Newly synthesized MAX phase Zr_2SeC: DFT insights into physical properties towards possible applications

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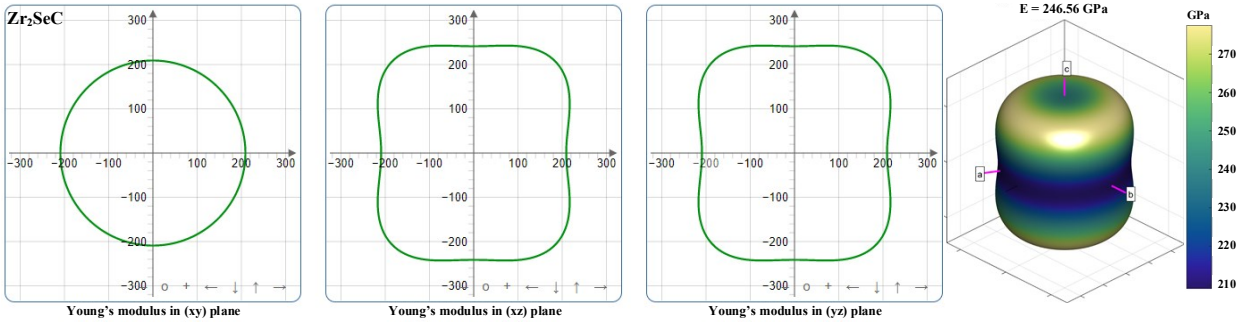
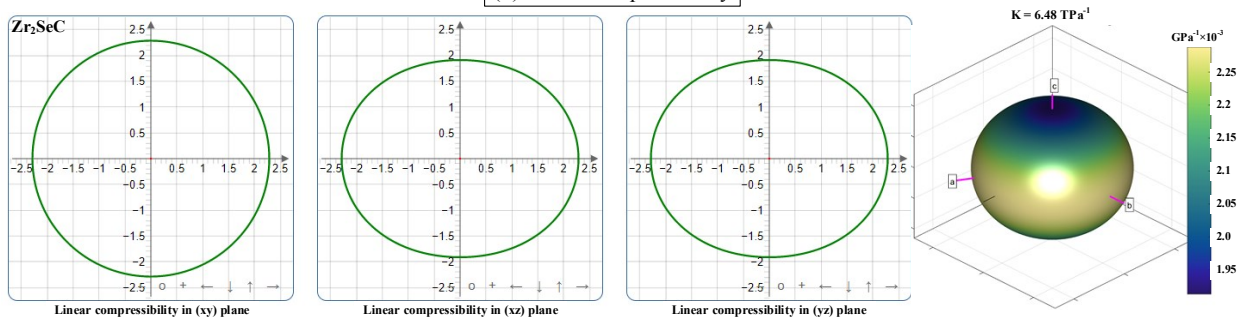
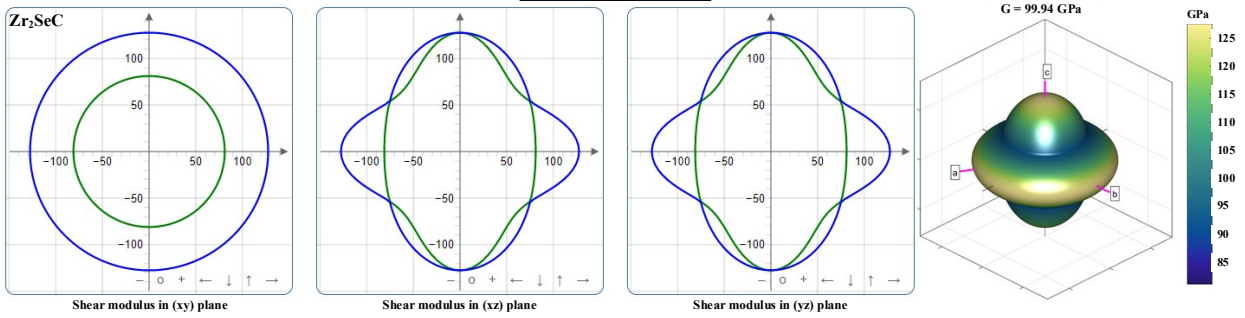
(a) Young's modulus



