Decoding the Atomic Structure of Ga_2Te_5 PLD Films for Memory Applications using Diffraction and First-Principles Simulations

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Supplementary Information

Figure S1. X-ray diffraction patterns of rapidly cooled Ga_2Te_5 melt and Ga_2Te_5 PLD film.

Figure S2. Scattering corrections for crystallized Ga_2Te_5 PLD film.

Figure S3. FSDP parameters for glassy Ga_xTe_{1-x} alloys.

Figure S4. Bond angle distribution $B_{\mathrm{TeGaTe}}(\theta)$ in simulated g-Ga_2Te_5.

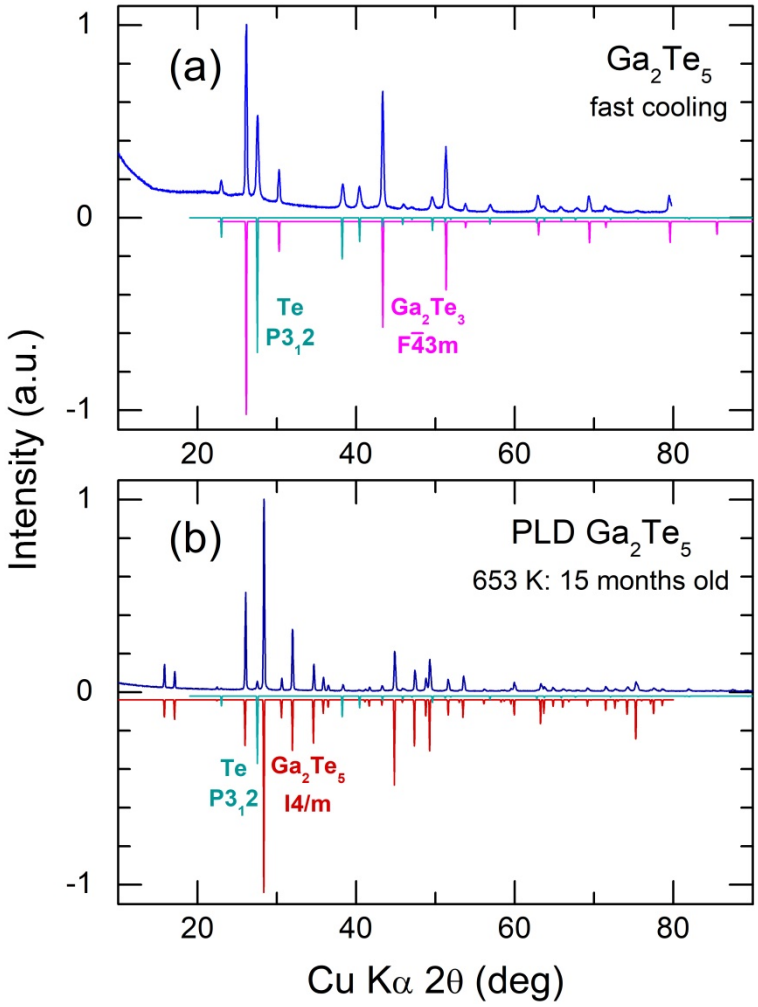

Figure S1. X-ray diffraction patterns of (a) rapidly cooled Ga_2Te_5 melt, and (b) Ga_2Te_5 PLD film heated to 653 K with a typical DSC rate of 10 K min^{-1}, cooled down to room temperature and stored for 15 months. Rapidly cooled Ga_2Te_5 appears to be a mixture of cubic Ga_2Te_3, space group $F\bar{4}3m$ [s1], and trigonal tellurium, $P3_12$ [s2]. Annealed 15-month old Ga_2Te_5 PLD film mostly contains tetragonal Ga_2Te_5, $I4/m$ [s3], metastable at room temperature [s4], and traces of trigonal Te.

