zr	6.51	1850
Hf	13.36	2230
V	6.11	1890
Nb	8.56	2468
Ta	16.6	2996

* decomposes

2.3 Thermal Properties

Thermal properties are summarized in Table 11.2.

Table 11.2: Thermal Properties of Interstitial Nitrides and Other Refractory Compounds

Compound	Specific Heat at 298K (J/mole·K)	Thermal Conductivity at 20°C (W/m·K)	Thermal Expansion at 20°C ($\times 10^{-6}/^{\circ}\text{C}$)
TiN	33.74	19.2	9.35
ZrN	40.39	20.5	7.24
HfN	38.01	21.7	6.9
VN	38.00	11.29	8.7
NbN	39.01	3.76	10.1
TaN	40.60	8.78	8.0
TiC	33.8	21	7.4
ZrC	37.8	20.5	6.7
HfC	33.4	20.0	6.6
VC	32.3	24.7	7.3
NbC	36.8	14.22	6.6
TaC	36.4	22.17	6.3
Ti	25.05	21.9	8.5
Zr	26.05	22.7	
Hf	26.27	23.0	6.0
V	24.75	30.7	8.0
Nb	24.43	53.7	7.3
Ta	25.33	57.5	6.5

2.4 Thermal Conductivity

A discussion on the thermal conductivity of refractory carbides and nitrides is given in Ch. 4, Sec. 2.4. As can be seen in Table 11.2, the nitrides of Groups IV and V, like the corresponding carbides, can be considered good thermal conductors, reflecting the metallic character of

Refractory

these materials.^[12] However, their thermal conductivity is still considerably lower than the best conductors such as aluminum nitride (220 W/m·K) (see Ch. 13, Sec. 3.0). Their thermal conductivity generally increases slightly with increasing temperature as shown in Fig. 11.1 (reliable data not available for NbN and TaN).^[5]

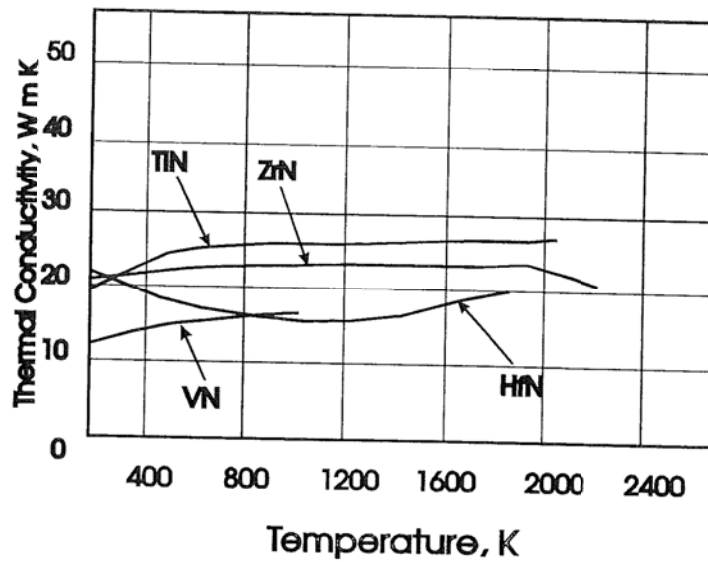


Figure 11.1: Thermal conductivities of the interstitial nitrides vs. temperature.

2.5 Thermal Expansion

The observations on thermal expansion of refractory carbides in Sec. 2.0 of Ch. 4 are applicable to the refractory nitrides. Table 11.3 shows that generally the higher the bond energy of the compound, the lower the expansion.

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Table 11.3: Bond energy and Thermal Expansion of Refractory Nitrides

Nitride	Bond Energy E_o , eV	Thermal Expansion at 20°C ($\times 10^{-6}/^{\circ}\text{C}$)
Group IV	TiN	9.35
	ZrN	7.24
	HfN	6.9
Group V	VN	8.7
	NbN	10.1
	TaN	8.8

As shown in Fig. 11.2, thermal expansion is essentially linear with increasing temperature (data available for Group IV nitrides only).^[5]

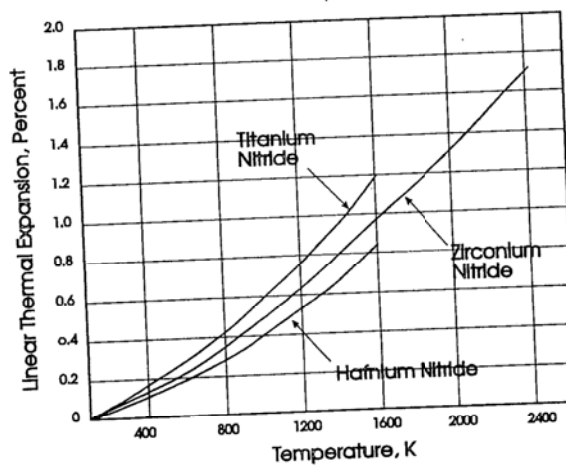


Figure 11.2: Linear thermal expansions of the interstitial nitrides vs. temperature.