(b) Linear compressibility



(c) Shear modulus



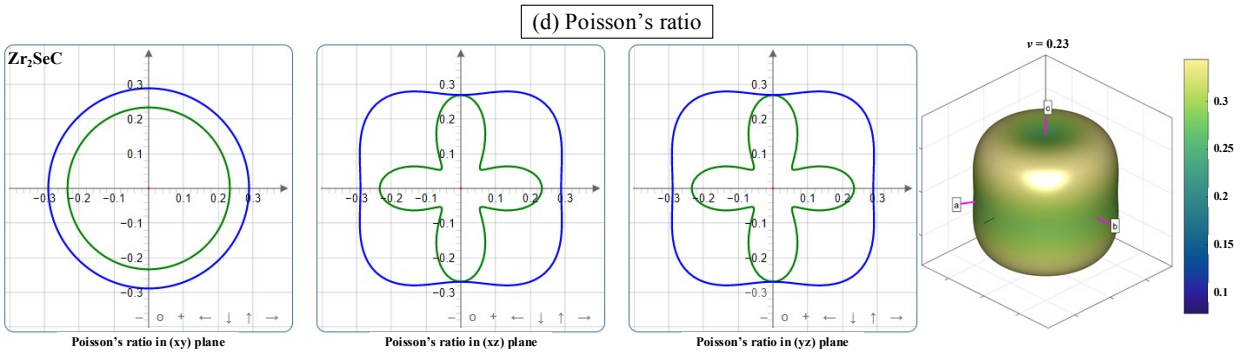
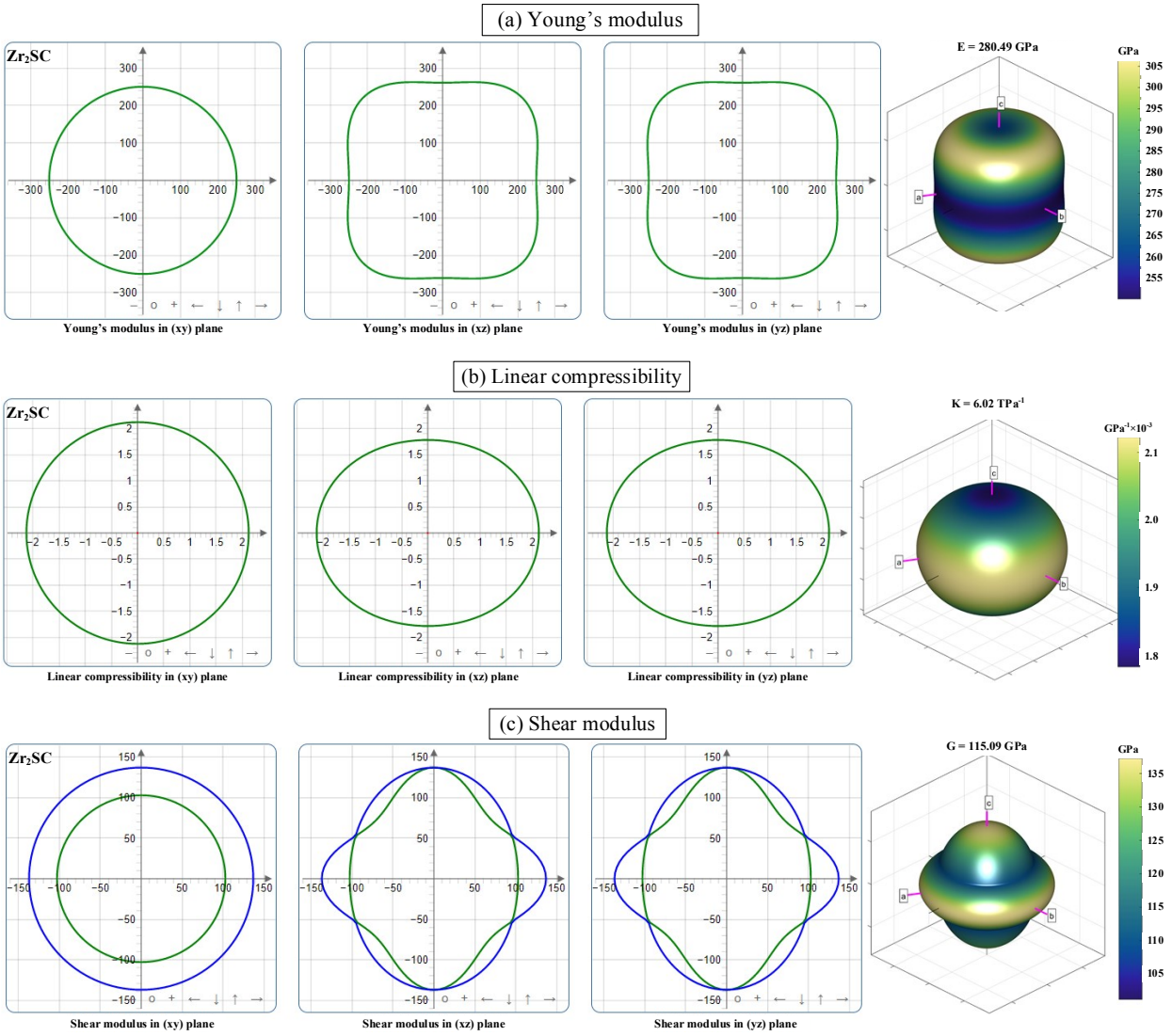


Fig. S1 The 2D projections and 3D plots of (a) Young's modulus, Y, (b) Linear compressibility, K, (c) shear modulus, G, and (d) Poisson's ratio, ν of Zr_2SeC MAX phase.



