The effect of iron doping on the electrophysical properties of $Cd_2P_2S_6$ crystals

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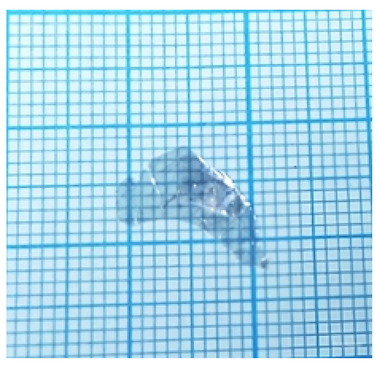
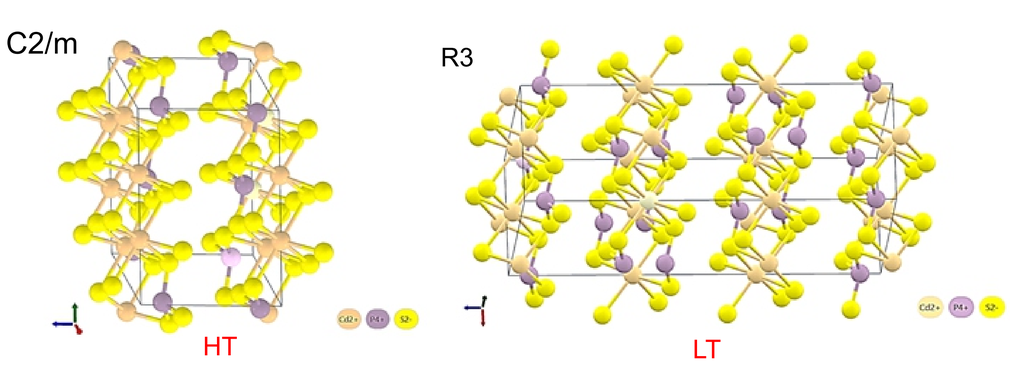
One way to continue progress in increasing the speed and reducing the size of electronic components is to migrate to spintronics, which uses not only the charge but also the spin of electrons to store, process, and transmit information. Van der Waals antiferromagnetic materials are considered very promising for creating such devices, as they can be exfoliated to a two-dimensional (2D) limit-structural monolayers-while retaining their antiferromagnetic properties.

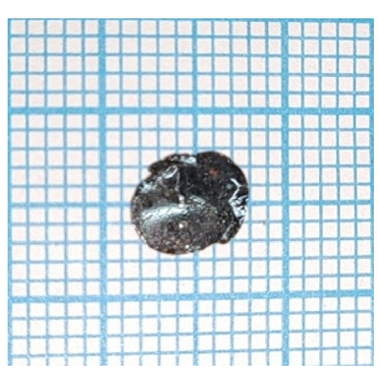
One example of a layered crystal with antiferromagnetic properties is cadmium trichalcogenophosphate ($Cd_2P_2S_6$) doped with iron. The properties of this material change significantly when every second cadmium (Cd) atom is replaced with iron (Fe), forming the compound $CdFeP_2S_6$. Although this material was synthesized in 1988, only three studies have been devoted to it, and almost nothing is known about its electrophysical properties. Therefore, our research focused on studying the temperature dependence of the conductivity and dielectric permittivity of $CdFeP_2S_6$ crystals.



