1. Manufacture of nitrogen-free diamond thin film

By Nishimori, Toshihiko
From Jpn. Kokai Tokkyo Koho (2001), JP 2001164366 A 20010619, Language: Japanese, Database: CAPLUS

A diamond film is manufd. in a vacuum chamber (vacuum degree: $\leq 1 \times 10^{-3}$ Torr) by using H atoms which are prepd. by exciting a H gas and a Me gas which is prepd. by thermally exciting a CMe_4 gas. The diamond film has few N atoms because not a conventional Me_2N_2 gas but a CMe_4 gas is used.

~0 Citings

2. Carbon-nitride, diamond-like-carbon and silicon-based films synthesized by electron cyclotron resonance chemical vapor deposition

By Moran, M. B.; Johnson, L. F.
From Materials Research Society Symposium Proceedings (1999), 555(Properties and Processing of Vapor-Deposited Coatings), 353-364. Language: English, Database: CAPLUS

Carbon nitride and diamond-like carbon films were deposited by electron cyclotron resonance chem. vapor deposition (ECR-CVD) using carbon precursors in either a nitrogen- or an argon-high-d. plasma. The carbon precursors were tetrachloroethylene (C_2Cl_4), ethylene (C_2H_4) and neopentane (C_5H_{12}). Electron spectroscopy for chem. anal. (ESCA) and Fourier transform IR (FTIR) spectroscopy showed three distinct chem. compns.: chlorine-doped carbon nitride (CN_x:Cl), hydrogenated carbon nitride (CN_x:H) and hydrogenated amorphous carbon (a-C:H). FTIR spectroscopy revealed a fourth compn.: chlorine-doped amorphous carbon (a-C:Cl). ESCA anal. of the a-C:Cl film was not performed. Microstructures ranging from amorphous to microcryst. were obsd. using differential interference contrast (DIC) optical microscopy and at. force microscopy (AFM). Plasma etching of the substrate prior to film growth and biasing of the stage during film growth strongly influence the resulting microstructure. 100-μM-size, stacked, pyramidal CN_x:Cl crystallites were deposited onto a glass microscope slide through a combination of substrate preetching and rf-biasing of the stage during film growth. In later expts., pulsed-dc-high-voltage biasing of the stage during the growth process resulted in the deposition of 1-μm-size, rectangular- and triangular-shaped CN_x:Cl crystallites onto fused silica. Chlorinated instead of hydrogenated precursors were used to eliminate hydrogen incorporation during the growth of the ECR-CVD carbon nitride films. Chlorinated hydrocarbon precursors like trichloroethylene (C_2HCl_3) and C_2Cl_4 reduce the amt. of hydrogen in the plasma and make the formation of CN bonds more favorable. The results also show that double-bonded CC precursors are needed for N_2 to react with carbon. However, when a hydrogenated precursor like C_2H_4 is used with a N_2 plasma, hydrogen reacts with the CC double bond to form CH and NH bonds faster than N_2 can react to form double- and single-bonded CN. The disadvantages of using chlorinated-carbon precursors are that the resulting CN_x:Cl films contain a small amt. of chlorine (Cl), are porous and are unstable with respect to moisture incorporation. It is much easier to obtain stable, dense films using chlorinated precursors if more conventional materials are deposited. Silicon dioxide (SiO_2) and silicon nitride (Si_3N_4) films were deposited by ECR-CVD using trichlorosilane ($SiHCl_3$). The films showed no degrdn. or moisture incorporation after several months.

~2 Citings

3. Carbon nitride and diamond-like carbon films synthesized by electron cyclotron resonance chemical vapor deposition

By Johnson, L. F.; Moran, M. B.
From Annual Technical Conference Proceedings - Society of Vacuum Coaters (1997), 40th, 192-197. Language: English, Database: CAPLUS

