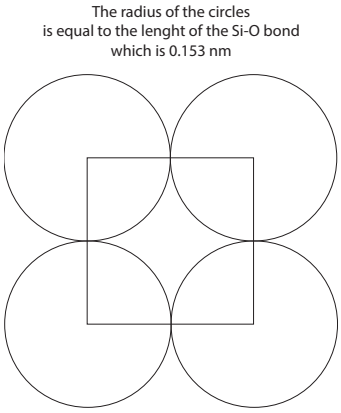
06A_HW Problem: Packing of Silica Tetrahedra

The question is to formulate a relationship between the length of the Si-O bond and the density of silica, α, with the assumption that the silica tetrahedra are close packed.

(i) Assume simple cubic packing

Approach:



•One cube contains one sphere since each sphere is shared by eight cubes

•The volume of the sphere is the third power of 2*bond length

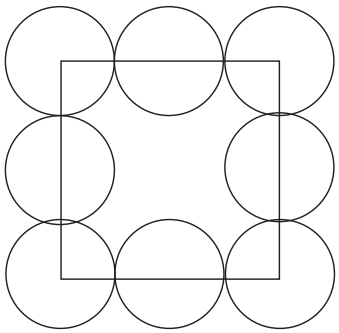
•The weight of one cube is give by the sum of the atomic weights of Si (28 g/mol) and two oxygens (2*16), divided by the Avogadro's number (6.02E23 per mole).

				Avgadro'a No	
				6.03E+23	per mole
bond length	bond len	Vol cube	Mol wt SiO2	One Molecule	density
nm	cm	cm^3	g/mol	g	g/cm^3
0.15	1.50E-08	2.7E-23	60	9.95E-23	3.69

The experimental density of fused (amorphous) silica is 2.2 g/cm^3

Therefore, the packing we have is too severe. Let us pose a different problem. Assume the packing to be as follows

Now the cube edge is 4*bond length, so the cube volume is x8 of the volume just above.



The number spheres per unit cell are 1 from the corner spheres and 3 from the spheres in the middle of the edges, since each edge is shared by four cubes, and because there are 12 edges altogether.

So the volume is 8 times bigger but the weight

We can conclude that the packing of the tetrahedra lies about half way between the two cube structure drawn above.

You can try other packings, for example body centered cubic.