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**HYPERFINE AND SUPERHYPERFINE TENSORS AS PROBES OF THE
LOCAL ENVIRONMENT OF DEEP-LEVEL DEFECT CENTERS***

Michael Cook^a and C. T. White^b

^aDepartment of Chemical Engineering
University of Massachusetts
Amherst, MA 01003

^bCode 6119
Naval Research Laboratory
Washington, D.C. 20375

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HYPERFINE AND SUPERHYPERFINE TENSORS AS PROBES
OF THE LOCAL ENVIRONMENT OF DEEP-LEVEL DEFECT
CENTERS.* Michael Cook,[†] Geo-Centers Inc., Ft. Washington, MD
20744; and Carter T. White, Theoretical Chemistry Section, Code
6119, Naval Research Laboratory, Washington, D.C. 20375.

In several recent theoretical studies, we have analyzed the local environment of deep-level defects through comparisons of theoretical and experimental hyperfine tensors.^{1,2} The principal hyperfine interactions sample the distribution of spin density near the center of the defect site, and are diagnostic of the local bonding conformation; the smaller hyperfine (superhyperfine) tensors, which are caused by couplings of the spin density with nuclei somewhat removed from the center of the defect, give valuable information about the embedding of the defect into the extended lattice of its solid-state host.

In the present article, we discuss the particular effect of dihedral angles on the second-neighbor superhyperfine interactions in broken-bond defects in silicon and SiO₂. This includes such defect centers as the P_b center at the Si/SiO₂ interface, the E' centers which occur in a-SiO₂ and quartz, and the D centers of hydrogenated amorphous silicon. The dihedral angle is found to affect the ability of the second-neighbor bonding atomic orbitals to couple to the defect hybrid and participate in the molecular orbital which carries the unpaired electron spin; the result is a significant dependence of second-neighbor superhyperfine splittings on the dihedral angle.

¹ M. Cook and C.T. White, *Phys. Rev. B* 38: 9674 (1988).

² M. Cook and C.T. White, *Semicond. Sci. Tech.* 4: 1012 (1989).

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[†] Present Address: Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003.

Michael Cook
Code 6119
Naval Research Laboratory
Washington, DC 20375-5000
(202) 767-2026

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Gainesville, FL 32611

Dr. T. Pavlopoulos (1)
Naval Ocean Systems Center
Code 521
San Diego, CA 92152-5000

Dr. Peter P. Schmidt (1)
Chemistry Division, Code 1113PS
Office of Naval Research
800 North Quincy Street
Arlington, VA 22217-5000

Dr. Larry R. Cooper (1)
Electronics Division, Code 1114SS
Office of Naval Research
800 North Quincy Street
Arlington, VA 22217-5000

Dr. George B. Wright (1)
Electronics Division, Code 1114SS
Office of Naval Research
800 North Quincy Street
Arlington, VA 22217-5000

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