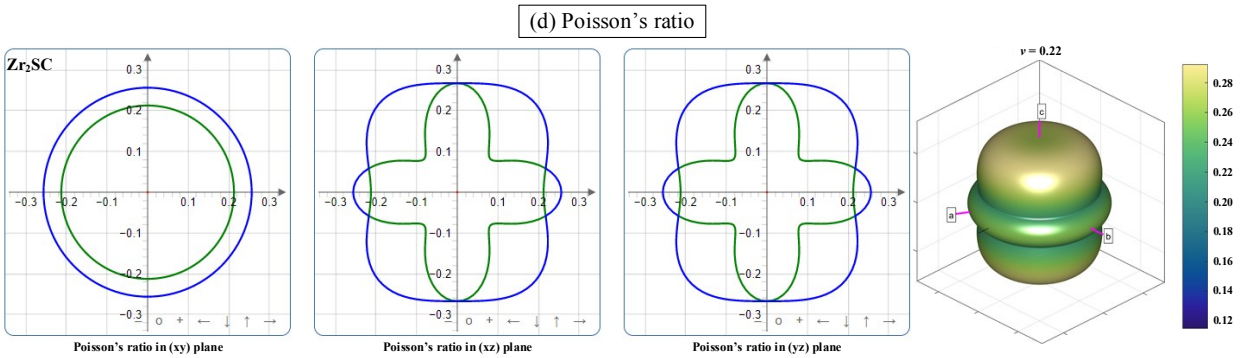


Fig. S2 The 2D projections and 3D plots of (a) Young's modulus, Y, (b) Linear compressibility, K, (c) shear modulus, G, and (d) Poisson's ratio, v of Zr_2SC MAX phase.