Carbon nitride and diamond-like carbon films were deposited by electron cyclotron resonance (ECR) chem. vapor deposition (CVD) using four different hydrocarbon precursors in either a nitrogen- or argon-high-d. plasma. The four hydrocarbon precursors investigated were trichloroethylene, tetrachloroethylene, neopentane and ethylene. Electron spectroscopy for chem. anal. (ESCA) and Fourier transform IR (FTIR) spectroscopy showed that these conditions resulted in four distinctly different chem. compns.; chlorine-doped carbon nitride (CN_x:Cl), hydrogenated carbon nitride (CN_x:H), hydrogenated amorphous carbon (a-C:H) and chlorine-doped amorphous carbon (a-C:Cl). Film microstructure was studied using at. force microscopy (AFM) and differential interference contrast (DIC) microscopy. The microstructures fell into three categories; colloidal deposits, continuous films, and cryst.-phase material. One set of exptl. conditions resulted in the deposition of 100-μm-size CN_x:Cl crystallites. The crystallites are stacked pyramids with rectangular bases. This structure may be a chlorine-doped version of the metastable α-rhombohedral phase of carbon nitride.

~0 Citings

4. Diamond-like-carbon films synthesized by electron cyclotron resonance chemical vapor deposition

By Moran, Mark B.; Johnson, Linda F.
From Proceedings of SPIE-The International Society for Optical Engineering (1997), 3060(Window and Dome Technologies and Materials V), 42-54. Language: English, Database: CAPLUS, DOI:10.1117/12.277064

The preceding paper in these proceedings provided a detailed discussion of colloidal and cryst.-phase Cl-doped C nitride (CN_x:Cl) films synthesized by electron cyclotron resonance (ECR) CVD.[1] This paper will focus on diamond-like C (DLC) and hydrogenated C-nitride (CN_x:H) films deposited by ECR-CVD in either a N- or an Ar-high-d. plasma using 1 of the following hydrocarbon precursors; trichloroethylene, tetrachloroethylene, neopentane or ethylene. For clarity, results and discussions for the CN_x:Cl deposits will be presented again. Electron spectroscopy for chem. anal. (ESCA) and FTIR spectroscopy will show that the ECR-CVD expts. so far resulted in 4 distinctly different chem. compns.; CN_x:Cl, CN_x:H, hydrogenated amorphous C (a-C:H) and Cl-doped amorphous C (a-C:Cl). The a-C:H films deposited from neopentane and N have the lowest refractive index and the highest bandgap. The a-C:Cl films exhibit a strong IR peak at ~1560 cm^{-1} indicating that they may contain a large amt. of microcryst. graphite.

~0 Citings

5. Solar-induced chemical vapor deposition of diamond-type carbon films

By Pitts, J. Roland; Tracy, C. Edwin; King, David E.; Stanley, James T.
From U.S. (1994), US 5346729 A 19940913, Language: English, Database: CAPLUS

The CVD method, for depositing transparent continuous coatings of sp^3-bonded diamond-type C films, comprises: (a) providing a volatile hydrocarbon gas/H_2 reactant mixt. in a cold wall vacuum/CVD chamber contg. a suitable substrate for the films, at pressure of ≈1-50 Torr; and (b) directing a concd. solar flux of ≈40-60 W/cm^2 through the reactant mixt. to produce substrate temps. of ≈750-950° to activate deposition of the film on the substrate.

~4 Citings

6. Methods for producing synthetic diamond films on substrates

By Huehne, Erwin Dieter
From Ger. (1992), DE 4115930 C1 19920827, Language: German, Database: CAPLUS

Methods for prepg. a polycryst. diamond film on a substrate entail placing a substrate in a detonation chamber, introducing an atm. which hinders oxidn. of the substrate surface while heating the substrate to a temp. adequate to explosively ignite a hydrocarbon-contg. and O_2-contg. atm. which replaces the oxidn.-inhibiting atm. after the substrate has been heated to the desired temp.; the resulting detonation produces the film.

~2 Citings

7. A quantum-mechanical calculation of interatomic interactions in diamond

By Mahon, P.; Pailthorpe, B. A.; Bacskay, G. B.
From Philosophical Magazine B: Physics of Condensed Matter: Statistical Mechanics, Electronic, Optical and Magnetic Properties (1991), 63(6), 1419-30. Language: English, Database: CAPLUS

Ab initio Hartree-Fock SCF-theory calcns. were performed on neopentane, a C5 cluster, subjected to bond stretching and bending distortions. The potential energy surface was fitted by a Stillinger-Weber potential reparametrized for carbon in the diamond form. This potential provides a good description of the C-C interaction and should be useful in mol. dynamics, simulations of diamond.

