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Theoretical study of the Cu_{PL} defect in Si ALEXANDRA CARVALHO, University of Aveiro, STEFAN K. ESTREICHER, Texas Tech University
— Copper is a common contaminant in Si processing. When in supersaturation, a fraction of 1% of the Cu in the sample forms an electrically-active defect easily seen by photoluminescence. This Cu_{PL} defect in Si has a no-phonon line at 1014 meV. It has long been believed to consist of an interstitial copper (Cu_i) weakly bound to a substitutional copper (Cu_s) : The $\{Cu_sCu_i\}$ pair. However, PL studies in isotopically pure ^{28}Si crystals have shown that the defect contains not two but four copper atoms [1]. We examine the possibility that the core of the defect consists of not one but two adjacent substitutional Cu atoms. This core traps two Cu_i atoms, resulting in defect with D_{3d} symmetry. We will discuss its formation mechanism and stability, and show that they are consistent with the conditions at which Cu_{PL} is observed. If this model is correct, then then DLTS lines associated with Cu_s should be re-assigned to $\{Cu_sCu_s\}$.

[1] M. Steger *et al.*, Phys. Rev. Lett. 100, 177402 (2008)

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