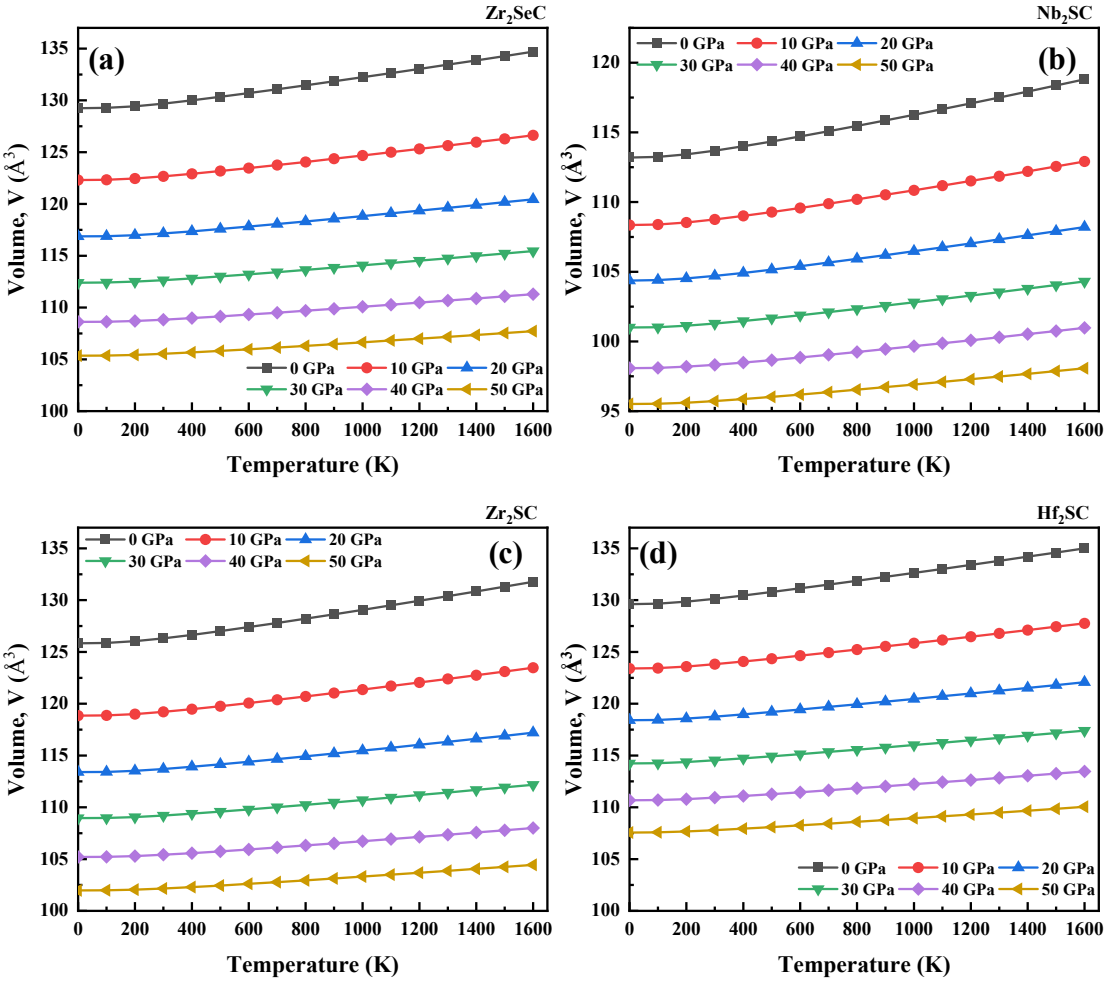


Fig. S3 Temperature effect on the volume of (a) Zr_2SeC, (b) Nb_2SC, (c) Zr_2SC, and (d) Hf_2SC MAX phases at different pressure.

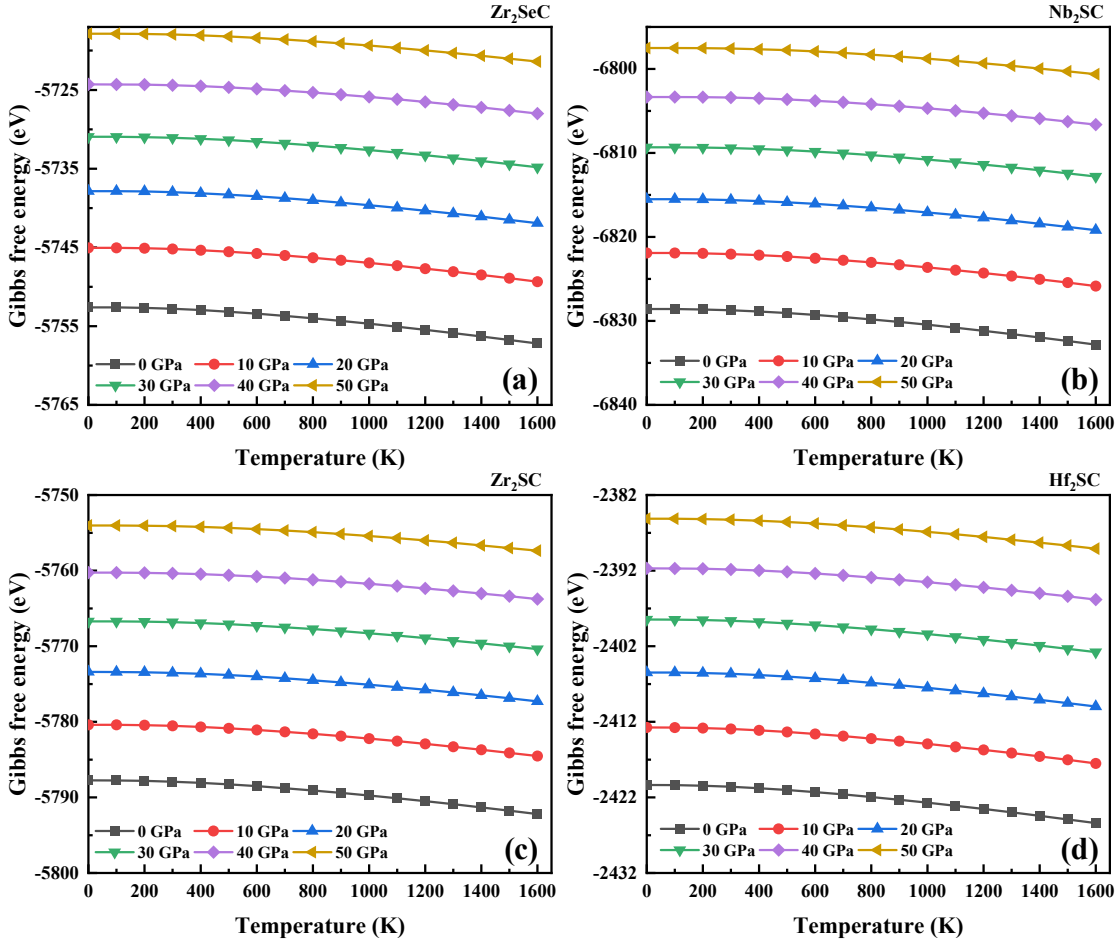


Fig. S4 Variation of Gibbs free energy with temperature for (a) Zr_2SeC, (b) Nb_2SC, (c) Zr_2SC, and (d) Hf_2SC MAX phases at different pressure.