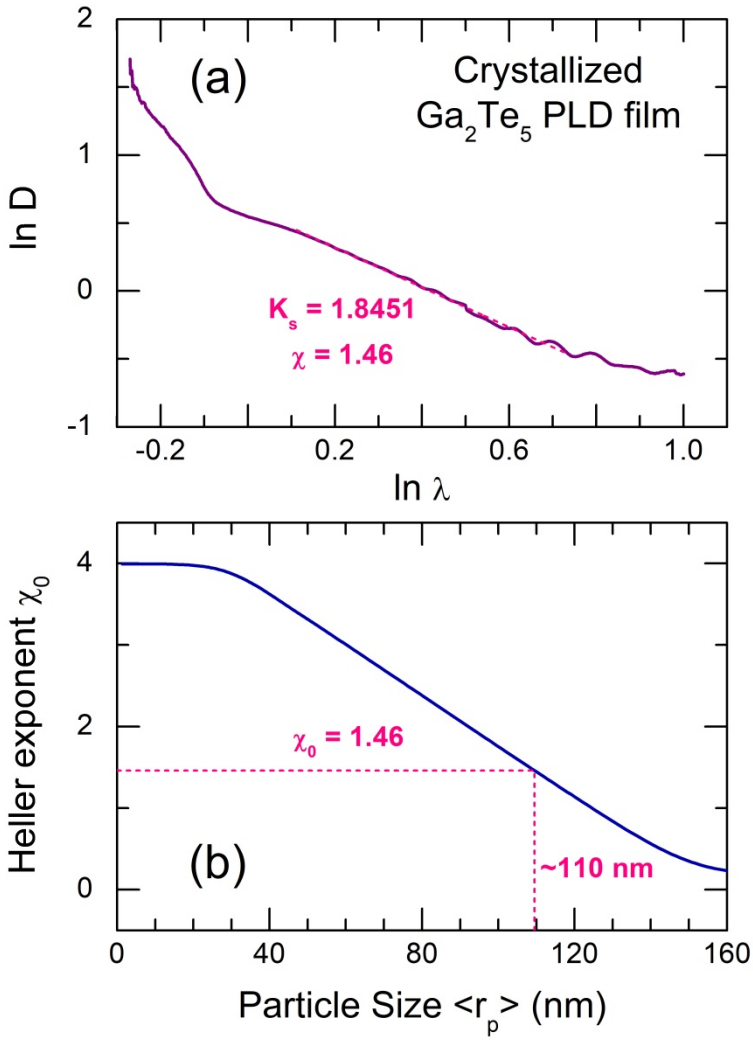

Figure S2. Scattering corrections for crystallized Ga_2Te_5 PLD film: (a) optical density D as a function of λ, plotted on a logarithmic scale; the derived scattering coefficient K_S and the wavelength exponent χ are indicated; (b) theoretical Heller wavelength exponent χ_0 as a function of the average particle size $\langle r_p \rangle$, yielding $\langle r_p \rangle \approx 110$ nm for the crystallized Ga_2Te_5 PLD film.

