

Abstract Submitted
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N.Q.R measurements of low energy Chiral structures in powdered glassy As_2Se_3 CHRIS NELSON, A.P.S — Experimental and theoretical work on the As-chalcogen glasses have shown that in the glassy state the local cylindrical symmetry associated with the elemental pyramidal unit is preserved. Here we introduce a local paracrystalline model of glassy As_2Se_3 . This model is based on a tight binding calculation of the electric field gradient (EFG) at the core of an As atom located at the apex of the pyramidal structure. This EFG is shown to be hyper sensitive to the bond angles and bond lengths the As atom forms with the chalcogen nearest neighbors, as well as the hybrid angle formed with second neighbor As atoms. A continuous variation of the bonding parameters produces a unique set of these pyramidal units which are shown to fit the NQR data for powdered glassy samples. The best fit to the NQR data indicates that the pyramidal units organize themselves into Chiral structures in the glass. A plot of the electronic energy per molecular site shows that the chiral structures have on average a lower electronic energy than a random configuration.

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