Methyl Silanes

Methylsilane (1MS), Dimethylsilane (2MS), Trimethylsilane (3MS) and Tetramethylsilane (4MS) have been used in Semiconductor manufacturing as precursors for the Chemical Vapor Deposition (CVD) of various layers, most often low dielectric constant (low-k) films. They also offer excellent barrier properties, typically used for a liner or a cap layer adjacent to other dielectric layers. These low-k layers vary in composition based on co-reactants combined with the Methylsilanes and result in Silicon Carbide (SiC), Silicon Carbonitride (SiCN), and Siliconoxyhydride (SiCO:H); the deposition reaction can typically be performed at relatively low temperature ranges.

- 1MS and 2MS are utilized mostly for low volume deposition of SiC, SiCN, or SiCO:H depending on the conditions and precursors used.
- 3MS has been used for SiC deposition or SiCO:H deposition, again depending on starting chemistries. This is a production-proven precursor, with current high volume application in Semiconductor fabrication.
- 4MS is currently used for SiC deposition on several advanced technology platforms and it is reported within several application patents.

Physical Properties of Organosilicon Precursors for CVD

Property	1MS	2MS	3MS	4MS	4M2S	6M2S
V.P. (°C)	-80 @241mm	-80@30mm	25@1218mm	20@589mm	27@195mm	20@23mm
B.P. (°C)	-57	-20	6.7	26.6	86	112
M.P. (°C)	(-157)	(-150)	(-136)	(-99)	(-93)	12
F.P. (°C)	<-40	<-20	<-20	-27	-26	-1
M.W.	46.14	60.17	74.20	88.22	118.32	146.38
CAS #	992-94-9	1111-74-6	993-07-7	75-76-3	814-98-2	1450-14-2

Compounds

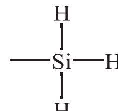
Name	MW	bp °C/mm (mp)	D_4^{20}	n_D^{20}

SIM6515.0
METHYLSILANE
1MS
CH_6Si — 46.14 — -57° — (-157°) — 0.628^{-58}

CAUTION: CAN FORM EXPLOSIVE MIXTURES WITH AIR

ΔHcomb: -2,612 kJ/mole
ΔHform: -29 kJ/mole
ΔHvap: 19.3 kJ/mole
Dipole moment: 0.73 debye

Flashpoint: <-40°C (<-40°F)
Autoignition temperature: 130°C
Vapor pressure, -80°: 241 mm
Vapor pressure, 21°: 14 atm (210 psia)
Critical temperature: 79.3˚C



Plasma polymerization yields dry process photoresist.[1]
Intermediate for poly(methylsilane) precursor to silicon carbide.[2]
Deposits SiC on Si and Ge at 400 - 500˚C.[3]
Source for hydrogenated amorphous silicon carbide films.[4]

1. Dabbagh, G. et al. J. Photopolym. Sci. Tech. 1998, 11, 651.
2. Fhang, Z. et al. J. Am. Ceram. Soc. 1991, 74, 670.
3. Takatsuka, T. et al. Appl. Surf. Sci. 2000, 162, 156.
4. Lee, M. et al. in "Chemical Aspects of Electronic Ceramics Processing" Arkles, B. ed., MRS Proc. 1998, 495, 153.

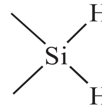
HYDROLYTIC SENSITIVITY: 9: reacts extremely rapidly with atmospheric moisture - may be pyrophoric - glove box or sealed system required

[992-94-9] TSCA EC 213-598-5 HMIS: 3-4-3-X

SID4230.0
DIMETHYLSILANE
2MS
C_2H_8Si — 60.17 — -20° — (-150°) — 0.68^{-20}

ΔHcomb: -2,612 kJ/mole
ΔHform: -96 kJ/mole
ΔHvap: 23.0 kJ/mole
Dipole moment: 0.75 debye

Flashpoint: <-40°C (<-40°F)
Vapor pressure, -80: 30 mm



CVD precursor for low k dielectric layers in damascene metallization applications
Generates cubic silicon carbide by plasma CVD.[1]
Epitaxial growth of cubic silicon carbide carried out by triode plasma CVD.[2]

1. Hashim, A. et al. Semiconductor Electronics, IEE Int'l. Conf. Proc. 2006, 646.
2. Yasuiet, K. et al. Appl. Surf. Sci. 2000, 159, 556.

