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A study on the sintering of fine-grained diamond-SiC composites

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APPENDICES

Appendix 1:

Calculation of the amount of powder required to achieve a 1μm TiC coating on 2μm diamond powder.

Molar mass of Ti = 48g, Molar mass of C = 12g, Molar mass of O_2 = 32g, Molar mass of NH_4Cl =53g, Density of TiC = 4.93g/cm^3, Density of Diamond = 3.54g/cm^3.

$$NH_4Cl + Ti + C \longrightarrow TiC + NH_3 + HCl$$

Unit volume of diamond (U) = $\frac{1g}{density} = \frac{1}{3.54} = 0.282\text{cm}^3$

Volume of diamond grain = $\frac{4}{3}\pi r^3 = \frac{4}{3}\pi\left(\frac{0.0002}{2}\right)^3 = 4.19 \times 10^{-12}\ \text{cm}^3$

Number of particles per g of diamond (n) = $\frac{UnitVol.}{Vol.ofgrain} = 6.74 \times 10^{10}$

Therefore: Specific surface area of diamond (SSA) = $4\pi r^2$ x No. of particles per gram (n)

$= 8.47 \times 10^3\text{cm}^2/\text{g}$

Vol. of coating per g of diamond powder (V) = SSA x thickness of coating on diamond (t) $= 8.47 \times 10^3\text{cm}^2/\text{g} \times 1 \times 10^{-4}\text{cm}$

$= 8.47 \times 10^{-1}\text{cm}^3$

Mass of TiC per g of diamond = density of coating compound x vol. of coating per g of diamond $= 4.18\text{g}$

Vol. fraction of TiC = $\frac{V}{V+U}$ = 0.75

Therefore: Vol. fraction of diamond (ignoring porosity) (V_p) = 1-0.75 = 0.25

Assuming 50% porosity of the preform:

Vol. fraction of diamond prior to infiltration (porosity included) = V_p x (1-0.5) = 0.125

Estimated vol. of sample (preform) = $\pi r^2 h = \pi (0.9)^2$ x 0.5 = 1.272cm^3

Therefore: Vol. of diamond in the sample = 0.125 x 1.272 = 0.159cm^3

Therefore: Mass of diamond in the sample = Vol. x Density = 0.159 x 3.52

= 0.560g

Final vol. of TiC in the sample (porosity included) = Vol. fraction of TiC x Porosity

= 0.75 x 0.5

= 0.375

Therefore: Vol. of TiC in sample = vol. frac. of TiC x vol. of sample

= 0.375 x 1.272cm^3

= 0.477cm^3

Hence: Mass of TiC in the sample = vol. of TiC x density of TiC

= 0.477cm^3 x 4.93g/cm^3

= 2.352g

Therefore: **Mass of Ti in the sample** = 2.352 x $\frac{48}{60}$ = **<u>1.882g</u>**

Hence: Balance C from TiC = 2.352 – 1.882 = 0.470g

Therefore: **Total mass of C (diamond) in the sample** = 0.470g + 0.560g = **1.030g**

Ratio of reacting moles from the equation = Ti : NH_4Cl = 1:1

Moles of Ti that reacted = Moles of NH_4Cl that reacted = $\frac{1.882}{48}$ = 0.0392 moles

Hence: **Mass of NH_4Cl reacted** = moles x Mr = 0.0392 x 53g = **2.078g**

Therefore the required quantities of the powders are**: Diamond = 1.030g**

: Ti =1.882g

: NH4Cl = 2.078g

Appendix 2:

Calculation of the amount of powder required to achieve a 1μm SiC coating on 2μm diamond powder.

Molar mass of Si = 28g, Molar mass of C = 12g, Molar mass of O_2 = 32g, Molar mass of NH_4Cl =53g, Density of SiC = 3.16g/cm^3, Density of Diamond = 3.54g/cm^3.

$$NH_4Cl + Si + C \longrightarrow SiC + NH_3 + HCl$$

Unit volume of diamond (U) = $\frac{1g}{density} = \frac{1}{3.54} = 0.282\text{cm}^3$

Volume of diamond grain = $\frac{4}{3}\pi r^3 = \frac{4}{3}\pi\left(\frac{0.0002}{2}\right)^3 = 4.19 \times 10^{-12}\ \text{cm}^3$

Number of particles per *g* of diamond (*n*) = $\frac{UnitVol.}{Vol.ofgrain} = 6.74 \times 10^{10}$

Therefore: Specific surface area of diamond (SSA) = $4\pi r^2$ x No. of particles per gram (*n*)

$= 8.47 \times 10^3 \text{cm}^2/\text{g}$

Vol. of coating per *g* of diamond powder (*V*) = SSA x thickness of coating on diamond (t)

$= 8.47 \times 10^3 \text{cm}^2/\text{g} \times 1 \times 10^{-4}\text{cm}$

$= 8.47 \times 10^{-1}\text{cm}^3$

Mass of SiC per *g* of diamond = density of coating compound x vol. of coating per g of diamond

$= 2.68\text{g}$

Vol. fraction of SiC = $\frac{V}{V+U} = 0.75$

Vol. fraction of diamond (ignoring porosity) (V_p) = 1-0.75 = 0.25

Assuming 50% porosity of the preform:

Vol. fraction of diamond prior to infiltration (porosity included) = V_p x (1-0.5) = 0.125

Estimated vol. of sample (preform) = $\pi r^2 h = \pi (0.9)^2 \times 0.5 = 1.272\text{cm}^3$

Therefore: Vol. of diamond in the sample = $0.125 \times 1.272 = 0.159\text{cm}^3$

Therefore: Mass of diamond in the sample = Vol. x Density = 0.159 x 3.52

$= 0.560\text{g}$

Final vol. of SiC in the sample (porosity included) = Vol. fraction of SiC x Porosity

$= 0.75 \times 0.5$

$= 0.375$

Therefore: Vol. of SiC in sample = vol. frac. of SiC x vol. of sample

$= 0.375 \times 1.272 cm^3$

$= 0.477 cm^3$

Hence: Mass of SiC in the sample = vol. of SiC x density of SiC

$= 0.477 cm^3 \times 3.16 g/cm^3$

$= 1.507 g$

Therefore: **Mass of Si in the sample** = $1.507 \times \frac{28}{40}$ = **<u>1.055g</u>**

Hence: Balance C from SiC = 1.507 – 1.055 = 0.452g

Therefore: **Total mass of C (diamond) in the sample** = 0.452g + 0.560g = **<u>1.012g</u>**

Ratio of reacting moles from the equation = Si : NH_4Cl = 1:1

Moles of Si that reacted = Moles of NH_4Cl that reacted = $\frac{1.055}{28}$ = 0.0377 moles

Hence: **Mass of NH_4Cl reacted** = moles x Mr = 0.0377 x 53g = **<u>1.998g</u>**

Therefore the required quantities of the powders are**: Diamond = 1.012g**

: Si =1.055g

: NH4Cl = 1.998g