3.0 ELECTRICAL PROPERTIES OF INTERSTITIAL NITRIDES

A discussion on the electrical properties of interstitial carbides and nitrides is given in Ch. 4, Sec. 3.0. The electrical properties of these materials are shown in Table 11.4.^{[4][10][11][13]}

Table 11.4: Electrical Properties of Group IV and V Interstitial Nitrides and Carbides at 20°C.

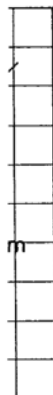
Compound	Electrical Resistivity at 20°C ($\mu\Omega\cdot\text{cm}$)	Hall Constant at 20°C ($10^{-4} \text{ cm}^3/\text{A}\cdot\text{s}$)	Magnetic Susceptibility* (10^{-6} emu/mol)
TiN	20 ± 10	-0.7 ± 0.2	+38
ZrN	7-21	-1.3	+22
HfN	33		
VN	85		
NbN	58	-0.52	+31
TaN	135		
TiC	68	-15.0	-7.5
ZrC	43	-9.41	-30
HfC	37	-12.4	-37
VC	60	-0.48	+35
NbC	35	-1.3	+20
TaC	25	-1.1	+12

As shown in the above table, the interstitial nitrides are relatively good electrical conductors although with a resistivity slightly higher than that of the corresponding carbides and the parent metals, but still reflecting the essentially metallic character of these compounds. The electrical resistivity of TiN (and presumably of the other interstitial nitrides) increases almost linearly with temperature as shown in Fig. 11.3.^[10]

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Superconductivity. The interstitial nitrides are all good superconductors but their transition temperatures may be considerably affected by the presence of vacancies and impurities such as oxygen (see Secs. 6–11 for values).^[13]

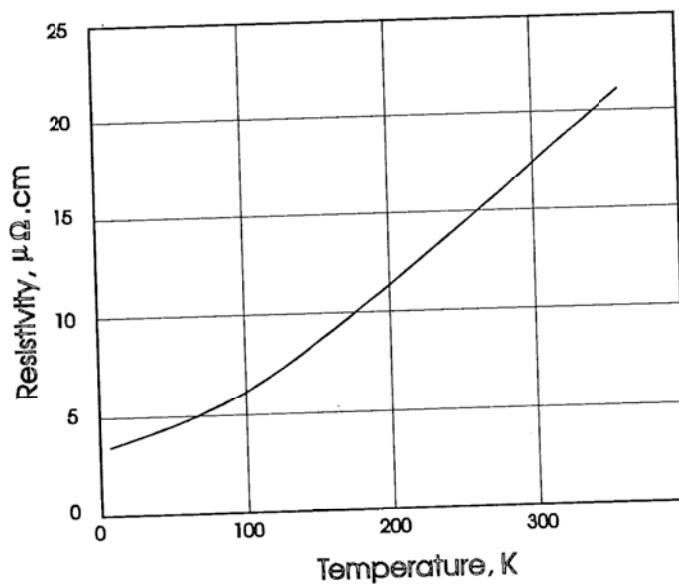


Figure 11.3: Resistivity of a single-crystal titanium nitride.

4.0 MECHANICAL PROPERTIES OF INTERSTITIAL NITRIDES

A discussion on the mechanical properties of both interstitial carbides and nitrides is given in Ch. 4, Sec. 4.0. Large spreads in the reported values are common and are related to differences in stoichiometry, impurity levels, and fabrication processes.

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4.1 Summary of Mechanical Properties

The observations on failure mechanism, ductile-brittle transition, and hardness of the interstitial carbides (Ch. 4, Secs. 4.3 and 4.4) are applicable to the interstitial nitrides. These materials have a ductile-brittle transition temperature of approximately 800°C.

Little information is available on the mechanical properties of the interstitial nitrides and what has been published is summarized in Table 11.5 and compared with properties of the equivalent interstitial carbides. The values are averages reported in the recent literature.^{[1][4]-[7][14][15]}

4.2 Hardness

As shown in Table 11.5, the hardness of the interstitial nitrides is somewhat lower than that of the corresponding carbides. The Group IV nitrides generally have higher hardnesses than those of Groups V. This reflects the greater contribution of M-N bonding found in these compounds.

Table 11.5: Mechanical Properties of Group IV and V Interstitial Nitrides and Carbides at 20°C

Compound	Vickers Hardness (GPa)	Young's Modulus of Elasticity (GPa)
TiN	18-21	251
ZrN	15.8	397
HfN	16.3	
VN	14.2	357
NbN	13.3	493
TaN	11.0	
TiC	28-35	410-510
ZrC	25.9	350-440
HfC	26.1	350-510
VC	27.2	430
NbC	19.6	338-580
TaC	16.7	285-560

Hardness vs. Composition. Hardness varies with composition as shown in Fig. 11.4.^{[1][11]} The hardness of the interstitial nitrides of Group IV (TiN, ZrN, and presumably HfN) reaches a maximum at stoichiometry while the maximum hardness of the nitrides of Group V (NbN, TaN, and presumably VN) occurs before stoichiometry is reached. A similar behavior is observed for the corresponding carbides (see Fig. 4.5 of Ch. 4).

