

## Multinuclear NMR study of the nitrogen-doped 6H-polytype silicon carbide

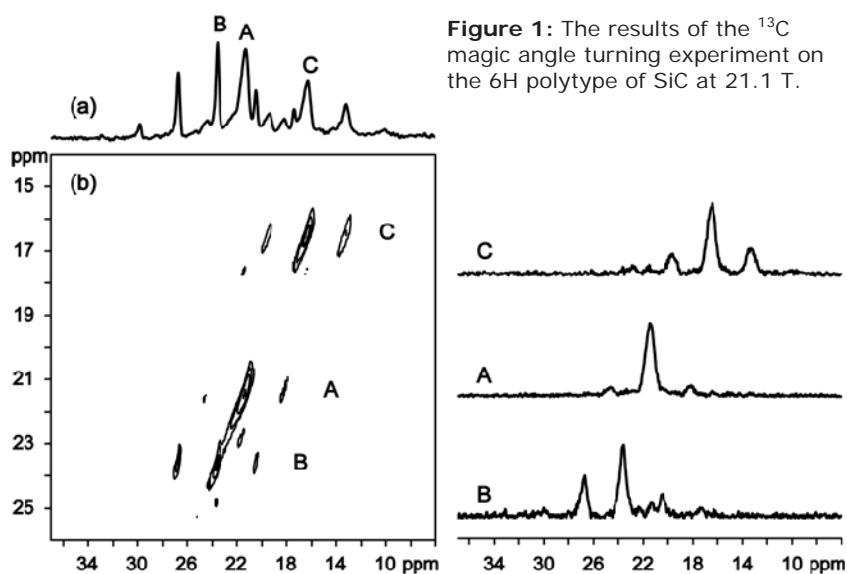
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Silicon carbide is a unique network solid in that it can crystallize in more than 200 polytypes: forms with different layer stacking sequences. All forms of silicon carbide are based on the diamond structure, with alternating Si and C atoms and with both Si and C tetrahedrally coordinated. Pure silicon carbide is an insulator, but nitrogen doping can turn it into a high-band-gap semiconductor, the dopant atoms entering into silicon carbide lattice sites. The unpaired electrons from the nitrogen dopant cause unusual  $^{13}\text{C}$  and  $^{29}\text{Si}$  spin-lattice relaxation effects. We still have no definitive information about where the nitrogen sits in the lattice. Our original proposal was to observe the  $^{14}\text{N}$  signals of the dopant atoms themselves. However we have been unsuccessful in this, with either powdered or single-crystal samples.

Our work on the 4H and 6H polytypes of silicon carbide has continued using  $^{13}\text{C}$  and  $^{29}\text{Si}$  MAS NMR. The Highfield NMR Facility for Solids was essential in our definitive assignment of their NMR signals, by allowing determination of chemical shift anisotropies at the different carbon and silicon sites. The high symmetry of the sites and resulting paucity of spinning sidebands required that this work be carried out at the highest possible magnetic field and the slowest possible stable spin rate. Use of the 21.1 Tesla instrument, with stable spinning at speeds down to 350 Hz, gave adequate spinning sideband patterns for CSA analysis, in all but one case.



**Figure 1:** The results of the  $^{13}\text{C}$  magic angle turning experiment on the 6H polytype of SiC at 21.1 T.

Slow-spin  $^{13}\text{C}$  spectra of the 6H polytype, even at 21.1 Tesla, had extensive peak overlap which prevented accurate CSA determination. Magic Angle Turning (MAT) experiments at 21.1 T allowed us to separate the spinning sideband patterns according to isotropic shift, giving the 2D spectrum shown in Figure 1, with clearly resolved spinning sideband patterns. This work has been recently published in the *Journal of Physical Chemistry C*:

J.S. Hartman, B. Berno, P. Hazendonk, C. Kirby, E. Ye, J. Zwanziger, A. Bain, "NMR Studies of Nitrogen Doping in the 4H Polytype of Silicon Carbide: Site Assignments and Spin-Lattice Relaxation", *J. Phys. Chem. C* **113** (2009) 15024-15036.