~10 Citings

8. A valence force field for diamond from ab initio molecular orbital cluster calculations

By Guth, Jason R.; Hess, Anthony C.; McMillan, Paul F.; Petuskey, William T.
From Journal of Physics: Condensed Matter (1990), 2(40), 8007-14. Language: English, Database: CAPLUS, DOI:10.1088/0953-8984/2/40/002

The lattice dynamics and elastic moduli of diamond are reinvestigated using a method based upon an ab initio valence force field obtained for the neopentane mol. The calcd. phonon dispersion relations are in very good agreement with expt. particularly with respect to the La, LO, TO vibrational modes. The results demonstrate the transferability of force fields from ab initio calcns. on suitably chosen mol. clusters to condensed phases, and also show that a five-parameter valence force field model is sufficient to reproduce most of the features of the lattice dynamics of diamond. Excellent agreement was found between calcd. and exptl. bulk moduli indicating adequate modeling of the bond stretching interactions. Deviations of the transverse acoustical vibration modes at low frequencies and the remaining elastic moduli are assocd. with bond angle interaction terms, which may be due to the omission of a longer range interaction force const.

~6 Citings

9. Donor levels and impurity-atom relaxation in nitrogen- and phosphorus-doped diamond

By Jackson, Koblar; Pederson, Mark R.; Harrison, Joseph G.
From Physical Review B: Condensed Matter and Materials Physics (1990), 41(18), 12641-9. Language: English, Database: CAPLUS

Properties were studied of the n-type impurities of N and P in diamond, using a first-principles cluster approach based on the local-d. approxn. Impurity-donor-level positions of 0.75 and 1.09 eV were detd., resp., for C:N and C:P, measured relative to the bottom of the conduction band. Energetics was investigated of impurity-atom relaxation along the ⟨111⟩ direction in the diamond lattice. While exptl. observations indicate a trigonal distortion about the impurity site, the on-center position for both impurity atoms was found to be stable against simple off-center relaxation.

~32 Citings

10. Chemical vapor deposition of diamond

By Haku, Hisao; Sayama, Katsunobu; Tarui, Hisaki; Matsuyama, Takao; Tsuda, Shinya; Nakano, Shoichi
From Jpn. Kokai Tokkyo Koho (1988), JP 63069795 A 19880329, Language: Japanese, Database: CAPLUS

The title method is characterized by use of a source gas contg. CMe_4. A diamond film was formed with a glow discharge at 200-300° in substrate temp., 0.02-0.2 μm/h in deposition rate, 100 W in 13.56 MHz high-frequency power, and 10-50 Pa in H_2-CMe_4 mixed gas supply.

~0 Citings

11. Diamond force constant reconciliation with crystal elastic constants, Raman frequency, bulk compressibility, and neopentane group frequency assignments

By Wall, R. S.; Riter, J. R., Jr.
From Journal of Chemical Physics (1980), 72(4), 2886-8. Language: English, Database: CAPLUS, DOI:10.1063/1.439394

The diamond force const. reconcilation was made with crystal elastic consts., Raman frequency, bulk compressibility, and neopentane group frequency assignments. The question of the validity of treating neopentane as a quasitetrahedral system with the resultant 4 group frequencies, or the equiv. one of the relative separability of the 4 skeletal XY_4 modes, was resolved in the affirmative by the potential energy distribution calcns. of R. G. Snyder and J. H. Schachtschneider (1965), using a generalized force field with 36 parameters derived from 308 obsd. vibrational frequencies of 17 alkane mols. The $\nu_1(A_1)$ was 100% C-C stretch, $\nu_2(E)$ was 97% C-C-C bend, and the lowest F_2 frequency, ν_4, was 85% C-C-C bend and 10% Me rock. The 2 other F_2 frequencies that are candidates for the assignment as the ν_3 fundamentals, 1253 and 923 cm^{-1}, had the largest admixt. of nonskeletal contributions of any of the quasitetrahedral group frequencies, viz. 50% C-C stretch, 31% Me rock, and 19% Me HCH sym. bending, and 60% C-C stretch and 35% Me rock, resp.