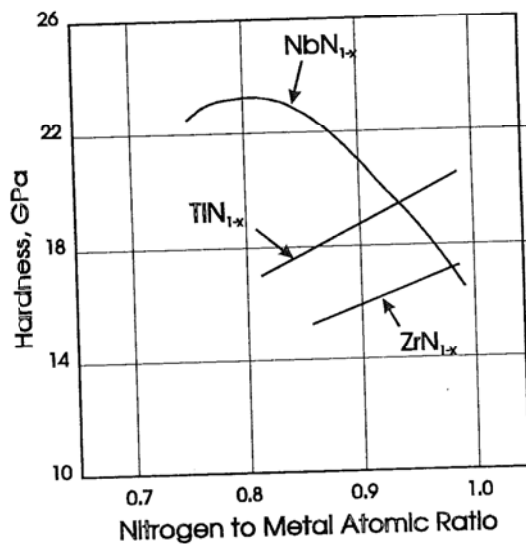


Figure 11.4: Hardnesses of the interstitial nitrides vs. nitrogen-to-metal atomic ratio.

Hardness vs. Crystal Orientation. The hardness varies depending on crystal orientation, the (111) orientation being the hardest as shown in Fig. 11.5.^[10] Extremely high hardness up to 50 GPa has been reported for epitaxial superlattices of interstitial nitrides such as NbN/TiN and VN/TiN.^[16]

Figure 11.4

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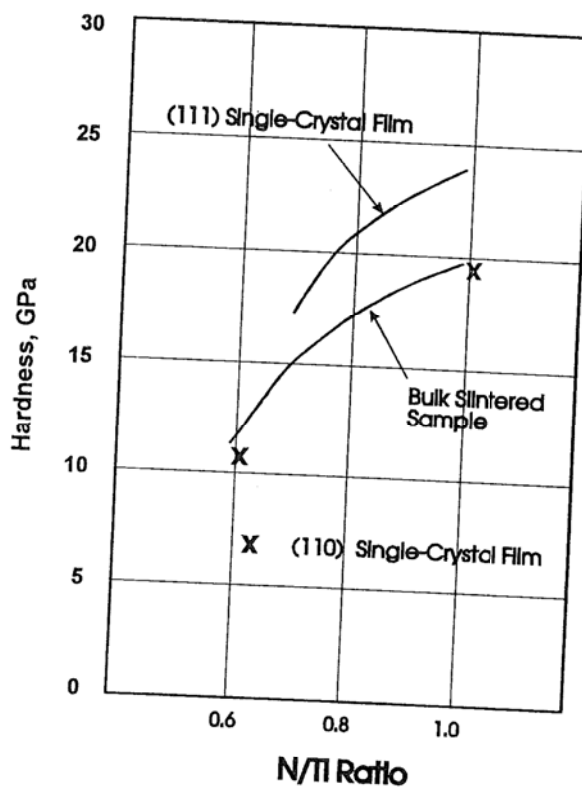


Figure 11.5: Hardnesses of single-crystal ($\{111\}$ orientation) TiN and bulk-sintered TiN as a function of N/Ti ratio.

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5.0 CHEMICAL PROPERTIES OF INTERSTITIAL NITRIDES

5.1 Mutual Solubilities

The existence of ternary carbides and nitrides was discussed in Ch. 4, Sec. 5.0. As shown in Fig. 11.6, TiN has complete mutual solubility with the other nitrides of Groups IV and V while mutual solubility with the

other nitrides is not as complete. With the partial exception of VN, they are also mutually soluble with the carbides of Groups IV and V (see Fig. 4.8 of Ch. 4).^[6]

5.2 Chemical Properties

The interstitial nitrides are chemically stable and have a chemical resistance similar to that of the Group IV and V carbides.

	TiN	ZrN	HfN	VN	NbN	TaN
TiN		○	○	X	○	○
ZrN	○		○	X	○	?
HfN	○	○		○	○	?
VN	○	X	X		○	?
NbN	○	○	○	○		?
TaN	○	○	○	○	○	

- Completely soluble
- X Insoluble or partially soluble
- ? Not reported

Figure 11.6: Mutual solubilities of interstitial nitrides.

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6.0 TITANIUM NITRIDE: SUMMARY OF PROPERTIES

6.1 Summary of Properties

The properties of titanium nitride are summarized in Table 11.6.

Table 11.6: Characteristics and Properties of Titanium Nitride.

Note: Test temperature is 20°C unless otherwise stated.

