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Structural refinement of vitreous silica bilayers[1] MAHDI SADJADI, Arizona State Univ, MARK WILSON, University of Oxford, M.F. THORPE, Arizona State Univ and University of Oxford — The importance of glasses resides not only in their applications but in fundamental questions that they put forth. The continuous random network model can successfully describe the glass structure, but determining details, like ring statistics, has always been difficult using only diffraction data. But recent atomic images of 2D vitreous silica bilayers can offer valuable new insights which are hard to be observed directly in 3D silica models/experiments [for references see (1)]. However, the experimental results are prone to uncertainty in atomic positions, systematic errors, and being finite. We employ special boundary conditions developed for such networks to refine the experimental structures. We show the best structure can be found by using various potentials to maximize information gained from the experimental samples. We find a range of densities, the so-called flexibility window, in which tetrahedra are perfect. We compare results from simulations using harmonic potentials, MD with atomic polarizabilities included and DFT. (1) Mark Wilson, Avishek Kumar, David Sherrington and M.F. Thorpe, Modeling vitreous silica bilayers, Phys. Rev. B 87, 214108, pages 1-9 (2013)

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