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Volume and structural analysis of super-cooled water under high pressure SOLOMON F. DUKI[1], Department of Physics and Astronomy, Rowan University, 201 Mullica Hill Road, Glassboro, NJ 08028-1701, MESFIN TSIGE[2], Department of Polymer Science, Goodyear Polymer Center 1021, The University of Akron, Akron, OH 44325-3909 — Motivated by recent experimental study of super-cooled water at high pressure [1], we performed atomistic molecular dynamic simulations study on bulk water molecules at isothermal-isobaric ensemble. These simulations are performed at temperatures that range from 40 K to 380 K using two different cooling rates, 10K/ns and 10K/5ns, and pressure that ranges from 1atm to 10000 atm. Our analysis for the variation of the volume of the bulk sample against temperature indicates a downward concave shape for pressures above certain values, as reported in [1]. The same downward concave behavior is observed at high pressure on the mean-squared-displacements (MSD) of the water molecules when the MSD is plotted against time. To get further insight on the effect of the pressure on the sample we have also performed a structural analysis of the sample.

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