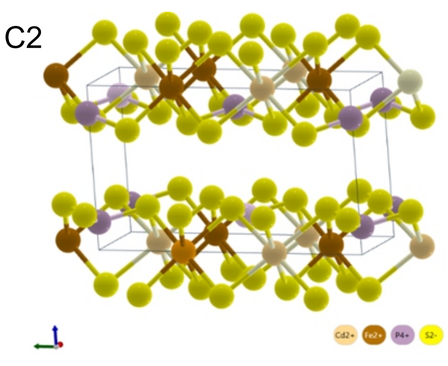
Appearance of the $Cd_2P_2S_6$ crystal



Crystal structure of $Cd_2P_2S_6$

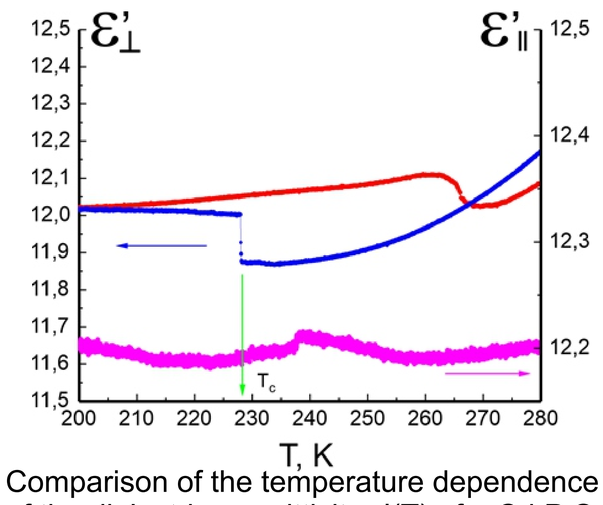


Appearance of the $CdFeP_2S_6$ crystal

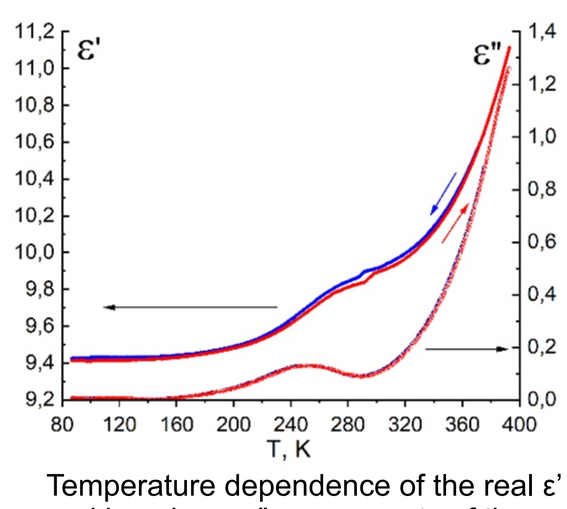


Crystal structure of $CdFeP_2S_6$

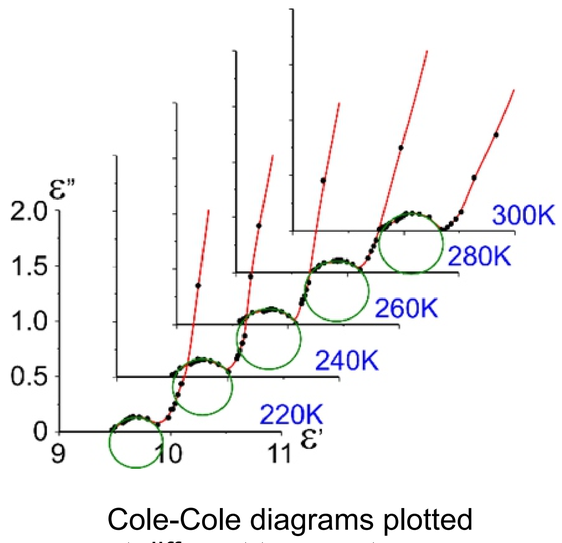
We studied the temperature dependence of the dielectric spectra of $CdFeP_2S_6$ single crystals within a temperature range of 80-400 K. Our measurements revealed that this material exhibits a change in the temperature-frequency behavior of its dielectric properties. The maximum anomaly of the imaginary part (ε”) and the corresponding break in the real component (ε’) of the complex dielectric permittivity (ε* = ε’ - iε”) occur at a temperature of 250 K and a measurement field frequency of 10 kHz. The observed dielectric spectra can be described by the Cole-Cole formula, with a relaxation time distribution parameter α of 0.4-0.6, which is very high and decreases upon cooling. This indicates a large relaxation time distribution, strong spatial and energy inhomogeneity, and a cooperative rather than Debye relaxation mechanism. The temperature dependence of the relaxation time is described by the Arrhenius law. Using this, the activation energy of the process was determined to be E_a = 0.347 eV.



