Sites and Dynamics for Muonium in III-V Semiconductors

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Muonium (Mu) can be considered as a light isotope of hydrogen with the same sites and defect chemistry as H. Far more experimental information exists on Mu defect states than on the analogous isolated H impurities. We review the stable and metastable locations obtained for each Mu charge-state in the III-V compounds. We also discuss the motional properties of each state and dynamics for observed site-change and charge-state transitions. For cubic zincblende systems, Mu⁰ either occupies a nearly bond-centered (BC) site having reacted with the lattice, or rapidly diffuses among tetrahedral (T) sites. Mu⁺ is stable at BC but motion involves the T_V sites as well, while Mu⁻ is stable at T_{III} and much less mobile. In the hexagonal wurtzite structured nitrides we find Mu⁻ located at the two inequivalent group-III anti-bonding (AB_{III}) locations, and Mu⁺ at AB_N with the ground state highly mobile. GaN and AlN show transient Mu⁰ signatures consistent with large negative U, while a shallow donor Mu⁰ is found in InN. Large differences are seen in the mobilities of different charge-states for Mu, leading us to infer that diffusion of H will likely be controlled by transitions into and out of a single highly mobile species in either structure: the T-site Mu⁰ in cubic systems and the channel Mu⁺ in the nitrides. Charge-state dynamics as well as the diffusivity and reactivity of a given hydrogen state will then be important to the efficiency of passivation reactions and any treatment to activate unintentionally passivated dopants. Reactions between Mu and dopants have been identified at very low T involving mobile Mu⁰ and the neutral dopants, and at high T by Coulomb capture of mobile Mu⁺ or Mu⁻ species by the ionized acceptors or donors.