Phase: TiN (major) (see Table 10.2 of Ch. 10)
 Structure and Lattice Parameter: fcc B1 (NaCl), $a = 0.424 \text{ nm}$
 Space Group: Fm3m
 Pearson Symbol: cF8
 Composition: $\text{TiN}_{0.6}$ to $\text{TiN}_{1.1}$
 Molecular Weight: 64.95
 Color: gold
 X-ray Density : 5.40 g/cm^3
 Melting Point: 2950°C
 Debye Temperature: 636K

Specific Heat (C_p): $33.74 \text{ J/mol}\cdot\text{K}$
 Heat of Formation ($-\Delta H_f$) at 298K: $338 \text{ kJ/g-atom metal}$
 Thermal Conductivity (K): $19.2 \text{ W/m}\cdot^\circ\text{C}$ (see Fig. 11.1)
 Thermal Expansion: $9.35 \times 10^{-6}/^\circ\text{C}$ (see Fig. 11.2)

Electrical Resistivity: $20 \pm 10 \mu\Omega\cdot\text{cm}$
 Superconductive Transition Temperature: 5.6 K
 Hall Constant: $-0.7 \pm 0.2 \times 10^{-4} \text{ cm}^3/\text{A}\cdot\text{s}$
 Magnetic Susceptibility: $+38 \times 10^{-6} \text{ emu/mol}$

Vickers Hardness: 18–21 GPa
 Modulus of Elasticity: 251 GPa

Oxidation Resistance: Begins to oxidizes in air at approximately 800°C
 Chemical Resistance: Chemically stable at room temperature. Slowly attacked by concentrated acid solution with rising temperature.

6.2 Isomorphism

Titanium nitride is completely and mutually soluble with nitrides of Groups IV and V (see Fig. 11.6). It is isomorphous with TiC as carbon can substitute for nitrogen to form a binary solid solution, titanium carbonitride, Ti(CN), over a wide range of composition. The properties of TiCN are comparable to those of TiC and TiN (see Ch. 4, Sec. 6.0 and Fig. 4.8).

6.3 Phase Diagram

The Ti-N phase diagram is shown in Fig. 11.7.^{[17][18]}

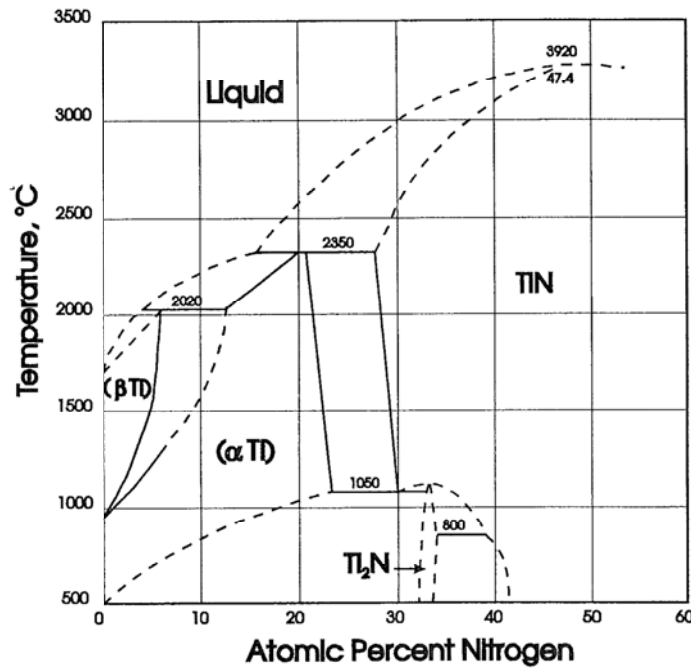


Figure 11.7: Nitrogen-titanium phase diagram.

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6.4 Summary of Fabrication Processes

TiN coatings are deposited by CVD, reactive evaporation, reactive sputtering, and ion-beam-assisted deposition. They can also be obtained by thermal spray. TiN powder is produced by the nitridation of Ti metal with nitrogen or ammonia at 1200°C (see Chs. 14 and 15).

6.5 Summary of Applications and Industrial Importance

Titanium nitride offers excellent protection against abrasive wear and has good lubricating characteristics. It is chemically resistant, thermally stable and, unlike titanium carbide, is an excellent diffusion barrier. It is a major industrial material. The following is a summary of its applications in production or development. More details are given in Ch. 16.

- Wear and erosion resistant coatings on cemented carbides, either singly or in combination with TiC, TiCN and Al₂O₃
- Coatings on tool steel for twist drills
- Diffusion barriers in semiconductor devices, between Si and Al, Ti and Pt, and between Ag and Si

7.0 ZIRCONIUM NITRIDE: SUMMARY OF PROPERTIES

7.1 Summary of Properties

The properties of zirconium nitride are summarized in Table 11.7.

7.2 Isomorphism

Zirconium nitride is completely and mutually soluble with the nitrides and carbides of Groups IV and V with the exception of VN and VC (see Fig. 11.6 and Fig. 4.8 of Ch. 4).

7.3 Phase Diagram

The Zr-N phase diagram is shown in Fig. 11.8.^{[17][18]}

Table 11.7: Characteristics and Properties of Zirconium Nitride.

Note: Test temperature is 20°C unless otherwise stated.

