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Calculation of Si L2,3-edge Non-Resonant Inelastic X-ray Scattering Spectra of Compressed Silica Glass KEITH GILMORE, European Synchrotron Radiation Facility, JOHN TSE, University of Saskatchewan — Despite the abundance of silica in Earth's crust and its corresponding importance to geological processes, debate continues as to the local coordination of Si in silica at geological pressures. Recent *ab initio* molecular dynamics simulations [M. Wu et al., Sci. Rep. 2, 398 (2012)] predicted a change from 4-fold coordinated Si at ambient pressure to 6-fold coordination by 22 GPa. This was consistent with experimental non-resonant inelastic x-ray scattering (NRIXS) measurements at the O K-edge that also suggested a conversion to 6-fold coordination by 22 GPa [J. Lin et al., Phys. Rev. B 75, 012201 (2007)]. However, NRIXS measured at the Si L-edge found the spectra to be largely independent of pressure up to 74 GPa [H. Fukui et al., Phys. Rev. B 78, 12203 (2008)] indicating that 4-fold coordination is maintained. The discrepancy may potentially be due to low instrument resolution of the Si L-edge measurements. We present calculated Si L-edge NRIXS spectra at multiple pressures between ambient and 150 GPa and for several momentum transfer values. This allows us to identify spectral features that may be used to better distinguish 4-fold and 6-fold coordinated environments as experimental resolutions improve.

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