Glassy GaS: transparent and unusually rigid thin films for visible to mid-IR memory applications

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Electronic Supplementary Information

Fig. S1. High-energy X-ray diffraction measurements at SPring-8 (Hyogo Prefecture, Japan).

Fig. S2. Experimental and simulated FPMD/PBEsol X-ray pair-distribution functions $g_{\mathrm{X}}(r)$ of glassy GaS.

Fig. S3. Mean-square displacements $\langle r^2(t)\rangle$ of Ga and S species as a function of FPMD time t and temperature T.

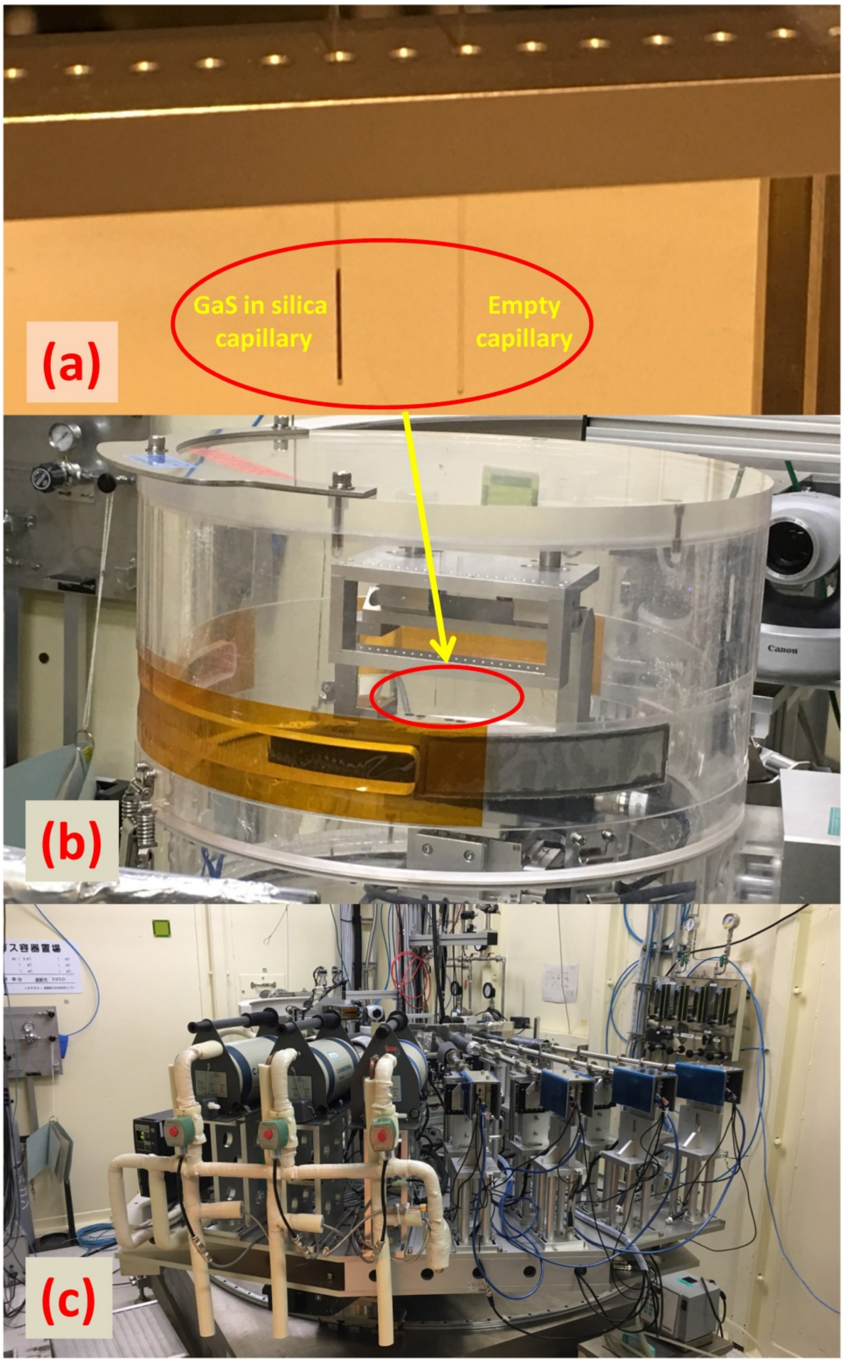

Fig. S1. High-energy X-ray diffraction measurements at SPring-8 (Hyogo Prefecture, Japan): (a) glassy GaS in thin-walled