The goal of the project is to model nano-porous SiC films. We hope to construct models that reproduce a subset of data from Pormoski et al JAP 2013 paper.[1](#_ENREF_1) We will start with crystalline SiC and carve out a pore while replacing the surface with hydrogens. The goal is to reproduce these results from Fig. 1 of Ref. 1:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  ( g /cm3) | K | % C | % Si | % O | % H | Eg (eV ) |
| 2.5 | 7.2 | 36.3 | 37.1 | 0.3 | 26.3 | 2.4 |
| 2.3 | 6.9 | 34.7 | 33.9 | 0.2 | 31.2 | 2.6 |
| 2.2 | 6.8 | 34.5 | 32.4 | 0.5 | 32.7 | 2.6 |
| 2.0 | 6.5 | 33.2 | 31.5 | 0.1 | 35.1 | 2.7 |
| 1.9 | 6.2 | 31.7 | 30.8 | 1.1 | 36.3 | 2.8 |

Our model results

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  ( g /cm3) | % C | % Si | % H | Radius Multiplier |
| 2.429 | 35.3 | 33.1 | 31.7 | 0.42 |
| 2.343 | 31.4 | 33.6 | 35 | 0.45 |
| 2.135 | 31.9 | 29.6 | 38.5 | 0.46 |
| 2.0496 | 27.82 | 30.08 | 42.1 | 0.5 |

1. T. A. Pomorski, B. C. Bittel, C. J. Cochrane, P. M. Lenahan, J. Bielefeld and S. W. King, Journal of Applied Physics **114** (7), 074501 (2013).