Phase: ZrN (major) (see Table 10.2 of Ch. 10)

Structure: fcc B1 (NaCl)

Lattice Parameter: $a = 0.4567$ nm

Space Group: Fm3m

Pearson Symbol: cF8

Composition: ZrN_{0.55} to ZrN_{1.0}

Molecular Weight: 105.23

Color: pale yellow

X-ray Density : 7.32 g/cm³

Melting Point: 2980°C

Debye Temperature: 515 K

Specific Heat (C_p): 40.39 J/mol·K

Heat of Formation ($-\Delta H_f$) at 298K: 365.4 kJ/g-atom metal

Thermal Conductivity (K): 20.5 W/m·°C (see Fig. 11.1)

Thermal Expansion: $7.4 \times 10^{-6}/^\circ\text{C}$ (see Fig. 11.2)

Electrical Resistivity: 7-21 $\mu\Omega\cdot\text{cm}$

Superconductive Transition Temperature: 10.7 K

Hall Constant: $-1.3 \times 10^{-4}\text{cm}^3/\text{A}\cdot\text{s}$

Magnetic Susceptibility: $+22 \times 10^{-6}$ emu/mol

Vickers Hardness: 15.0 GPa

Modulus of Elasticity: 397 GPa

Oxidation Resistance: Begins to oxidizes in air at approximately 800°C
Chemical Resistance: Chemically stable at room temperature. Slowly attacked by concentrated acid solution with rising temperature.

Fig

7.4

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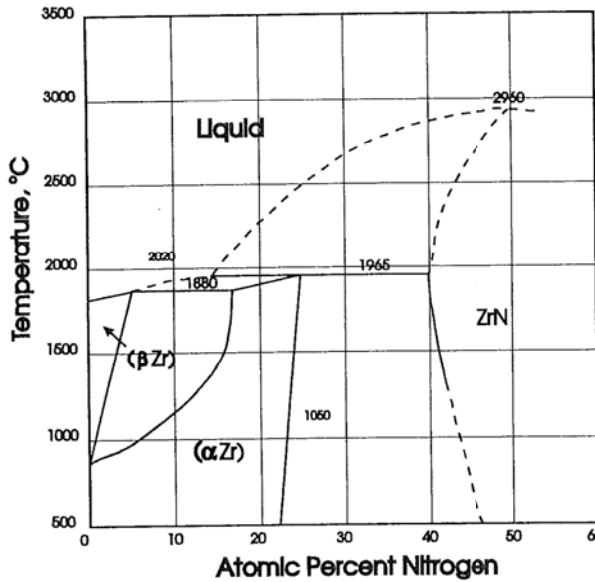


Figure 11.8: Nitrogen-zirconium phase diagram.

7.4 Summary of Fabrication Processes

Zirconium nitride is produced mostly on an experimental basis. Coatings are deposited by CVD, reactive evaporation, and reactive sputtering. They can also be obtained by thermal spray. ZrN powder is produced by the nitridation of Zr metal with nitrogen or ammonia at 1200°C (see Chs. 14 and 15).

7.5 Summary of Applications and Industrial Importance

Applications are presently limited to experimental studies.

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8.0 HAFNIUM NITRIDE. SUMMARY OF PROPERTIES

8.1 Summary of Properties

The properties of hafnium nitride are summarized in Table 11.8.

Table 11.8: Characteristics and Properties of Hafnium Nitride.

Note: Test temperature is 20°C unless otherwise stated.

Phase: HfN (major) (see Table 10.2 of Ch. 10)

Structure: fcc B1 (NaCl),

Lattice Parameter: $a = 0.452 \text{ nm}$

Space Group: Fm3m

Pearson Symbol: cF8

Composition: HfN_{0.75} to HfN_{1.12}

Molecular Weight: 192.497

Color: greenish yellow

X-ray Density: 13.8 g/cm^3

Melting Point: 3387°C

Debye Temperature: 421 K

Specific Heat (C_p): $38 \text{ J/mol}\cdot\text{K}$

Heat of Formation ($-\Delta H_f$) at 298K: $369.4 \text{ kJ/g-atom metal}$

Thermal Conductivity (K): $21.7 \text{ W/m}\cdot^\circ\text{C}$ (see Fig. 11.1)

Thermal Expansion: $6.9 \times 10^{-6}/^\circ\text{C}$ (see Fig. 11.2)

Electrical Resistivity: $33 \mu\Omega\cdot\text{cm}$

Superconductive Transition Temperature: 2–8.7 K (varies with composition)

Vickers Hardness: 16.3 GPa

Oxidation Resistance: Begin to oxidizes in air at approximately 800°C

Chemical Resistance: Chemically stable at room temperature. Slowly attacked by concentrated acid solution with rising temperature.

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Temperature, °C

Figure 1:

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8.2 Isomorphism

Hafnium nitride is completely and mutually soluble with the nitrides and carbides of Groups IV and V with the exception of VN and VC (see Fig. 11.6 and Fig. 4.8 of Ch. 4).

11.8.

