"Nanoscale physics"

Nanoscale mechanism of rare-earth doping in chalcogenide glass: an insight from free-volume tracing with annihilating positrons

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Free-volume structure of arsenic selenide As_2Se_3 glass modified with Sb (substituting As) and codoped with Ga to $Ga_2(As_{0.28}Sb_{0.12}Se_{60})_{98}$ composition is traced by annihilating positrons in lifetime measuring mode treated in terms of two-state trapping model. The most efficient positron traps in parent As_2Se_3 glass are shown to be imaged as free-volume voids formed within cycle-type arrangement of directly corner-sharing trigonal $AsSe_{3/2}$ pyramids, composed of atomic-accessible geometrical holes arrested by surrounding atomic-inaccessible Se-based bond-free solid angles. Positron trapping is mostly depressed in Ga-codoped $Ga_2(As_{0.40}Se_{0.60})_{98}$ glass due to agglomeration of free-volume voids, thus leading to gradual decrease in trapping rate and fraction of trapped positrons. Partial As replacement by heavier Sb atoms to form $Ga_2(As_{0.28}Sb_{0.12}Se_{0.60})_{98}$ glass occurs stabilizing effect on rare-earth doping, partially recovering void structure of parent glass with increased trapping in defects. Effect of 500 wppm of Pr^{3+} incorporated in $Ga_2(As_{0.28}Sb_{0.12}Se_{0.60})_{98}$ glass is explained in terms of competitive contribution of changed occupancy sites available for rare-earth ions and annihilating positrons being trapped in Ga-modified glassy network. Under doping, the Pr^{3+} ions are stabilized due to Pr^{3+}-Se-Ga linkages, thus eliminating neighboring void as potential positron trapping sites. Effect of rare-earth doping in the studied glass results in notably reduced positron trapping rate in free-volume voids, originated from their decreased content and rather slightly altered volume.