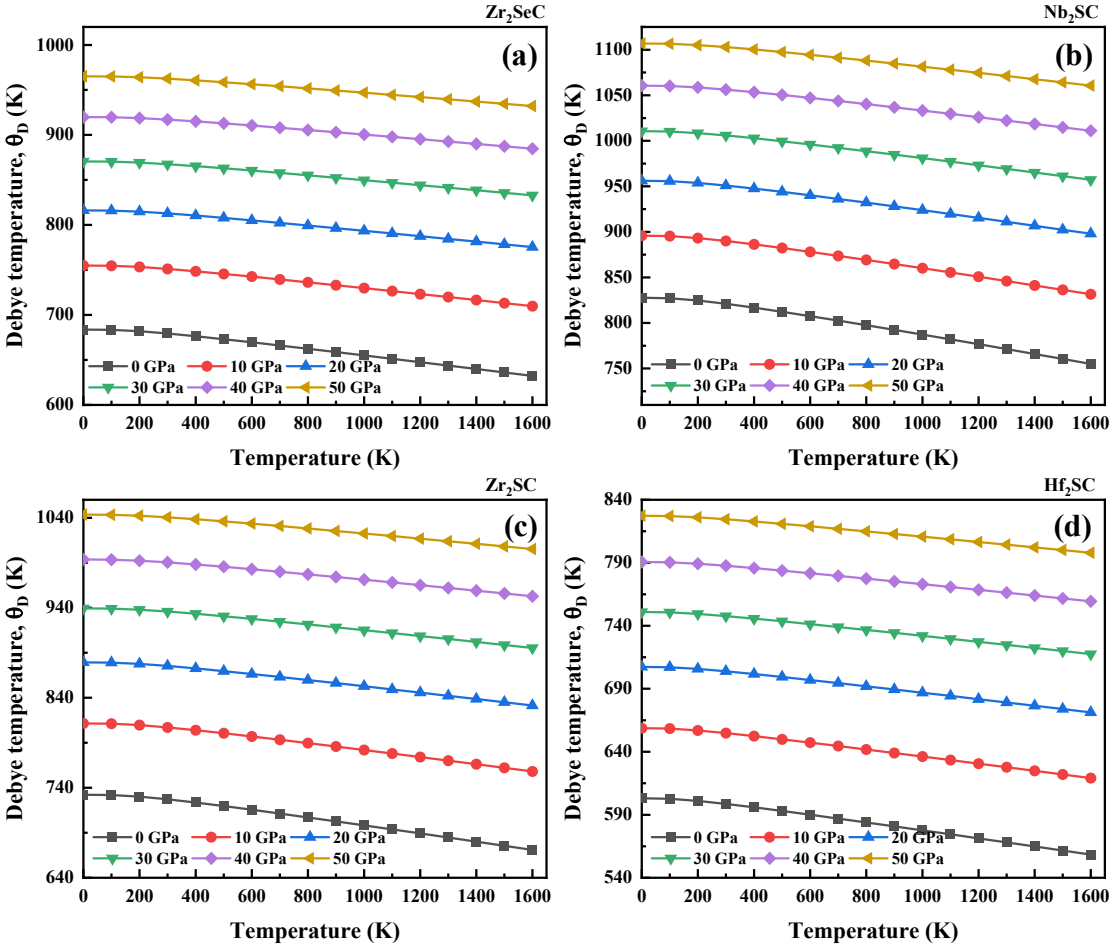


Fig. S5 Temperature effect on the Debye temperature of (a) Zr_2SeC, (b) Nb_2SC, (c) Zr_2SC, and (d) Hf_2SC MAX phases at different pressure.

