Dielectric Properties and the Pressure–Temperature Phase Diagram of Layered $CuInP_2S_6$ Crystals

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Crystals of $CuInP_2S_6$ belong to the family of layered van der Waals materials that attract considerable attention due to the combination of ferroelectric ordering and ionic conductivity. Their unique physical properties arise from the fact that ferroelectric ordering occurs at room temperature and is preserved down to thicknesses of only a few nanometers, making these materials highly promising for next-generation electronic, optoelectronic, and sensing devices.

These theses present the results of studies on the effect of hydrostatic pressure on the dielectric parameters and specific features of the $p–T$ phase diagram of $CuInP_2S_6$ crystals. The investigations were performed on single crystals grown by the Bridgman method. The complex dielectric permittivity was measured in the temperature range 77–450 K at a frequency of 1 MHz using a high-pressure chamber in the range p = 0–6000 atm.

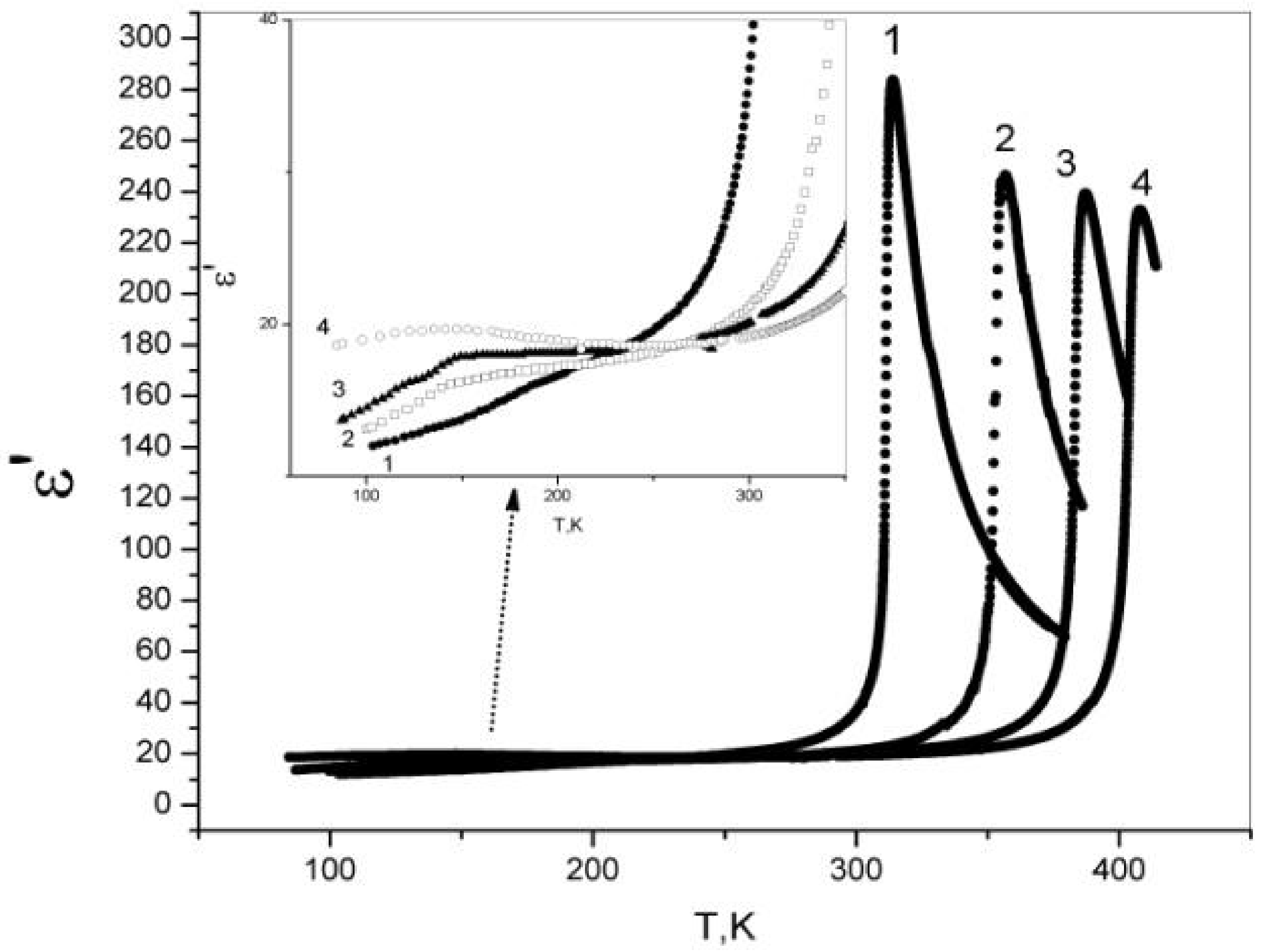


Fig. 1. Temperature dependence of the real part of the dielectric permittivity of a $CuInP_2S_6$ crystal at a frequency of 1 MHz under different pressures p (atm): 1 — atmospheric; 2 — 2000; 3 — 3000; 4 — 5000.

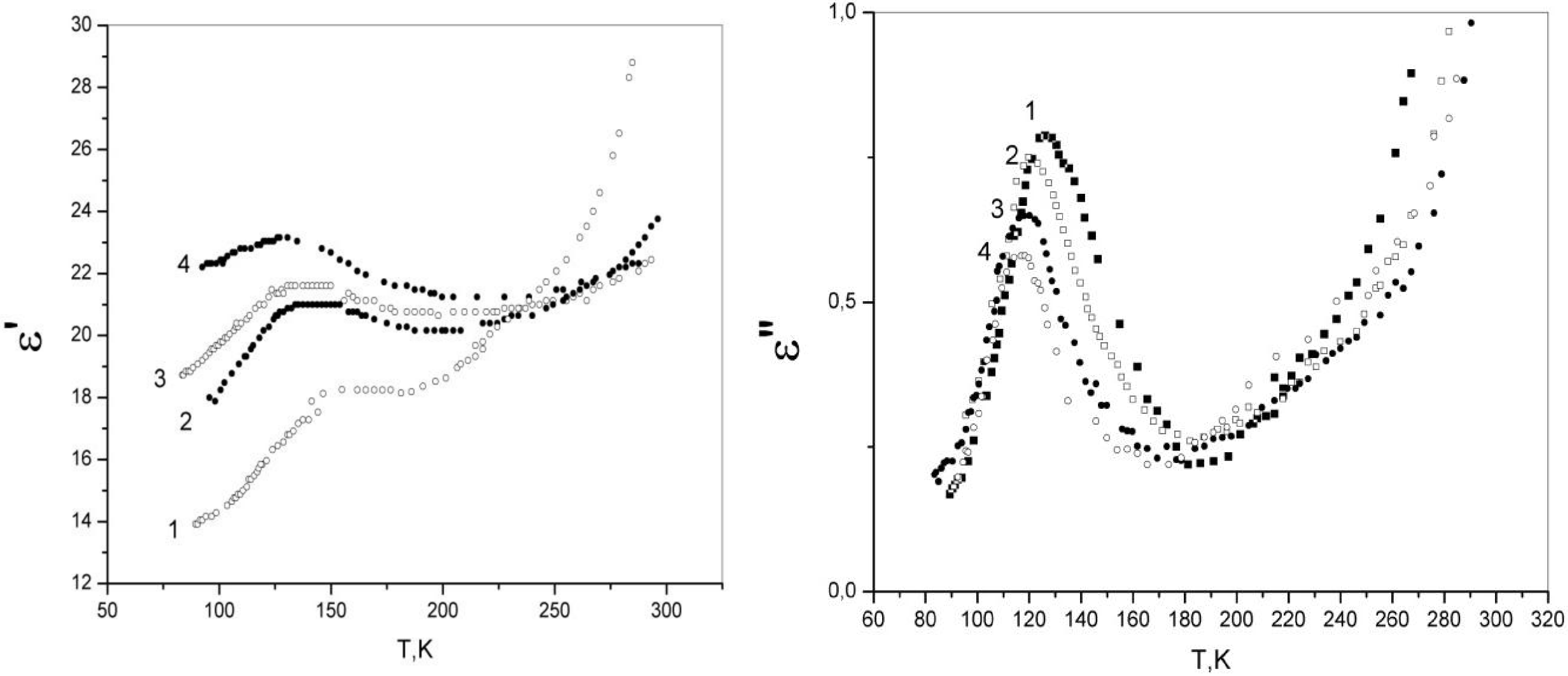
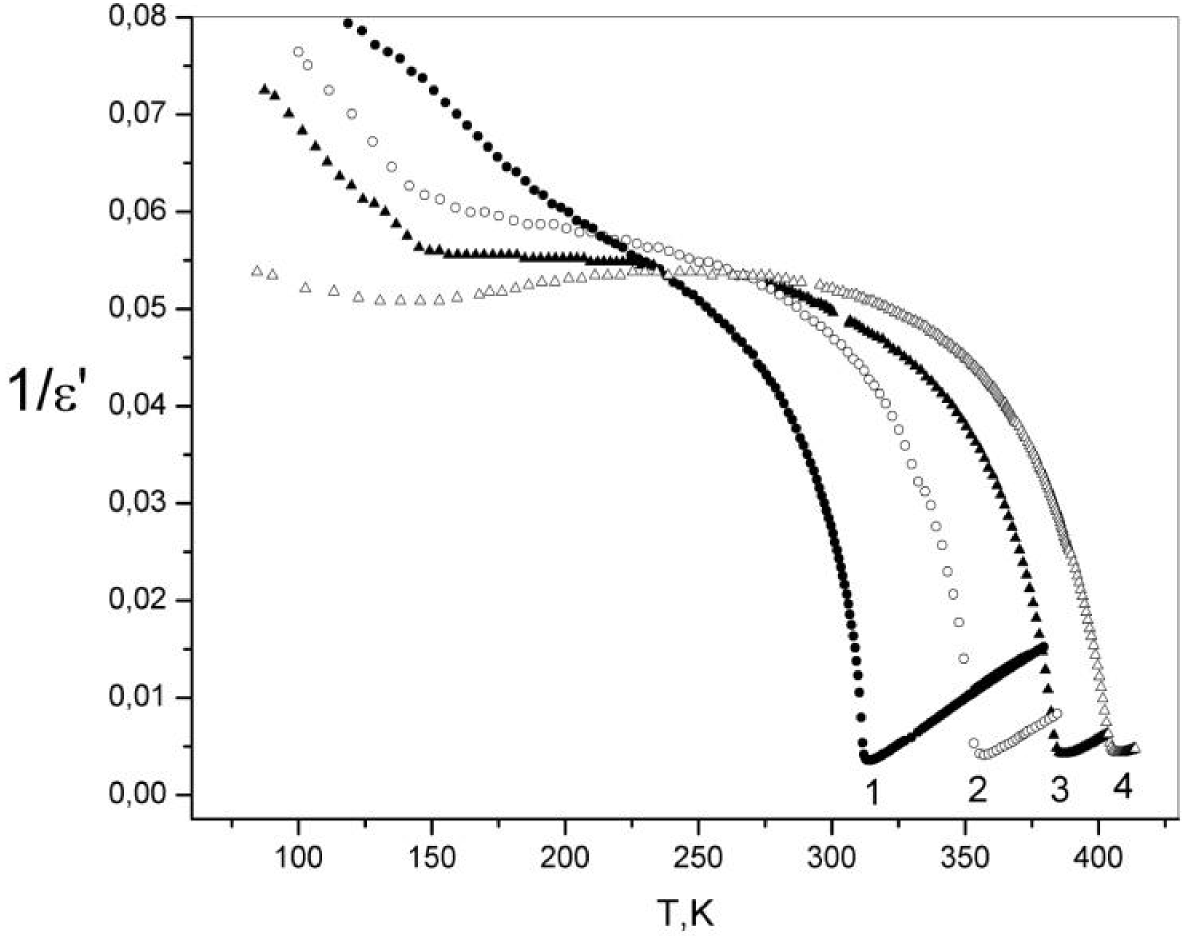


