- the carbosilane being 1,3,5,-trisilapentane (CAS No.: 5637-99-0) or 1,3,5-trisilacyclohexane (CAS No.: 291-27-0);
- the carbosilane being 1,3,5,-trisilapentane (CAS No.: 5637-99-0);
- the carbosilane being 1,3,5-trisilacyclohexane (CAS No.: 291-27-0);
- the polycarbosilazane polymer or oligomer is produced by a catalytic dehydrocoupling (DHC) reaction of
    a) two carbosilanes with two amines, wherein one of the two carbosilanes contains more than two -SiH_2R groups;
    b) two carbosilanes with two amines, wherein one of the two amines contains more than two N-H bonds; or
    c) more than two carbosilanes with more than two amines,
    where R is H, a C_1 to C_6 linear or branched alkyl group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, a C_3-C_6 cyclic alkenyl– group or combination thereof; and
- a catalyst used in the catalytic DHC reaction being NH_4Cl.

[0018a] In one aspect, there is provided a reaction mixture for producing a film forming polycarbosilazane polymer or oligomer, the reaction mixture comprising carbosilanes and amines, wherein the carbosilanes contain at least two –SiH2– moieties, either as terminal groups (–SiH2R) or embedded in a carbosilane cyclic compound, wherein R is H, a C1 to C6 linear or branched alkyl group, a C3-C6 cyclic alkyl– group, a C2 to C6 linear or branched alkenyl– group, a C3-C6 cyclic alkenyl– group or combination thereof, and wherein the reaction mixture is capable of forming the film forming polycarbosilazane polymer or oligomer, wherein the reaction mixture further comprises a polysilane that contains more than two –SiH_2R function groups, wherein R is H, a C_1 to C_6 linear or branched alkyl– group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, or a C_3-C_6 cyclic alkenyl– group.

[0018b] In another aspect, the present disclosure provides a method of forming a silicon and carbon containing film on a substrate, the method comprising the steps of producing a film forming polycarbosilazane polymer or oligomer by a polymerization of a reaction mixture of carbosilanes with amines; forming a solution containing the film forming polycarbosilazane polymer or oligomer; and contacting the solution with the substrate via a spin–on coating, spray coating, dip coating, or slit coating technique to form the silicon and carbon containing film, wherein the carbosilanes contain at least two –SiH_2– moieties, either as terminal groups (–SiH_2R) or embedded in a carbosilane cyclic compound, wherein R is H, a C_1 to C_6 linear

or branched alkyl group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, a C_3-C_6 cyclic alkenyl– group or a combination thereof, wherein the reaction mixture further comprises a polysilane that contains more than two $–SiH_2R$ function groups, wherein R is H, a C_1 to C_6 linear or branched alkyl– group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, or a C_3-C_6 cyclic alkenyl– group.

[0018c] In yet another aspect, the present disclosure provides a silicon and carbon containing film forming composition comprising a film forming polycarbosilazane polymer or oligomer that has a backbone comprising –Si–N– units, $–Si–N–C_n–N–Si–$ units, –Si–N–Si– units or combinations thereof, wherein $n \geq 1$, wherein the backbone includes cross–linked –Si–N– units, $–Si–N–C_n–N–Si–$ units or –Si–N–Si– units, branched –Si–N– units, $–Si–N–C_n–N–Si–$ units or –Si–N–Si– units, or combinations thereof, wherein the film forming polycarbosilazane polymer is produced from a reaction mixture of carbosilanes, amines, and a polysilane, the polysilane contains more than two $–SiH_2R$ function groups, wherein R is H, a C_1 to C_6 linear or branched alkyl– group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, or a C_3-C_6 cyclic alkenyl– group

Notation and Nomenclature

[0019] The following detailed description and claims utilize a number of abbreviations, symbols, and terms, which are generally well known in the art, and include:

[0020] As used herein, the indefinite article “a” or “an” means one or more.

[0021] As used herein, “about” or “around” or “approximately” in the text or in a claim means ±10% of the value stated.

[0022] As used herein, “room temperature” in the text or in a claim means from approximately 20°C to approximately 25°C.

[0023] The term “ambient temperature” refers to an environment temperature approximately 20°C to approximately 25°C.