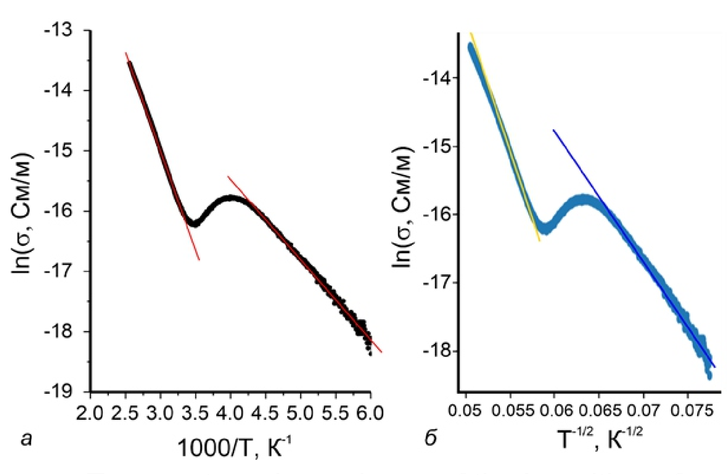
Comparison of the temperature dependence of the dielectric permittivity ε’(T) of a $Cd_2P_2S_6$ crystal along and across the structural layers at a frequency of 10 kHz.



Temperature dependence of the real ε’ and imaginary ε” components of the complex dielectric permittivity ε* = ε’iε” of the $CdFeP_2S_6$ crystal



Cole-Cole diagrams plotted at different temperatures

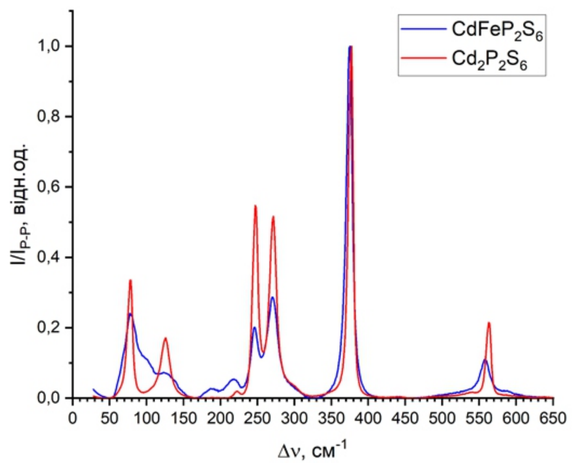


Temperature dependence of the logarithm of conductivity as a function of the inverse temperature – a, and $T^{1/2}$ – b.

In order to verify the most probable charge transfer mechanisms in these crystals, we measured the temperature dependence of the electrical conductivity of $CdFeP_2S_6$ crystals at a constant current. Two regions with different activation energies were observed in this dependence.

In the high-temperature region (1000/T = 2.5 - 3.2), we obtained an activation energy of E_{a1}= 0.3 - 0.35 eV. For the low-temperature region (1000/T = 4.2 - 5.8), E_{a2} = 0.12-0.15 eV.

These results enable us to determine the conduction mechanisms in $CdFeP_2S_6$ crystals more accurately. E_{a2} ~ 0.33 eV is more characteristic of polaron conduction caused by thermally activated charge carrier jumps, which is consistent with the mechanism associated with Fe^{2+}/Fe^{3+} centers. E_{a2} ~ 0.13 eV is most likely associated with hopping conduction, charge transfer between localized states and correlated defect transport. The nonlinearity between the two is indicative of a transition between the two mechanisms.



Comparison of the combinatorial scattering spectra of $Cd_2P_2S_6$ and $CdFeP_2S_6$ crystals obtained at a wavelength of 532 nm.

[1] S. Lee, P. Colombet, G. Ouvrard and R. Brec, Inorg. Chem. 27, 1291 (1988). http://dx.doi.org/10.1021/ic00280a041
[2] A. Bhomwick, B. Bal, S. Ganguly, M. Bhattacharya and M.L. Kundu, J. Phys. Chem. Solidv 53(10) 1279 (1992). http://dx.doi.org/10.1016/0022-3697(92)90246-A
[3] A. Le’austic, E. Rivie’re, R. Cle?ment, E. Manova and I. Mitov, J. Phys. Chem. B 103, 4833 (1999). http://dx.doi.org/10.1021/jp9904623