8.3 Phase Diagram

The Hf-N phase diagram is shown in Fig. 11.9.^{[17][18]}

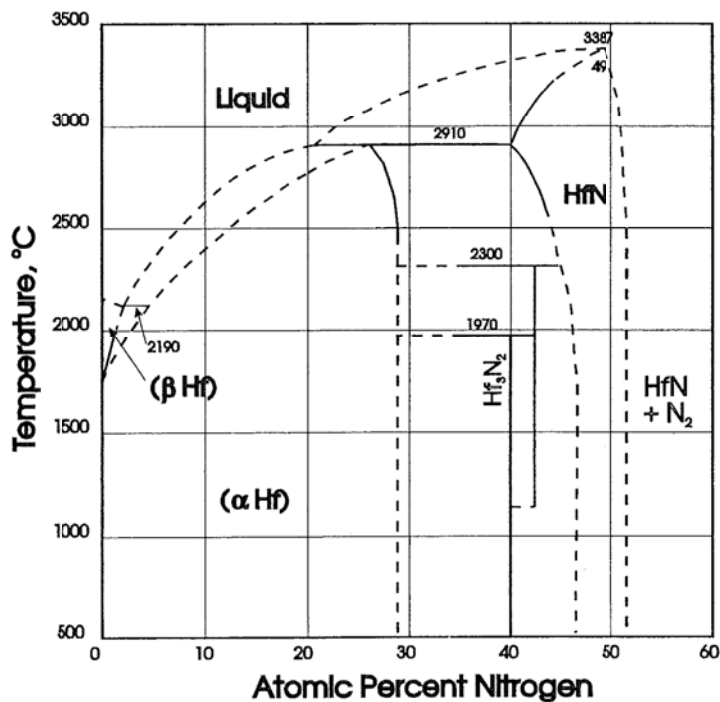


Figure 11.9: Nitrogen-hafnium phase diagram.

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8.4 Summary of Fabrication Processes

HfN coatings are deposited by CVD, reactive evaporation, and reactive sputtering (see Chs. 14 and 15). HfN powder is produced by the nitridation of Hf metal with nitrogen or ammonia at 1200°C.

8.5 Summary of Applications and Industrial Importance

- Coatings for cutting tools
- Tribological and corrosion resistant coatings
- Diffusion barriers for microelectronic devices (experimental)
- Whiskers^[19]
- Coatings on tungsten wires^[20]

9.0 VANADIUM NITRIDE: SUMMARY OF PROPERTIES

9.1 Summary of Properties

The properties of vanadium nitride are summarized in Table 11.9.

9.2 Isomorphism

VN, VC, and VO have isotypical structures and form solid solutions where nitrogen or oxygen can substitute for carbon over a wide range of composition. These solutions may be considered as V(C,N,O) mixed crystals. VN forms solid solutions with TiN and NbN, and with TiC, NbC, and TaC (see Fig. 11.6 and Fig. 4.8 of Ch. 4).

9.3 Phase Diagram

The V-N phase diagram is shown in Fig. 11.10.^{[17][18]}

9.4 Summary of Fabrication Processes

Vanadium nitride is produced mostly on an experimental basis. Coatings are deposited by CVD, reactive evaporation, reactive sputtering,

and ion-beam
nitridation of V m

Table 11.9

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Phases: V₂N
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and ion-beam-assisted deposition. VN powder is produced by the nitridation of V metal with nitrogen or ammonia at 1200°C (see Chs. 14 and 15).

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Table 11.9: Characteristics and Properties of Vanadium Nitride.

Note: Unless otherwise stated, test temperature is 20°C and quoted properties are those of the mononitride

Phases: V₂N, VN (see Table 10.2 of Ch. 10)

Structure and Lattice Parameters:

V₂N hex: a = 0.2835 nm, c = 0.4541 nm

VN fcc B1 (NaCl), a = 0.4126 nm

Space Group:

V₂N C6₃2

VN Fm3m

Pearson Symbol:

V₂N hP9

VN cF8

Composition (VN): VN_{0.72} to VN_{1.0}

Molecular Weight (VN): 64.95

Color: brown

X-ray Density: 6.8 g/cm³

Melting Point: 2177°C (decomposes)

Debye Temperature: 420 K

Specific Heat (C_p): 38.0 J/mol·K

Thermal Conductivity (K): 11.29 W/m·°C

Thermal Expansion: 8.7 × 10⁻⁶/°C

Electrical Resistivity: 85 μΩ·cm

Superconductive Transition Temperature: 8.2 K

Vickers Hardness: 14.2 GPa

Modulus of Elasticity: 357 GPa

Oxidation Resistance: Oxidation begins in air at approximately 800°C

Chemical Resistance: Resistant to cold acids, except HCl. Dissolved by hot oxidizing acids.