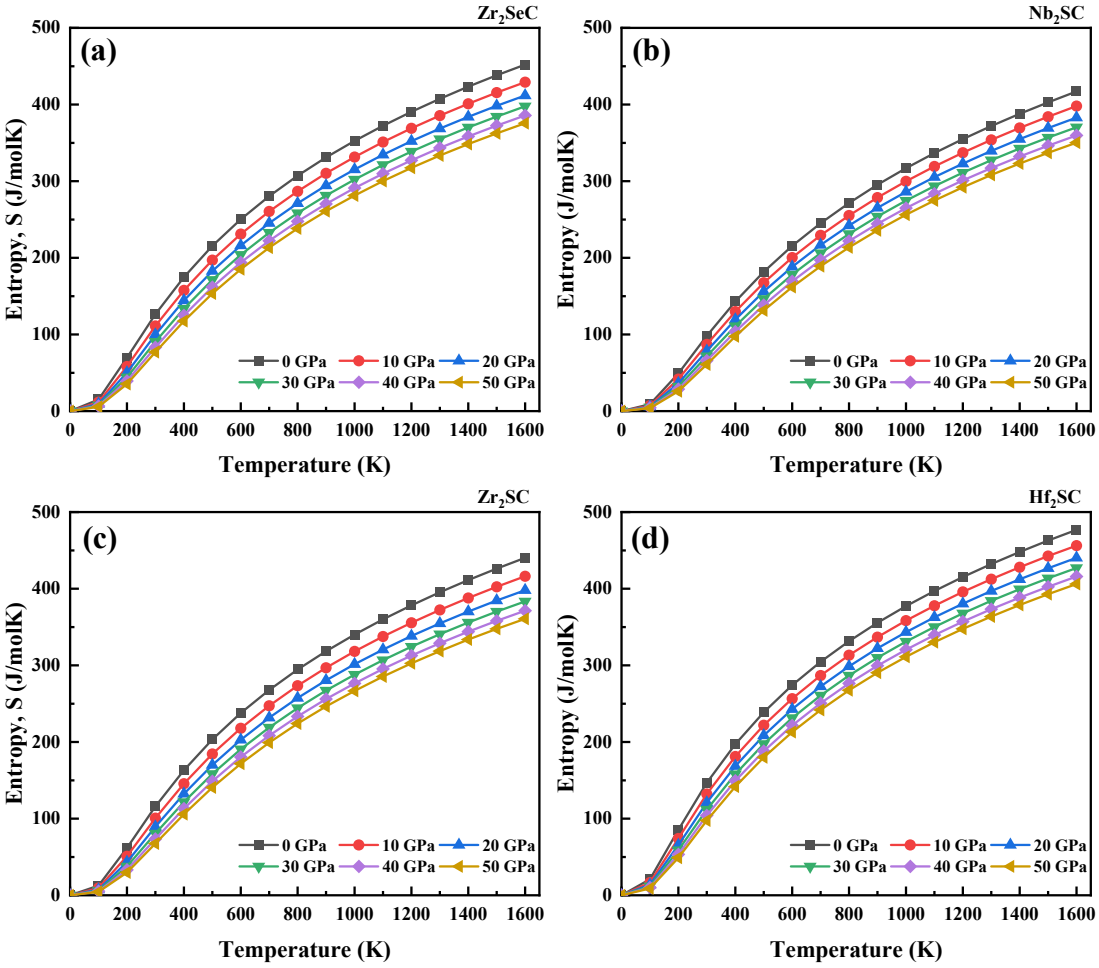


Fig. S6 Temperature effect on the entropy of (a) Zr_2SeC, (b) Nb_2SC, (c) Zr_2SC, and (d) Hf_2SC MAX phases at different pressure.