[0024] The term “substrate” refers to a material or materials on which a process is conducted. The substrate may refer to a wafer having a material or materials on which a process is conducted. The substrates may be any suitable wafer used in semiconductor, photovoltaic, flat panel, or LCD-TFT device manufacturing. The substrate may also have one or more layers of differing materials already deposited upon it from a previous manufacturing step. For example, the wafers may include silicon layers (e.g., crystalline, amorphous, porous, etc.), silicon containing layers (e.g., SiO_2, SiN, SiON, SiCOH, etc.), metal containing layers (e.g., copper, cobalt, ruthenium, tungsten, platinum, palladium, nickel, ruthenium, gold, etc.)

What is claimed is:

1. A reaction mixture for producing a film forming polycarbosilazane polymer or oligomer, the reaction mixture comprising carbosilanes and amines,

wherein the carbosilanes contain at least two $–SiH_2–$ moieties, either as terminal groups ($–SiH_2R$) or embedded in a carbosilane cyclic compound, wherein R is H, a C_1 to C_6 linear or branched alkyl group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, a C_3-C_6 cyclic alkenyl– group or combination thereof, and

wherein the reaction mixture is capable of forming the film forming polycarbosilazane polymer or oligomer,

wherein the reaction mixture further comprises a polysilane that contains more than two $–SiH_2R$ function groups, wherein R is H, a C_1 to C_6 linear or branched alkyl– group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, or a C_3-C_6 cyclic alkenyl– group.

2. The reaction mixture of claim 1, wherein the film forming polycarbosilazane polymer or oligomer has a backbone that comprises –Si–N– units, $–Si–N–C_n–N–Si–$ units, –Si–N–Si– units or combinations thereof, wherein $n \geq 1$, wherein the backbone includes cross-linked –Si–N– units, $–Si–N–C_n–N–Si–$ units, or –Si–N–Si– units, branched –Si–N– units, $–Si–N–C_n–N–Si–$ units, or –Si–N–Si– units, or combinations thereof.

3. The reaction mixture of claim 1, wherein the carbosilane has the formula:

$$R^1{}_aSi[–(CH_2)_b–SiH_2R^2]_c \qquad (I)$$

wherein R^1, R^2 are independently H, a C_1 to C_6 linear or branched alkyl group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, a C_3-C_6 cyclic alkenyl– group or combination thereof; a = 0 to 2; b = 1 to 4; c = 4 – a; or

$$R^3{}_eC[–(CH_2)_f–SiH_2R^4]_g \qquad (II)$$

wherein R^3, R^4 are independently H, a C_1 to C_6 linear or branched alkyl group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, a C_3-C_6 cyclic alkenyl– group or combination thereof; e = 0 to 2; f = 0 to 3; g = 4 – e; or

$$[\text{scaffold}]–[–(CH_2)_m–SiH_2R^5]_n \qquad (III)$$

wherein R^5 is H, a C_1 to C_6 linear or branched alkyl group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, a C_3-C_6 cyclic alkenyl– group or combination thereof; m = 0 to 4; n = 2 to 4; and the scaffold is a hydrocarbon scaffold; or

R^6_x–1,3,5–trisilacyclohexane (IV)

wherein R^6 is a C_1 to C_6 linear or branched alkyl group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, a C_3-C_6 cyclic alkenyl– group; x = 0 to 3.

4. The reaction mixture of claim 3, wherein the hydrocarbon scaffold is a hydrocarbon scaffold including a C_3 to C_{10} cyclic hydrocarbon scaffold containing silyl– group, –NH group, or –O– ether group.

5. The reaction mixture of claim 1, wherein the carbosilane contains –Si–C_n–Si– unit (n ≥ 1) unit(s) or a 1,3,5–trisilacyclohexane (TSCH) backbone.

