



Decoding the Atomic Structure of Ga₂Te₅ Pulsed Laser Deposition Films for Memory Applications Using Diffraction and First-Principles Simulations

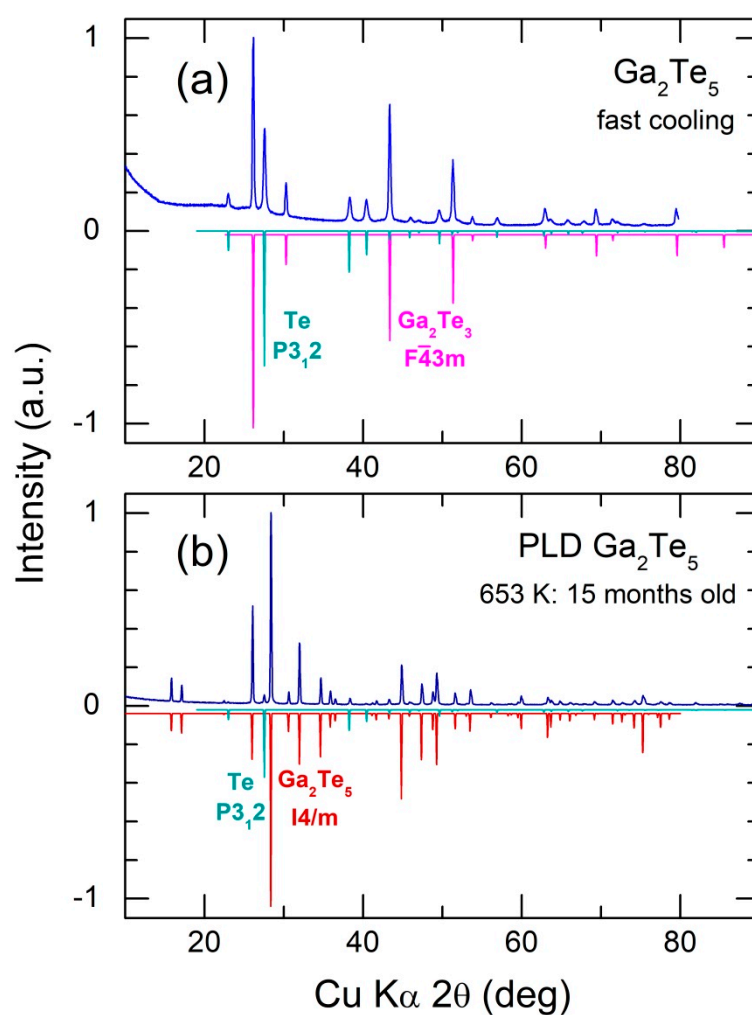


Figure S1. X-ray diffraction patterns of (a) rapidly cooled Ga₂Te₅ melt, and (b) Ga₂Te₅ PLD film heated to 653 K with a typical DSC rate of 10 K min^{−1}, cooled down to room temperature and stored for 15 months. Rapidly cooled Ga₂Te₅ appears to be a mixture of cubic Ga₂Te₃, space group *F*43*m* [1], and trigonal tellurium, *P*3₁2 [2]. Annealed 15-month old Ga₂Te₅ PLD film mostly contains trigonal Ga₂Te₅, *I*4/*m* [3], metastable at room temperature [4], and traces of trigonal Te.

