

Abstract Submitted
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Evidence for Quasi Tetrahedral $S=As(S_{1/2})_3$ local structures in As_xS_{1-x} glasses PING CHEN, P. BOOLCHAND, C. HOLBROOK, Univ. Cincinnati, K. JACKSON, Central Mich., D. GEORGIEV, Univ. of Toledo, M. MICOULAUT, Univ. Paris — Raman scattering and modulated DSC on bulk As_xS_{1-x} glasses in the $0.08 < x < 0.41$ range is studied¹. Vibrational spectroscopy results supported by first principles cluster calculations reveal that modes near 335, 380 and 490 cm^{-1} represent respectively symmetric stretch, asymmetric stretch and As=S stretch of Quasi- Tetrahedral (QT) $S=As(S_{1/2})_3$ local structures. Mode at 365 cm^{-1} is attributed to both symmetric and asymmetric stretch of pyramidal (PYR) $As(S_{1/2})_3$ units. In addition, modes of S_n chains near 460 cm^{-1} and those of S_8 rings near 475, 430, 217, and 150 cm^{-1} are observed at $x < 0.25$. Scattering strengths of modes of QT units are found to display a broad global maximum in the $0.20 < x < 0.30$ composition range, while modes of PYR units increase monotonically with x , and modes of S_n and S_8 rings monotonically decrease with x in the range examined. These findings are in harmony with the existence of a reversibility window (RW) in the $0.20 < x < 0.30$ range. ¹ D.G. Georgiev Ph.D. Thesis, Univ. of Cincinnati (unpublished) 2003. ² D.G. Georgiev and P. Boolchand Phil. Mag. 83, 2941(2003). * Supported by NSF grant DMR 04-56472

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