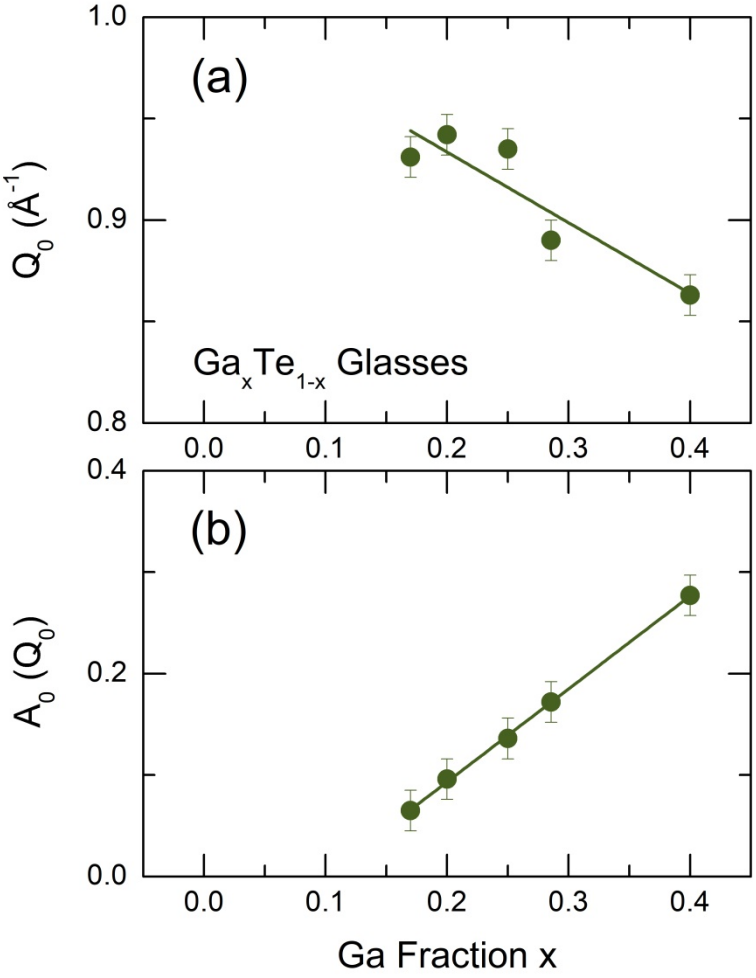

Figure S3. FSDP parameters for glassy Ga_xTe_{1-x} alloys: (a) the FSDP position Q_0, and (b) the amplitude $A_0(Q_0)$ as a function of x.

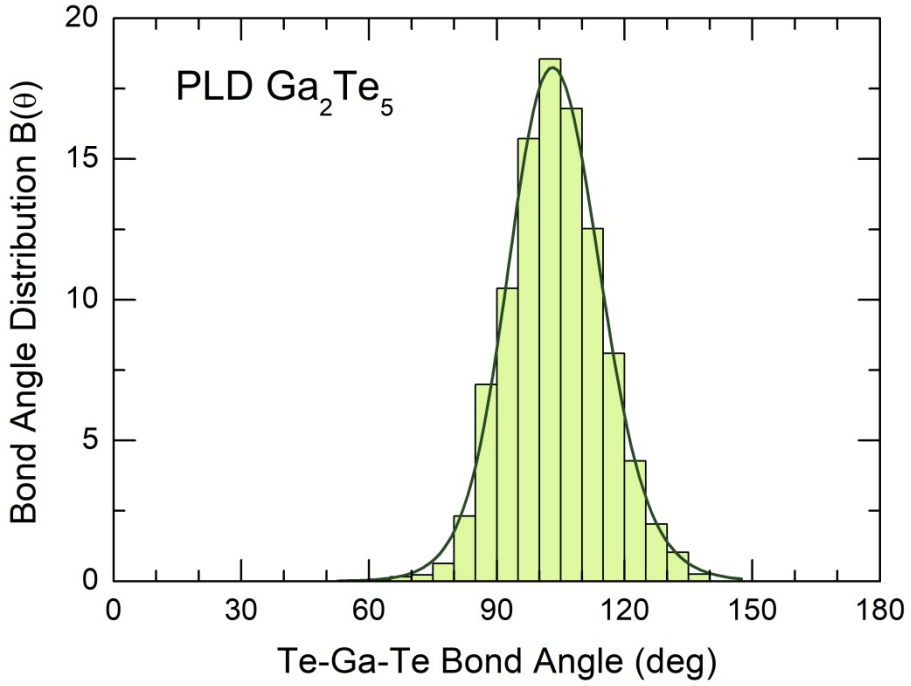

Figure S4. Bond angle distribution $B_{\mathrm{TeGaTe}}(\theta)$ in simulated g-Ga_2Te_5.

Additional references

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