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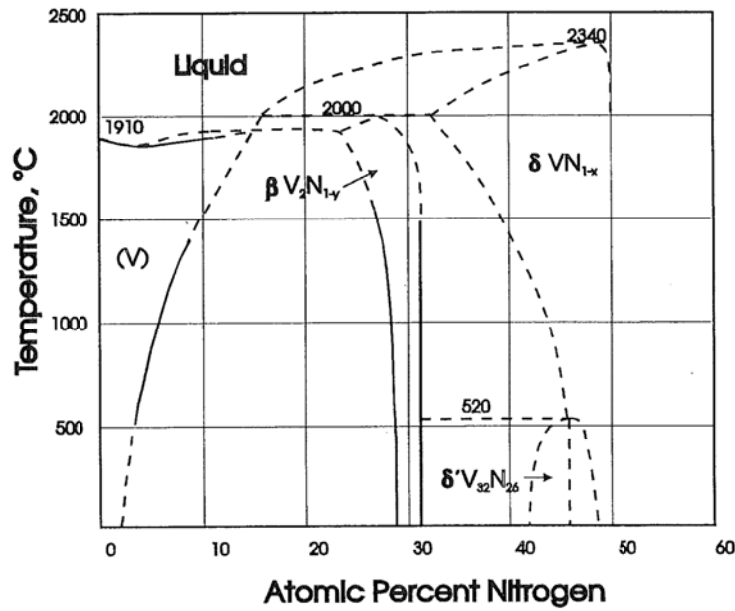


Figure 11.10: Nitrogen-vanadium phase diagram.

9.5 Summary of Applications and Industrial Importance

Applications are presently limited to experimental studies.

10.0 NIOBIUM NITRIDE: SUMMARY OF PROPERTIES

10.1 Summary of Properties

The properties of niobium nitride are summarized in Table 11.10.

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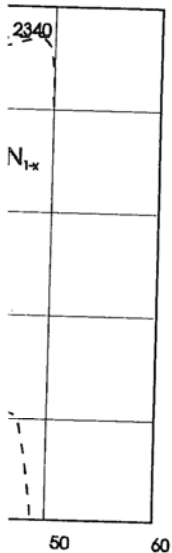
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Table 11.10: Characteristics and Properties of Niobium Nitride.

Note: Unless otherwise stated, test temperature is 20°C and quoted properties are those of the mononitride.



Phases: Nb₂N, Nb₄N₃, NbN (see Table 10.2 of Ch. 10)

Structure and Lattice Parameters:

Nb₂N hex: a = 0.3054 nm, c = 0.5005 nm

NbN hcp: a = 0.4395 nm, c = 0.4338 nm

Space Group:

Nb₂N P3 1m

NbN P6₃/mmc

Pearson Symbol:

Nb₂N hP9

NbN hP8

Composition (NbN): NbN_{0.92} to NbN_{1.06}

Molecular Weight (NbN): 106.91

Color: dark gray

X-ray Density: 7.3 g/cm³

Melting Point: near 2400°C

Debye Temperature: 307 K

Specific Heat (C_p): 39.01 J/mol.K

Heat of Formation (-ΔH_f) at 298K: 236 kJ/g-atom metal

Thermal Conductivity (K): 3.76 W/m·°C

Thermal Expansion: 10.01 × 10⁻⁶/°C

Electrical Resistivity: 58 μΩ·cm

Superconductive Transition Temperature: 16 K

Hall Constant: -0.52 × 10⁻⁴ cm³/A·s

Magnetic Susceptibility: +31 × 10⁻⁶ emu/mol

Vickers Hardness: 13.3 GPa

Modulus of Elasticity: 493 GPa

Oxidation Resistance: Begins to oxidize in air at approximately 800°C

Chemical Resistance: Chemically stable at room temperature. Slowly attacked by concentrated acid solution with rising temperature.

ble 11.10.

10.2 Isomorphism

Niobium nitride is completely and mutually soluble with the nitrides and carbides of Groups IV and V (see Fig. 11.6 and Fig. 4.8 of Ch. 4).

10.3 Phase Diagram

The Nb-N phase diagram is shown in Fig. 11.11.^{[17][18]}

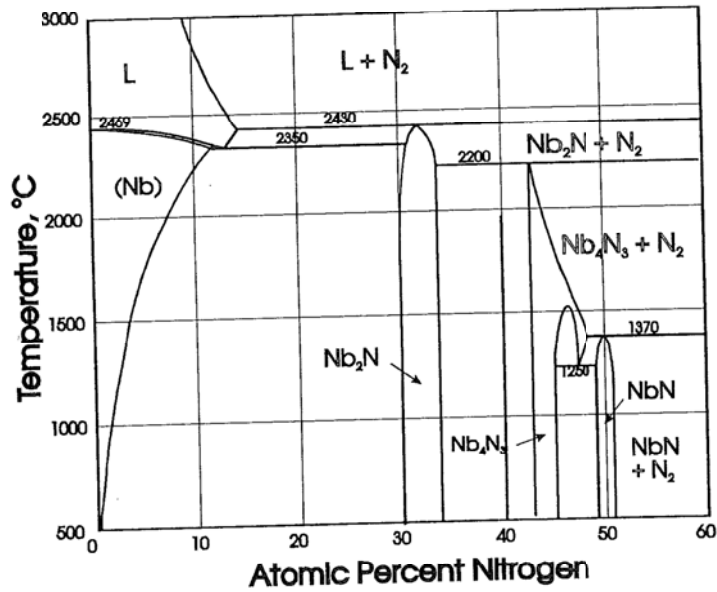


Figure 11.11: Nitrogen-niobium phase diagram.