6. The reaction mixture of claim 1, wherein the carbosilane is selected from the group consisting of $Si[–(CH_2)–SiH_3]_4$, $Si[–(CH_2)_2–SiH_3]_4$, $Si[–(CH_2)_3–SiH_3]_4$, and $Si[–(CH_2)_4–SiH_3]_4$, $R^1Si[–(CH_2)–SiH_3]_3$, $R^1Si[–(CH_2)_2–SiH_3]_3$, $R^1Si[–(CH_2)_3–SiH_3]_3$, and $R^1Si[–(CH_2)_4–SiH_3]_3$, $H_3Si–CH_2–SiH_2–CH_2–SiH_3$ (bis(silylmethyl)silane), $H_3Si–(CH_2)_2–SiH_2–(CH_2)_2–SiH_3$ (bis(2–silylethyl)silane), $H_3Si–(CH_2)_3–SiH_2–(CH_2)_3–SiH_3$ (bis(3–silylpropyl)silane), and $H_3Si–(CH_2)_4–SiH_2–(CH_2)_4–SiH_3$ (bis(4–silylbutyl)silane), $C[–SiH_3]_4$ (tetrasilylmethane), $C[–(CH_2)–SiH_3]_4$ (2,2–bis(silylmethyl)propane–1,3–diyl)bis(silane)), $C[–(CH_2)_2–SiH_3]_4$ (3,3–bis(2–silylethyl)pentane–1,5–diyl)bis(silane)), and $C[–(CH_2)_3–SiH_3]_4$ (4,4–bis(3–silylpropyl)heptane–1,7–diyl)bis(silane)), $R^1C[–SiH_3]_3$, $R^1C[–(CH_2)–SiH_3]_3$, $R^1C[–(CH_2)_2–SiH_3]_3$, and $R^1C[–(CH_2)_3–SiH_3]_3$, $H_3Si–CH_2–SiH_3$ (bisilylmethane), $H_3Si–(CH_2)_5–SiH_3$ (1,5–disilylpentane)), and $H_3Si–(CH_2)_7–SiH_3$ (1,7–disilylheptane)), 1,3–disilylcyclopentane, 1,2–disilylcyclopentane, 1,4–disilylcyclohexane, 1,3–disilylcyclohexane, 1,2–disilylcyclohexane, 1,3,5–trisilylcyclohexane and 1,3,5–trisilylbenzene, 2–Me–TSCH, 2–Et–TSCH, 2–iPr–TSCH, 2–nPr–TSCH, 2–nBu–TSCH, 2–tBu–TSCH, 2–sBu–TSCH, 2–iBu–TSCH, 2,4–Me_2–TSCH, 2,4–Et_2–TSCH, 2,4–iPr_2–TSCH, 2,4–nPr_2–TSCH, 2,4–nBu_2–TSCH, 2,4–iBu_2–TSCH, 2,4–tBu_2–TSCH, 2,4–sBu_2–TSCH, 2,4,6–Me_3–TSCH, 2,4,6–Et_3–TSCH, 2,4,6–iPr_3–TSCH, 2,4,6–nPr_3–TSCH, 2,4,6–nBu_3–TSCH, 2,4,6–iBu_3–TSCH, 2,4,6–tBu_3–TSCH, 2,4,6–sBu_3–TSCH, and combinations thereof, wherein R^1 is H, a C_1–C_6 linear, branched, or cyclic alkyl– group, a C_1–C_6 linear, branched, or cyclic alkenyl– group, or combinations thereof.

7. The reaction mixture of claim 1, wherein the carbosilane is 1,3,5–trisilapentane (CAS No.: 5637–99–0) or 1,3,5–trisilacyclohexane (CAS No.: 291–27–0).

8. The reaction mixture of claim 1, wherein the amine is selected from one or more of ammonia, amidine, hydrazine, hydroxylamine, monoalkylamine, diamines including ethylene diamine, or polyamines, which polyamines contain at least two N–H bonds either on the same nitrogen atom or on separate nitrogen atoms.

9. The reaction mixture of any one of claims 1 to 8, wherein the polysilane is selected from one or more of neopentasilane ($Si(SiH_3)_4$), n–tetrasilane ($SiH_3(SiH_2)_2SiH_3$), 2–silyl–tetrasilane ($(SiH_3)_2SiHSiH_2SiH_3$), trisilylamine ($N(SiH_3)_3$), or trisilyamine derivatives.

10. A method of forming a silicon and carbon containing film on a substrate, the method comprising the steps of:

producing a film forming polycarbosilazane polymer or oligomer by a polymerization of a reaction mixture of carbosilanes with amines;

forming a solution containing the film forming polycarbosilazane polymer or oligomer; and

contacting the solution with the substrate via a spin–on coating, spray coating, dip coating, or slit coating technique to form the silicon and carbon containing film,

wherein the carbosilanes contain at least two $–SiH_2–$ moieties, either as terminal groups ($–SiH_2R$) or embedded in a carbosilane cyclic compound, wherein R is H, a C_1 to C_6 linear or branched alkyl group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, a C_3-C_6 cyclic alkenyl– group or a combination thereof,

wherein the reaction mixture further comprises a polysilane that contains more than two $–SiH_2R$ function groups, wherein R is H, a C_1 to C_6 linear or branched alkyl– group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, or a C_3-C_6 cyclic alkenyl– group.