~0 Citings

12. The spherical Compton profile of neopentane and the carbon-carbon single bond of diamond

By Reed, W. A.; Snyder, L. C.; Eisenberger, P.; Pinder, X. J.; Weber, T.; Wasserman, Z.
From Journal of Chemical Physics (1977), 67(1), 143-6. Language: English, Database: CAPLUS,
DOI:10.1063/1.434558

The spherically averaged Compton profile of CMe4 is measured and also calcd. from an ab initio SCF-MO wave function.
The measured Compton profile of diamond, corresponding to a C-C bond, is compared with empirical C-C profiles
computed from exptl. and theor. profiles for CMe4, C2H6, and CH4. The localized-bond model works well in all cases
examd.

~1 Citing

13. Electronic structure of saturated hydrocarbons in the semiempirical equivalent orbital method. 2. Through space interactions from the data for diamond and neopentane

By D'yachkov, P. N.; Levin, A. A.
From Theoretica Chimica Acta (1975), 36(3), 181-94. Language: English, Database: CAPLUS,
DOI:10.1007/BF00572558

The problem of obtaining the matrix elements of Hartree-Fock Hamiltonians for alkanes using the equiv. orbital (EO)
method is considered. The data on the electronic spectra of diamond together with t/e splitting in the neopentane
photoelectron spectrum help produce an EO parameter scale which involves even through space interactions. In terms
of the EO method the photoelectron spectra of propane, butane, and neopentane are interpreted. The valence band
structure of polyethylene in analytical form is obtained.

~1 Citing

14. Electronic structure of saturated hydrocarbons in the semiempirical equivalent orbital method. 1. Matrix elements in valence approximation from data for methane, ethane, and diamond

By Dyachkov, P. N.; Levin, A. A.
From Theoretica Chimica Acta (1974), 33(4), 323-8. Language: English, Database: CAPLUS,
DOI:10.1007/BF00551159

Matrix elements of Hartree-Fock operators in the equiv. orbital basis are reported for CH4, C2H6, diamond, and (in part)
propane and neopentane. The data are discussed in relation to electronic structure (spectra) calcns.

~0 Citings

15. A general valence force field for diamond

By Musgrave, M. J. P.; Pople, J. A.
From Proc. Roy. Soc. (London) (1962), Ser. A 268, 474-84. Language: Unavailable, Database: CAPLUS

Expressions were obtained which relate the force consts. of a general valence force field to the macroscopic elastic
consts. and the Raman frequency of diamond-type crystals. When values of the valence force consts. derived from the
frequencies of the neopentane molecule were used in these expressions, poor agreement was found with the observed
phys. consts. of diamond. It was suggested that the interaction const. assocg. bond extension with angular deformation
is most seriously altered in the diamond structure, but a more definite conclusion must await improved exptl. detns. of the
elastic consts.

~1 Citing

16. Relation between the molecular structures and the heats of formation of cyclohexane, methyl derivatives of cyclohexane, and decahydronaphthalene isomers

By Ito, Kazuo
From Nippon Kagaku Kaishi (1921-47) (1949), 70(Pure Chem. Sect.), 21-4. Language: Unavailable, Database:
CAPLUS

cf. preceding abstr. The assumptions described above were used. The heat of formation of cyclohexane can be calcd. from the heats of formation of <mark>diamond</mark>, C_2H_6, C_3H_8, butane, pentane, isobutane, and <mark>neopentane</mark> as ΔH = -19.4 kcal./mole, whereas the observed value is -20.02 kcal./mole. The differences in the heats of formation of cyclohexane, methyl- and ethylcyclohexane, and the 7 dimethylcyclohexane isomers can be calcd. from the heats of formation of CH_4, C_2H_6, C_3H_8, dimethylbutane, etc., giving results in agreement with expt. Among various conceivable forms of decahydronaphthalene (I) the most stable is that of 2 cyclohexane rings in the chair form combined in parallel. The calcd. heat of formation is -44.7 kcal./mole as compared with the observed value for trans-I of -44.4 kcal./mole. The next most stable form is that of the chair form combined in another way. The calcd. energy of isomerization is 2.2 kcal./mole at 0°K. The observed heat of formation for cis-I is -42.3 kcal./mole. Hence the heat of isomerization is 2.1 kcal./mole at 298°K. in the liquid state, in agreement with the theoretical deductions.

~0 Citings