10.4 Summary of Fabrication Processes

Niobium nitride is produced mostly on an experimental basis. Coatings are deposited by CVD, reactive evaporation, reactive sputtering, and

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ion-beam-assisted deposition. NbN powder is produced by the nitridation of Nb metal with nitrogen or ammonia at 1200°C (see Chs. 14 and 15).

10.5 Summary of Applications and Industrial Importance

Applications are presently limited. A potential area is as a superconducting coating.

11.0 TANTALUM NITRIDE. SUMMARY OF PROPERTIES

11.1 Summary of Properties

The properties of tantalum nitride are summarized in Table 11.11.

11.2 Isomorphism

Tantalum nitride is completely and mutually soluble with the nitrides and carbides of Groups IV and V with the exception of VN and VC (see Fig. 11.6 and Fig. 4.8 of Ch. 4).

11.3 Phase Diagram

The Ta-N phase diagram is shown in Fig. 11.12.^{[17][18]}

11.4 Summary of Fabrication Processes

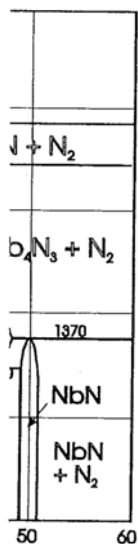
TaN is produced mostly on an experimental basis. Coatings are deposited by CVD, reactive evaporation, reactive sputtering, and ion-beam-assisted deposition. TaN powder is produced by the nitridation of Ta metal with nitrogen or ammonia at 1200°C (see Chs. 14 and 15).

11.5 Summary of Applications and Industrial Importance

TaN is used as a decorative coating for jewelry and similar items to impart a pleasing metallic shine.

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of Ch. 4).

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puttering, and

Table 11.11: Characteristics and Properties of Tantalum Nitride.

Note: Unless otherwise stated, test temperature is 20°C and quoted properties are those of the mononitride.

Phases: Ta₂N, TaN (see Table 10.2 of Ch. 10)

Structure and Lattice Parameters:

Ta₂N hcp: a = 0.5191 nm, c = 0.2906 nm

ΔTaN fcc (NaCl) a = 0.4336 nm

Space Group:

Ta₂N P6₃/mmc

TaN Fm3m

Pearson Symbol:

Ta₂N hP3

TaN cF8

Molecular Weight (TaN): 194.95

Color: yellowish gray

X-ray Density: 14.3 g/cm³

Melting Point: 3093°C (only melts under high N₂ pressure)

Specific Heat (C_p): 40.60 J/mol·K

Heat of Formation (-ΔH_f) at 298 K: 251 kJ/g-atom metal

Thermal Conductivity (K): 8.78 W/m·°C (see Fig. 11.1)

Thermal Expansion: 8.0 × 10⁻⁶/°C (see Fig. 11.2)

Electrical Resistivity: 135 μΩ·cm

Superconductive Transition Temperature (Ta₂N): 1.2 K

Vickers Hardness: 11 GPa

Oxidation Resistance: Begins to oxidize in air at approximately 800°C

Chemical Resistance: Chemically stable at room temperature. Slowly attacked by concentrated acid solution with rising temperature.

Temperature, °C

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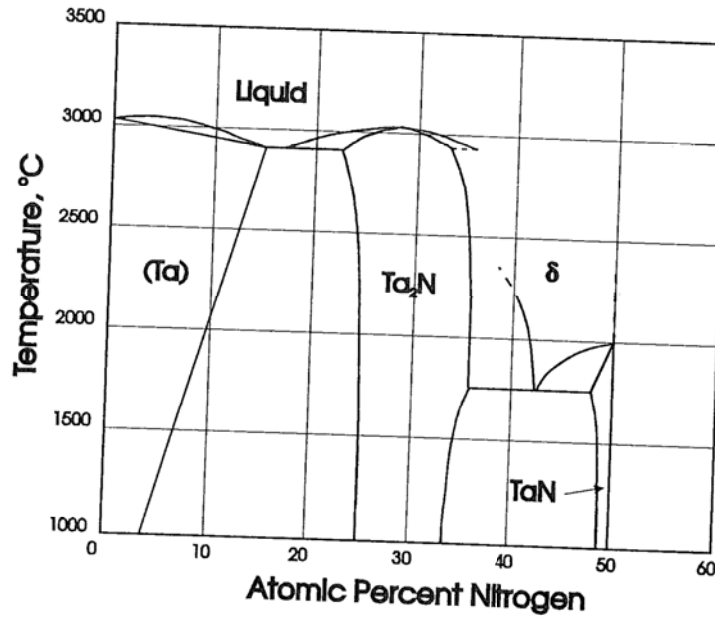


Figure 11.12: Nitrogen-tantalum phase diagram.

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