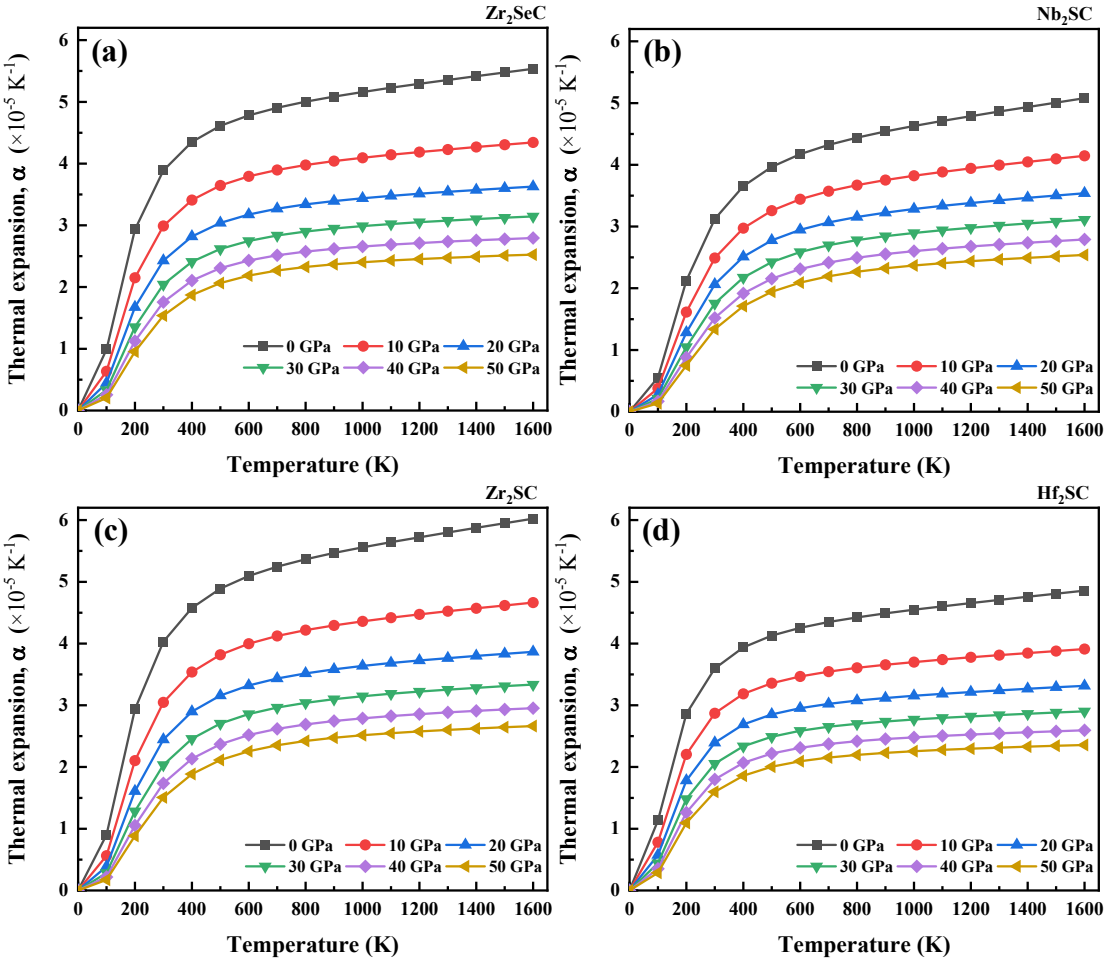


Fig.S7 Temperature effect on the thermal expansion coefficient of (a) Zr_2SeC, (b) Nb_2SC, (c) Zr_2SC, and (d) Hf_2SC MAX phases at different pressure.