silica capillary and empty capillary for background subtraction, (b) a vacuum chamber of the dedicated two-axis BL04B2 diffractometer, (c) a 7-detector setup of BL04B2 including four cadmium telluride detectors at low angles and three Ge diodes at high diffraction angles.

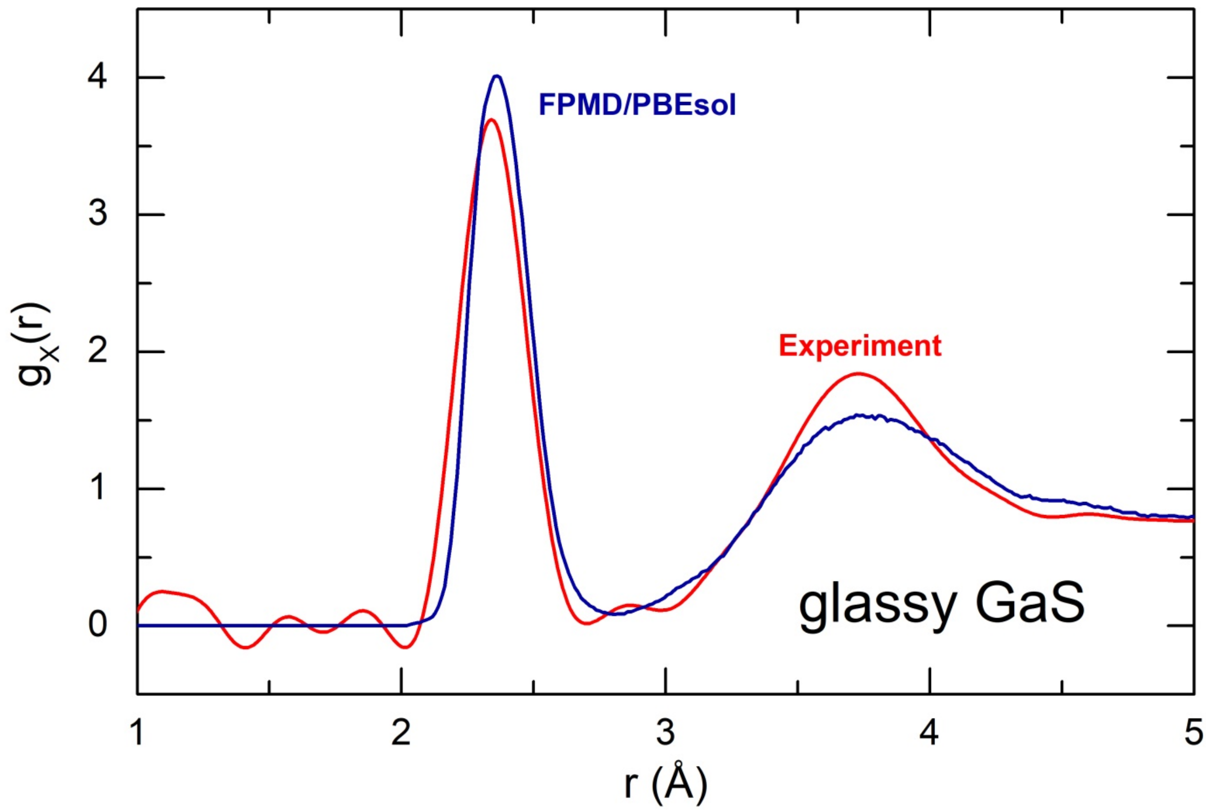

Fig. S2. Experimental (red) and simulated FPMD/PBEsol (blue) X-ray pair-distribution functions $g_X(r)$ of glassy GaS. A typical problem of FPMD simulations using the general gradient approximation with classical PBEsol exchange-correlation functional resides in overestimation of the nearest neighbor interatomic distances resulting in a higher-r shift of the NN peak.

