Sulfur-related metastable luminescence center in silicon

Mason, P.W.[ac], Sun, H.J.[ad], Ittermann, B.[ae], Ostapenko, S.S.[af], Watkins, G.D.[a], Jeyanathan, L.[bg], Singh, M.[bh], Davies, G.[b] and Lightowlers, E.C.[b]

[a] Department of Physics, Lehigh University, Bethlehem, PA 18015, United States
[b] Physics Department, King's College London, Strand, London WCR 2LS, United Kingdom
[c] Lucent Technologies, 9333 S. John Young Pkwy., Orlando, FL 32819, United States
[d] Philips Semiconductors, 9201 Pan American Fwy. NE, Albuquerque, NM 87113, United States
[e] Fachbereich Physik, Phillips-Universität Marburg, 35032 Marburg, Germany
[f] Center for Microelectronics Research, University of South Florida, 4202 Fowler Ave., Tampa, FL 33620, United States
[g] Department of Physics, University of Jaffna, Jaffna, Sri Lanka
[h] Department of Materials Engineering, Brunel University, Uxbridge, Middlesex UB8 3PH, United Kingdom

Abstract

Optical detection of magnetic resonance (ODMR) and photoluminescence (PL) studies are described for the sulfur-related metastable defect in silicon first reported by Brown and Hall. It is established that its two configurations, A and B, are of triclinic (C_1) symmetry, and the incorporation of a single impurity atom with nuclear spin I=3/2 is confirmed directly by resolving its hyperfine structure in each ODMR spectrum. Detailed study of the conversion kinetics indicates the dominant A →B mechanism under below band-gap excitation to be the result of direct optical excitation, not the result of exciton capture or the energy release accompanying the luminescence. The barrier for thermally activated B→A return is 0.10±0.01 eV, with no evidence of an intermediate configuration. Stress-induced splittings of the PL are satisfactorily analyzed as the sum of that for a highly localized hole plus that for a shallow Coulombically bound effective-mass electron. A tentative model is proposed involving a substitutional sulfur atom paired with an interstitial copper atom in two different nearby configurations. The low symmetry results from the tendency of the Cu interstitial to go off-center from the tetrahedral interstitial position.