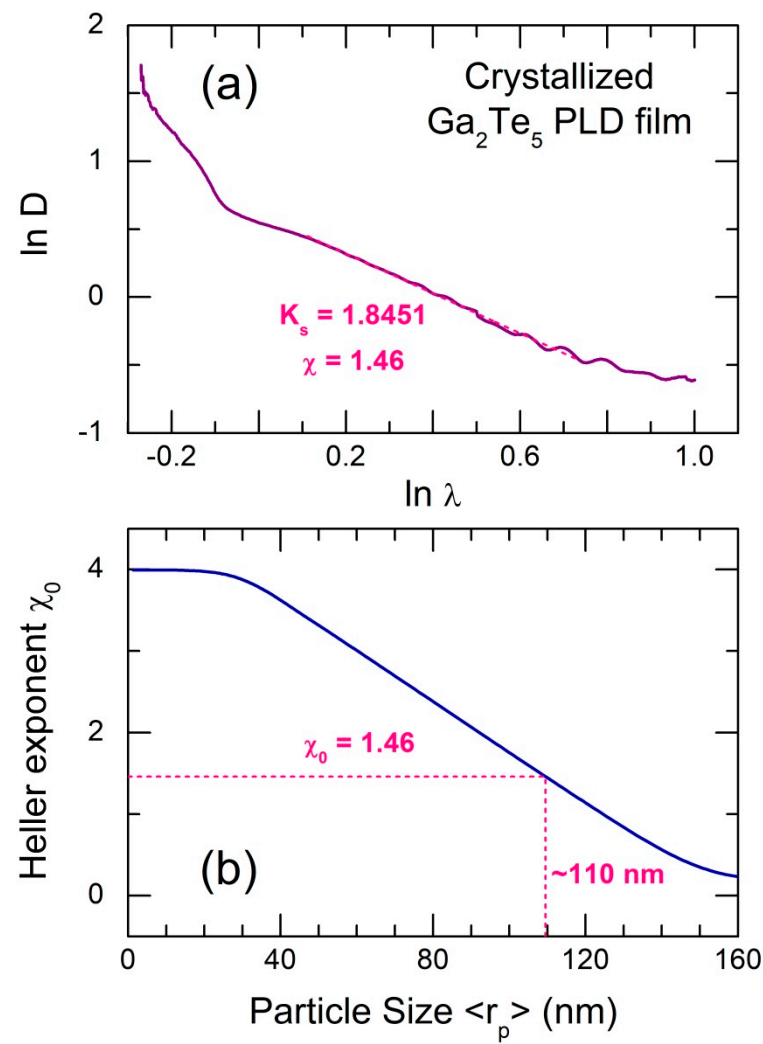


Figure S2. Scattering corrections for crystallized Ga_2Te_5 PLD film: **(a)** optical density D as a function of λ , plotted on a logarithmic scale; the derived scattering coefficient K_s and the wavelength exponent χ are indicated; **(b)** theoretical Heller wavelength exponent χ_0 as a function of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

