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Presence of α phase domains in the phonon-glass thermoelectric β-Zn_4Sb_3 from atomic pair distribution function (PDF) analysis H. J. KIM, E. S. BOZIN, S. J. L. BILLINGE, Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, S. HAILE, Materials Science, California Institute of Technology, Pasadena, CA 91125, G. J. SNYDER, Jet Propulsion Laboratory, 4800 Oak Grove Drive, Pasadena, CA 91109 — The promisingly high ZT of β-Zn_4Sb_3 between 450 K and 670 K is known to be due to its exceptionally low thermal conductivity. The discovery of significant Zn interstitial disorder in β-Zn_4Sb_3 provides foundation for better understanding of the origin of the glass-like thermal conductivity[1]. Furthermore, it has been reported that Zn interstitial atoms become ordered in α-phase[2]. We report on the *local* structural study of β-Zn_4Sb_3 using PDF technique, which has been successfully applied to solve the structures of crystallographically challenged materials[3,4]. Prominent diffuse scattering is found both in neutron and x-ray data. The PDF analysis suggests that the average β-structure consists of locally α-structure like domains where Zn interstitial atoms are ordered. This provides an important local structural insight into not well understood α to β order-disorder phase transition in Zn_4Sb_3 at 260 K. [1] G. J. Snyder *et al.* Nat. Mater. **3**, 458 (2004) [2] J. Nylén *et al.* J. Am. Chem. Soc. **126**, 16306 (2004) [3] T. Egami and S. J. L. Billinge, *Underneath the Bragg peaks*, Pergamon Press, Elsevier, Oxford, England, 2003 [4] S. J. L. Billinge and M. G. Kanatzidis, Chem. Commun., 749 (2004)

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