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Revealing Structural Details of SiCO Ceramics with GIPAW Calculations of Model Structures and Analysis of Experimental ^{29}Si Nuclear Magnetic Resonance Spectroscopy JOHN NIMMO, PETER KROLL, The University of Texas at Arlington — The occurrence of the various SiCxO4-x ($1 \leq x \leq 4$) mixed tetrahedra in silicon oxycarbide (SiCO) is often quantified by means of experimental 29Si nuclear magnetic resonance. The structural centers are assigned to individual peaks in the spectrum, which can be integrated to give the relative populations. Using a recently-developed method, we show that is is also possible to recover information on the connectivity of these tetrahedra. By combining a huge library of model structures an GIPAW calculations, we show that simple relations exist between the Si-O-Si linking angles and the 29Si NMR chemical shift. In this work, we perform detailed analyses of SiCO 29Si NMR spectra available in literature. We extract angular distributions in agreement with the experimental X-ray and neutron diffraction data. Furthermore, in glasses with large amounts of so-called "free" carbon, we observe a significant portion of the {Si}O4 tetrahedra which have disproportionately large angles. These angles indicate the presence of internal SiO2 surfaces or cages-like voids, similar to those found in zeolites or clathrates. This analysis suggests that in SiCO, the "free" carbon is incorporated into these voids, which produces strain on the bonding angles of the surrounding host glass.

John Nimmo
The University of Texas at Arlington

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