HYDROLYTIC SENSITIVITY: 3: reacts with aqueous base

[1111-74-6] TSCA EC 214-184-7 HMIS: 3-4-1-X

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Name	MW	bp °C/mm (mp)	D_4^{20}	n_D^{20}

SIT8570.0
TRIMETHYLSILANE
3MS
$C_3H_{10}Si$ — 74.20 — 6.7° — (-135.9°) — $0.638^{6.7}$

ΔHcomb: -3,206 kJ/mole
ΔHform: -163 kJ/mole
ΔHvap: 24.3 kJ/mole
Dipole moment: 0.52 debye

Flashpoint: <-20°C (<-4°F)
TOXICITY: ihl rat, LC50: >5,000 ppm/1H
Autoignition temperature: 320˚C
Vapor pressure, 25˚: 1,218 mm
Critical temperature: 158.85°C
Critical pressure: 31.48 atm

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Forms trimethylsilylalkanes from olefins w/Pt catalyst
Employed in plasma treatment of surfaces.[1]
Treatment of titanium alloys and stainless steel surfaces inhibits biofilm formation.[2]
1. Hendricks, N. et al. Semiconductor Int'l. 2000, 23, 95.
2. Ma, Y. et al. Antimicrob. Agents Chemother. 2012, 56, 5923.
F&F: Vol. 1, p 1235; Vol. 2, p 441; Vol. 13, p 101; Vol. 16, p 292.
HYDROLYTIC SENSITIVITY: 3: reacts with aqueous base
[993-07-7] TSCA EC 213-603-0 HMIS: 2-4-1-X

SIT7555.0
TETRAMETHYLSILANE, 99+%
4MS, TMS
$C_4H_{12}Si$ — 88.22 — 26.6-26.7° — (-99°) — 0.641 — 1.3588

NMR grade
Viscosity: 0.4 cSt
ΔHcomb: 3,851 kJ/mole
ΔHform: -232 kJ/mole
ΔHfus: 6.7 kJ/mole
ΔHvap: 26.8 kJ/mole
Photoionization threshold: 8.1 eV
Ce: 1.838×10^{-3}

Flashpoint: -27°C (-17°F)
TOXICITY: ihl rat, LC50: >5,000 ppm/4H
Autoignition temperature: 450˚C
Vapor pressure, 20°: 589 mm
Critical temperature: 185˚C
Critical pressure: 33 atm
Heat capacity: 195.2 joules/mole-K
Dielectric constant: 1.92

Intermediate for α-SiC:H thin films by PECVD.[1]
1. Kim, D. et al. Thin Solid Films 1996, 283, 109.
See also GET7550
HYDROLYTIC SENSITIVITY: 1: no significant reaction with aqueous systems
[75-76-3] TSCA EC 200-899-1 HMIS: 1-4-0-X

SIT7541.0
1,1,2,2-TETRAMETHYLDISILANE
4M2S,
$C_4H_{14}Si_2$ — 118.32 — 86-7° — (-93°) — 0.7202 — 1.429
Flashpoint: -26°C (-15°F)

Forms low k carbon doped silicon dioxide films.
Forms SiC nanowires by APCVD.[1]
1. Rho, D., Mat. Res. Soc. Symp. Proc., 2005, 832, 317.
HYDROLYTIC SENSITIVITY: 3: reacts with aqueous base
[814-98-2] TSCA HMIS: 2-4-1-X

SIH6109.0
HEXAMETHYLDISILANE
6M2S, HMD
$C_6H_{18}Si_2$ — 146.38 — 112-3° — 12-14° — 0.7293 — 1.4214

Viscosity: 1.0 cSt
ΔHcomb: 5,909 kJ/mole
ΔHform (gas): -494 kJ/mole
ΔHvap: 39.8 kJ/mole

Flashpoint: -1°C (30°F)
Vapor pressure, 20°: 22.9 mm
Ea decomposition at 545°K: 337 kJ/mole
Rotational barrier, Si-Si: 4.40 kJ/mole
Secondary NMR reference: δ = 0.045

Precursor for CVD of silicon carbide.[1]
1. *Thin Solid Films* 1999, 252, 13.
HYDROLYTIC SENSITIVITY: 1: no significant reaction with aqueous systems
[1450-14-2] TSCA EC 215-911-0 HMIS: 2-4-0-X 25g $36.00 100g $117.00 1.5kg $360.00

SIT7308.0
TETRAKIS(TRIMETHYLSILYL)SILANE
$C_{12}H_{36}Si_5$ — 320.85 — (267° sub.)

m.p. (sealed tube): 319-21°C
NMR standard

Precursor for CVD of amorphous hydrogenated silicon - carbon films.[1]
1. Wrobel, A. et al. *Chem. Mater.* **1995,** *7*, 1403.
HYDROLYTIC SENSITIVITY: 1: no significant reaction with aqueous systems
[4098-98-0] HMIS: 2-2-0-X 5g $82.00 25g $328.00