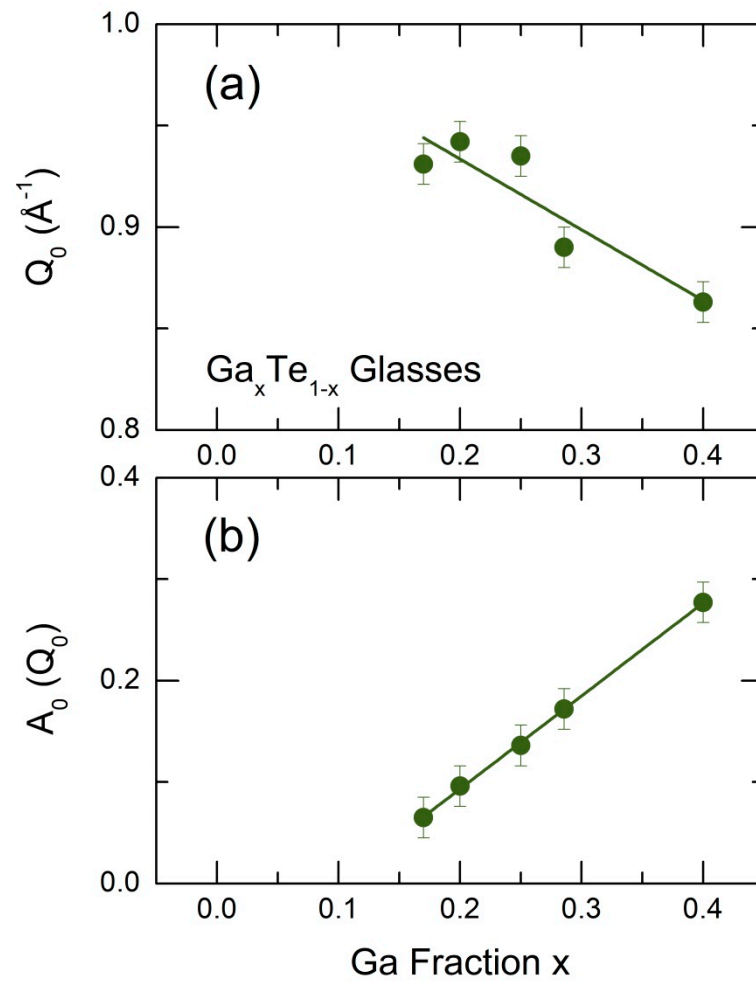


Figure S3. FSDP parameters for glassy $\text{Ga}_x\text{Te}_{1-x}$ alloys: **(a)** the FSDP position Q_0 , and **(b)** the amplitude $A_0(Q_0)$ as a function of x .

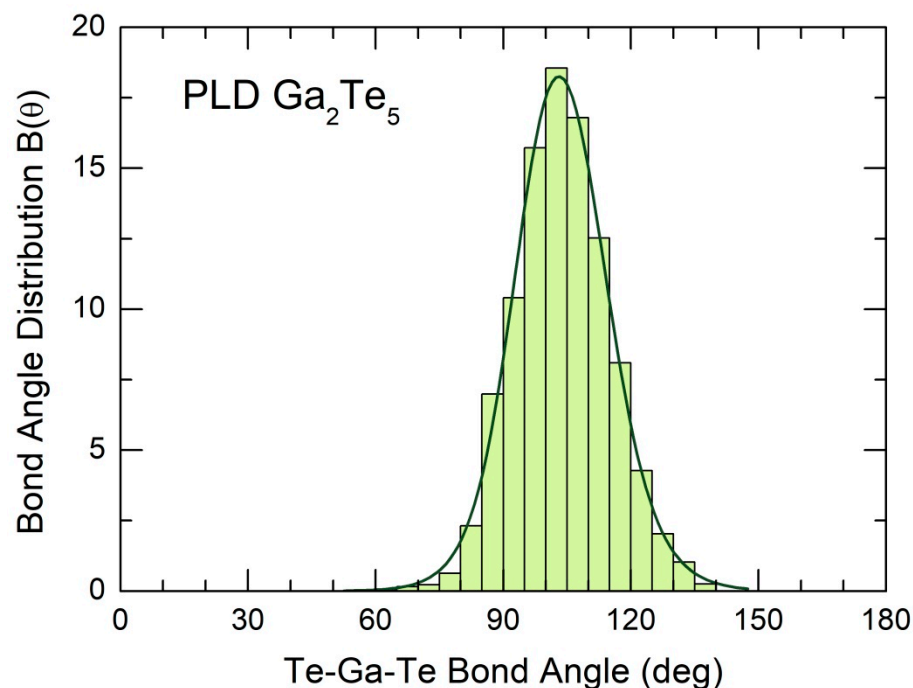


Figure S4. Bond angle distribution $B_{\text{TeGaTe}}(\theta)$ in simulated g- Ga_2Te_5 .

References

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2. Cherin, P.; Unger, P. Two-dimensional refinement of the crystal structure of tellurium. *Acta Crystallogr. B* **1967**, *23*, 670–671.
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4. Alapini, F.; Flahaut, J.; Guittard, M.; Jaulmes, S.; Julien-Pouzol, M. Système gallium–tellure. Diagramme de phases, étude structurale de GaTe , Ga_2Te_5 et de $\text{Ga}_6\text{SnTe}_{10}$. *J. Solid State Chem.* **1979**, *28*, 309–319.