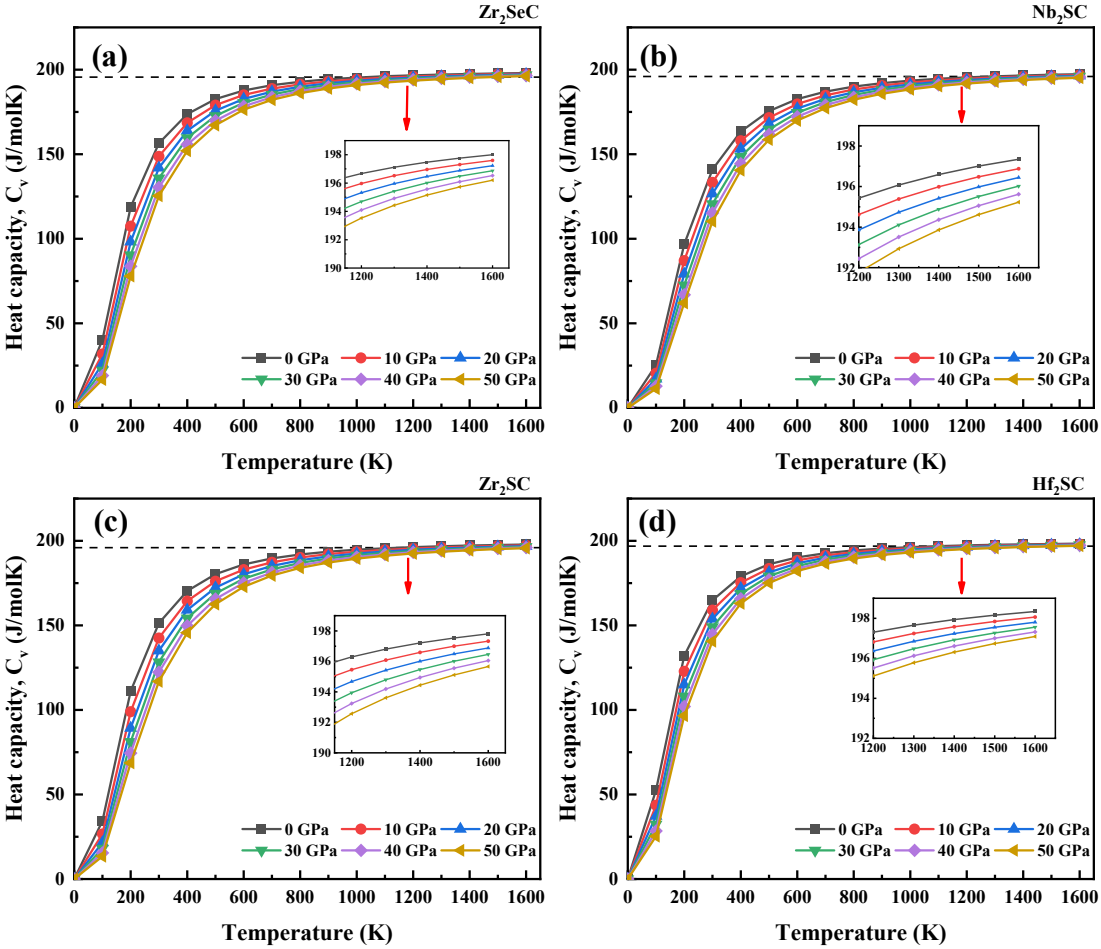


Fig. S8 Temperature effect on the heat capacity at constant volume (C_v) of (a) Zr_2SeC, (b) Nb_2SC, (c) Zr_2SC, and (d) Hf_2SC MAX phases at different pressure.

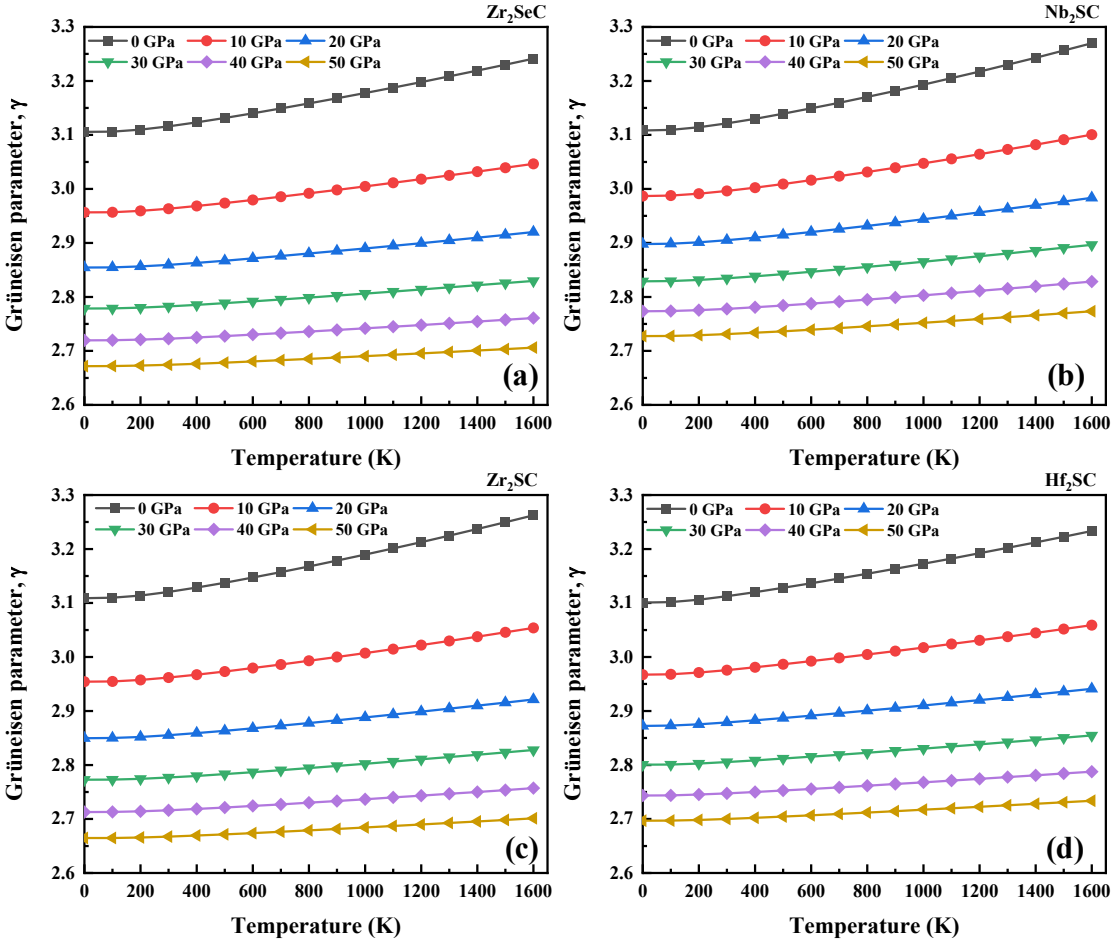


Fig. S9 Effect of temperature on Grüneisen parameter of (a) Zr_2SeC, (b) Nb_2SC, (c) Zr_2SC, and (d) Hf_2SC MAX phases at different pressure.