Fig. 2. Temperature dependence of the real and imaginary parts of the dielectric permittivity of a $CuInP_2S_6$ crystal under different pressures at a frequency of 1 kHz:

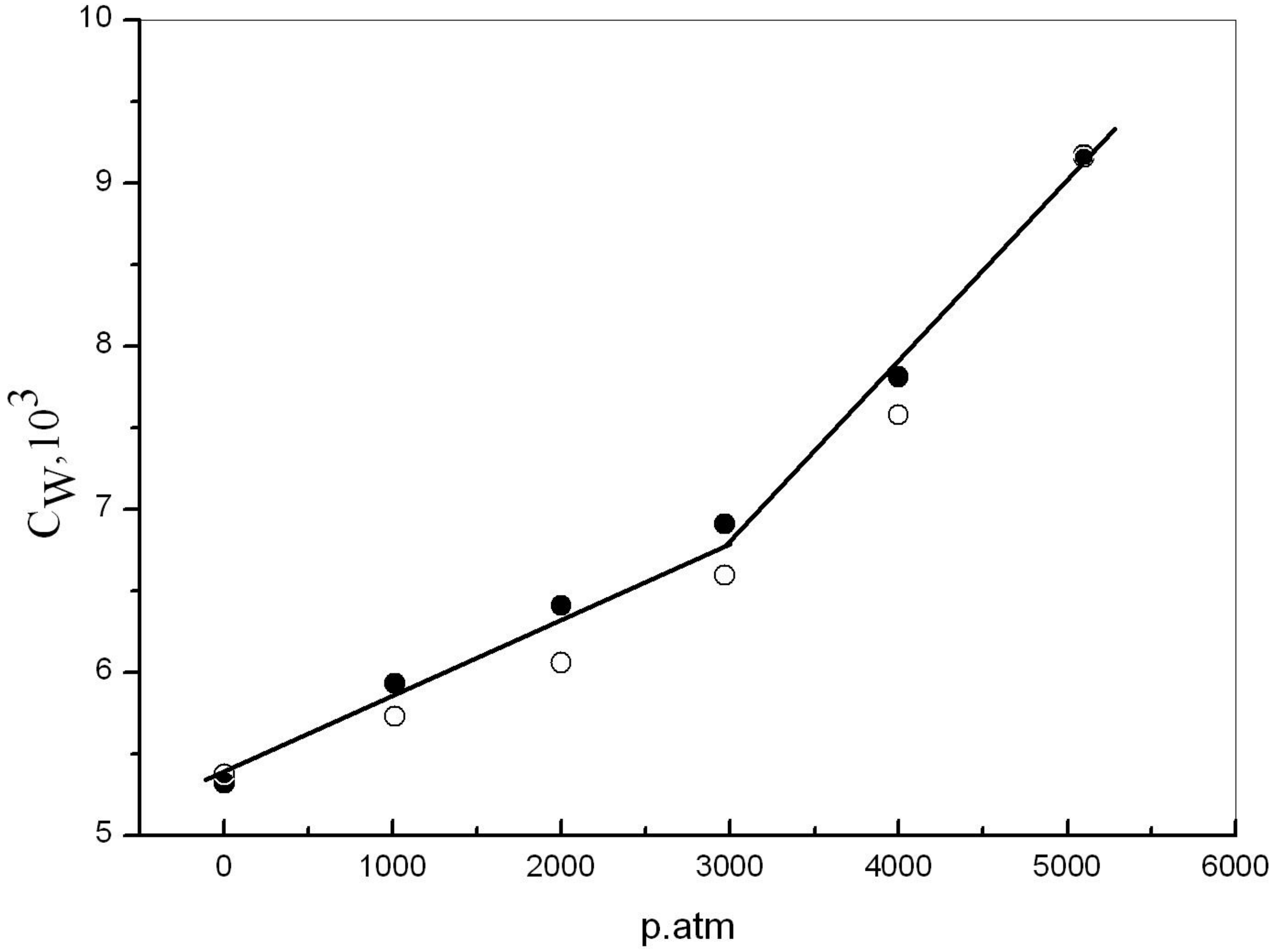
p=1atm; 2) p=2000atm; 3) p=3000atm; 4) p=5000atm.

In the low-temperature region (*T* < 200 K), relaxation behavior of the dielectric permittivity is detected in $CuInP_2S_6$ crystals. Under pressure, this relaxation anomaly becomes more pronounced and shifts toward lower temperatures, which is associated with changes in the lifetime of relaxators and with a reduction in potential barriers for thermally activated hopping polarization.



Above the phase transition temperature, the dielectric permittivity follows the Curie–Weiss law

Fig. 3. Temperature dependence of $1/\varepsilon'$ of a $CuInP_2S_6$ crystal under different pressures at a frequency of 1 MHz: $p = 1$ atm; 2) $p = 2000$ atm; 3) $p = 3000$ atm; 4) $p = 5000$ atm.



Increasing pressure leads to a rise in the Curie–Weiss constant, and a distinctive kink is observed near 2600 atm, which correlates with the deviation from linearity in the $p-T$ phase diagram.

Fig. 4. Pressure dependence of the Curie–Weiss constant in $CuInP_2S_6$ crystals.