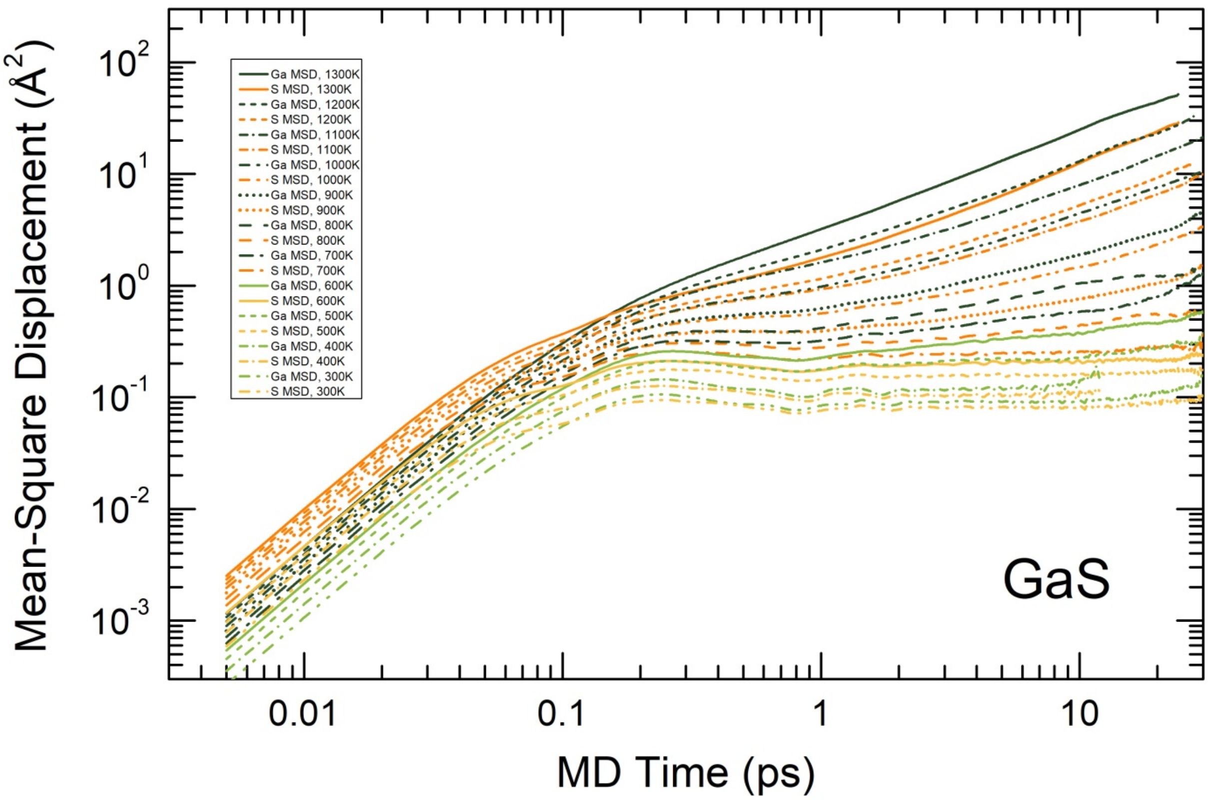

Fig. S3. Mean-square displacements $\langle r^2(t) \rangle$ of Ga and S species as a function of FPMD time t and temperature T. Three characteristic regimes are clearly seen: (1) the ballistic regime below $t \lesssim 30$ fs, $\langle r^2(t) \rangle \propto t^2$, (2) the intermediate regime related to vibrations and local diffusion, $\langle r^2(t) \rangle \propto t^s$, where $0 \le s < 1$, and (3) the long-range diffusion motion at high T and t, $\langle r^2(t) \rangle \propto t^1$.