11. The method of claim 10, further comprising the step of

pre–baking the silicon and carbon containing film under N_2 atmosphere at a temperature ranging from approximately 50°C to 400°C; and

subsequently hardbaking the silicon and carbon containing film by a heat–induced radical reaction or a UV–Vis photo induced radical reaction in an atmosphere of O_2, O_3, H_2O, H_2O_2, N_2O, or NO, air, compressed air, or combinations thereof at a temperature range of 200–1000°C to convert the silicon and carbon containing film to a SiOC or SiOCN containing film.

12. The method of claim 10, wherein the film forming polycarbosilazane polymer or oligomer has a backbone that comprises –Si–N– units, –Si–N–C_n–N–Si– units, –Si–N–Si– units or combinations thereof, wherein n ≥ 1, wherein the backbone includes cross–linked –Si–N– units, –Si–N–C_n–N–Si– units or –Si–N–Si– units, branched –Si–N– units, –Si–N–C_n–N–Si– units or –Si–N–Si– units, or combinations thereof.

13. The method of claim 10, wherein the carbosilane has the formula:

$$R^1{}_aSi[–(CH_2)_b–SiH_2R^2]_c \qquad (I)$$

wherein R^1, R^2 are independently H, a C_1 to C_6 linear or branched alkyl group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, a C_3-C_6 cyclic alkenyl– group or combination thereof; a = 0 to 2; b = 1 to 4; c = 4 – a; or

$$R^3{}_eC[–(CH_2)_f–SiH_2R^4]_g \qquad (II)$$

wherein R^3, R^4 are independently H, a C_1 to C_6 linear or branched alkyl group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, a C_3-C_6 cyclic alkenyl– group or combination thereof; e = 0 to 2; f = 0 to 3; g = 4 – e; or

$$[scaffold]–[–(CH_2)_m–SiH_2R^5]_n \qquad (III)$$

wherein R^5 is H, a C_1 to C_6 linear or branched alkyl group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, a C_3-C_6 cyclic alkenyl– group or combination thereof; m = 0 to 4; n = 2 to 4; and the scaffold is a hydrocarbon scaffold; or

$$R^6{}_x–1,3,5–trisilacyclohexane \qquad (IV)$$

wherein R^6 is a C_1 to C_6 linear or branched alkyl group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, a C_3-C_6 cyclic alkenyl– group; x = 0 to 3.

14. The method of claim 10, wherein the carbosilane is selected from the group consisting of $Si[–(CH_2)–SiH_3]_4$, $Si[–(CH_2)_2–SiH_3]_4$, $Si[–(CH_2)_3–SiH_3]_4$, $Si[–(CH_2)_4–SiH_3]_4$, $R^1Si[–(CH_2)–SiH_3]_3$, $R^1Si[–(CH_2)_2–SiH_3]_3$, $R^1Si[–(CH_2)_3–SiH_3]_3$, $R^1Si[–(CH_2)_4–SiH_3]_3$, $H_3Si–CH_2–SiH_2–CH_2–SiH_3$ (bis(silylmethyl)silane), $H_3Si–(CH_2)_2–SiH_2–(CH_2)_2–SiH_3$ (bis(2–silylethyl)silane), $H_3Si–(CH_2)_3–SiH_2–(CH_2)_3–SiH_3$ (bis(3–silylpropyl)silane), and $H_3Si–(CH_2)_4–SiH_2–(CH_2)_4–SiH_3$ (bis(4–silylbutyl)silane), $C[–SiH_3]_4$ (tetrasilylmethane), $C[–(CH_2)–SiH_3]_4$ (2,2–bis(silylmethyl)propane–1,3–diyl)bis(silane)), $C[–(CH_2)_2–SiH_3]_4$ (3,3–bis(2–silylethyl)pentane–1,5–diyl)bis(silane)), and $C[–(CH_2)_3–SiH_3]_4$ (4,4–bis(3–silylpropyl)heptane–1,7–diyl)bis(silane)), $R^1C[–SiH_3]_3$, $R^1C[–(CH_2)–SiH_3]_3$, $R^1C[–(CH_2)_2–SiH_3]_3$, and $R^1C[–(CH_2)_3–SiH_3]_3$, $H_3Si–CH_2–SiH_3$ (bisilylmethane), $H_3Si–(CH_2)_5–SiH_3$ (1,5–