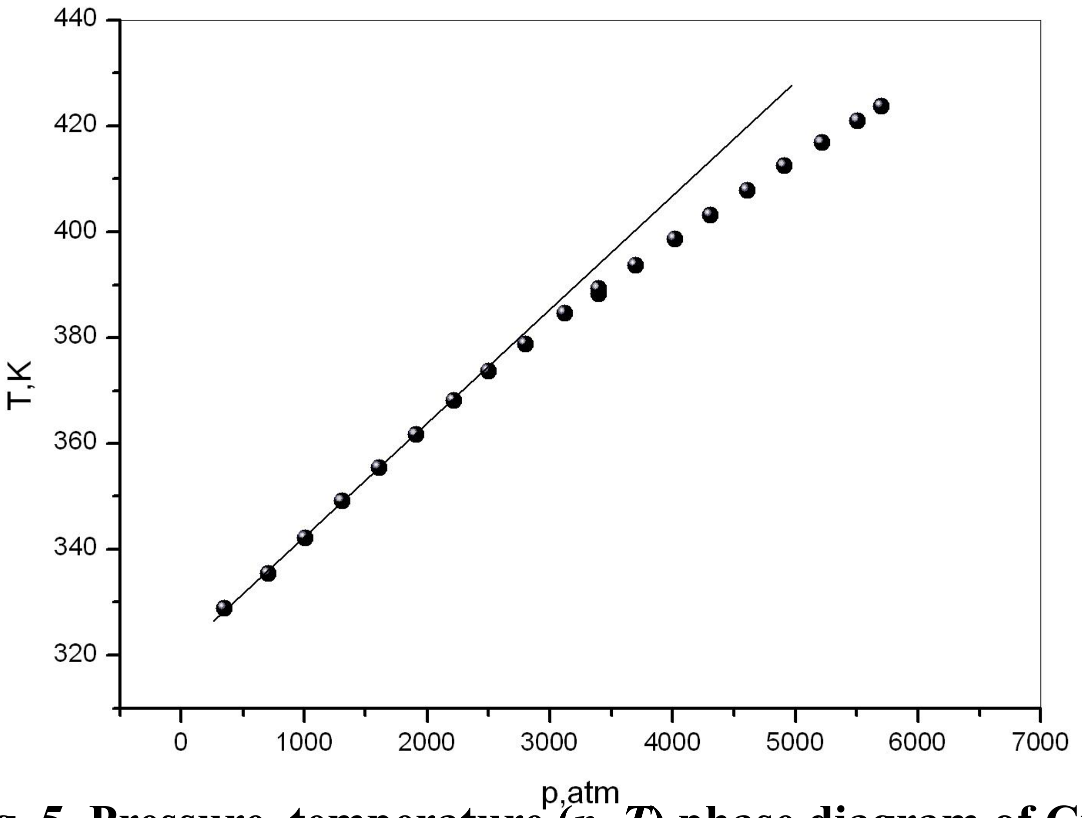


Fig. 5. Pressure–temperature (p–T) phase diagram of $CuInP_2S_6$ crystals.

It was established that in the initial pressure region up to p = 2600 atm, the dependence of the PT temperature on pressure is linear, with an exceptionally high positive pressure coefficient of 210 K/GPa. Such a value is atypical for order – disorder type transitions and indicates that even a small applied pressure can push the ferroelectric state far above room temperature. At higher pressures (p > 2600 atm), deviations of the phase boundary from linear behavior are observed. This behavior is evidently related to the anomalous enhancement of polarization in van der Waals $CuInP_2S_6$ under pressure in the range from 0.26 to 1.40 GPa [1,2]

[1] 1.X. Yao, Y. Bai, C. Jin, X. Zhang, Q. Zheng, Z. Xu, L. Chen, S. Wang, Y. Liu, J. Wang, and J. Zhu, Anomalous polarization enhancement in a van der Waals ferroelectric material under pressure, Nature Communications 14, 4301 (2023) . http://dx.doi.org/10.1038/s41467-023-40075-6 .

[2] Y. Li, Y. Luo, X. Yao, Y. Bai, J. Wang, and J. Zhu, Phase diagram of $CuInP_2S_6$ across wide temperature and pressure ranges. *Appl. Phys. Rev.* 12, 041425 (2025) https://doi.org/10.1063/5.0299899