disilylpentane), and $H_3Si–(CH_2)_7–SiH_3$ (1,7–disilylheptane), 1,3–disilylcyclopentane, 1,2–disilylcyclopentane, 1,4–disilylcyclohexane, 1,3–disilylcyclohexane, 1,2–disilylcyclohexane, 1,3,5–trisilylcyclohexane and 1,3,5–trisilylbenzene, 2–Me–TSCH, 2–Et–TSCH, 2–iPr–TSCH, 2–nPr–TSCH, 2–nBu–TSCH, 2–tBu–TSCH, 2–sBu–TSCH, 2–iBu–TSCH, 2,4–Me_2–TSCH, 2,4–Et_2–TSCH, 2,4–iPr_2–TSCH, 2,4–nPr_2–TSCH, 2,4–nBu_2–TSCH, 2,4–iBu_2–TSCH, 2,4–tBu_2–TSCH, 2,4–sBu_2–TSCH, 2,4,6–Me_3–TSCH, 2,4,6–Et_3–TSCH, 2,4,6–iPr_3–TSCH, 2,4,6–nPr_3–TSCH, 2,4,6–nBu_3–TSCH, 2,4,6–iBu_3–TSCH, 2,4,6–tBu_3–TSCH, 2,4,6–sBu_3–TSCH, and combinations thereof; and wherein R^1 is H, a C_1 to C_6 linear or branched alkyl group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, a C_3-C_6 cyclic alkenyl– group or a combination thereof.

15. The method of claim 10, wherein the carbosilane is 1,3,5–trisilapentane (CAS No.: 5637–99–0) or 1,3,5–trisilacyclohexane (CAS No.: 291–27–0).

16. The method of 10, wherein the step of the producing the film forming polycarbosilazane polymer or oligomer comprises the step of adding a catalyst to the reaction mixture, wherein the film forming polycarbosilazane polymer or oligomer is produced by a polymerization of the reaction mixture through a catalytic dehydrocoupling (DHC) reaction.

17. The method of claim 16, wherein the catalyst is NH_4Cl.

18. The method of claim 10, wherein the step of the producing the film forming polycarbosilazane polymer or oligomer comprises the step of adding a polysilane that contains more than two $–SiH_2R$ function groups to the reaction mixture for enhancing the polymerization of the carbosilanes with amines, wherein R is H, a C_1 to C_6 linear or branched alkyl group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, a C_3-C_6 cyclic alkenyl– group or a combination thereof.

19. The method of 18, wherein the polysilane is selected from one or more of neopentasilane (or 2,2–disilyltrisilane) ($Si(SiH_3)_4$), n–tetrasilane ($SiH_3(SiH_2)_2SiH_3$), 2–silyl–tetrasilane ($(SiH_3)_2SiHSiH_2SiH_3$), trisilylamine ($N(SiH_3)_3$), or trisilyamine derivatives such as alkylamino–substituted trisilylamines or oligomers of trisilylamines.

20. The method of any one of claims 10 to 19, wherein the film forming polycarbosilazane polymer or oligomer is produced by the polymerization of the carbosilanes with amines through the catalytic dehydrocoupling (DHC) reaction selected from one or more of

i) two carbosilanes with two amines, wherein one of the two carbosilanes contains the at least two –SiH_2– moieties, either as the terminal groups (–SiH_2R) or embedded in the carbosilane cyclic compound;

ii) two carbosilanes with two amines, wherein one of the two amines contains more than two N–H bonds; and

iii) more than two carbosilanes with more than two amines,

wherein R is H, a C_1 to C_6 linear or branched alkyl group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, a C_3-C_6 cyclic alkenyl– group or a combination thereof.

21. A silicon and carbon containing film forming composition comprising:

a film forming polycarbosilazane polymer or oligomer that has a backbone comprising –Si–N– units, –Si–N–C_n–N–Si– units, –Si–N–Si– units or combinations thereof, wherein n ≥ 1,

wherein the backbone includes cross–linked –Si–N– units, –Si–N–C_n–N–Si– units or –Si–N–Si– units, branched –Si–N– units, –Si–N–C_n–N–Si– units or –Si–N–Si– units, or combinations thereof,

wherein the film forming polycarbosilazane polymer is produced from a reaction mixture of carbosilanes, amines, and a polysilane, the polysilane contains more than two –SiH_2R function groups, wherein R is H, a C_1 to C_6 linear or branched alkyl– group, a C_3-C_6 cyclic alkyl– group, a C_2 to C_6 linear or branched alkenyl– group, or a C_3-C_6 cyclic alkenyl– group.