Frequency Dependent Conductivity In Vanadium Intercalated $MnPSe_3$ Bulk Single Crystal

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Abstract

We observe large dielectric constant of 10^3 at 380 K in low frequency regime which decreases to 40 at 10^6 Hz for $MnPSe_3$ single crystal. We have also synthesized vanadium intercalated $MnPSe_3$ with varying concentration x which is represented as V_xMnPSe_3. Suppression of the dielectric constant is found for low vanadium concentration ($0 < x < 0.05$) at low frequency whereas it shows increasing nature above this $x = 0.05$. Moreover we have also measured frequency dependent polarization conductivity of the same intercalated system which shows hopping type behavior of mobile charge carriers contributed by vanadium.

Keywords: Single crystal, intercalation, dielectric, polarization, hopping.

1. Introduction

Discovery of graphene has also initiated a race which has focused on developing other types of new generation semiconductors with multifunctional properties [1–3]. Layered metal thiophosphates with chemical formula MPX_3 where M is a metal and X is a chalcogen have emerged as a novel group of semiconductors having access to fine tunable band gap[4,5]. $MnPSe_3$ is one of the promising Van der Waal magnetic material with rich physics and many undiscovered physical phenomenon's. The major advantage of this material is the ability to host various transitional metal atoms such as Mn, Fe, Co at the M (Transitional metal) site which corresponds to diverse physical and chemical properties [6–8]. Moreover the Chalcogenide of $MnPSe_3$ can be replaced by other atoms in the same group like Sulphur while keeping the same crystal structure. On the other hand, car- rier doping and transitional metal adsorption can induces a random magnetic moment whose precise control still hinders the fabrication of these layered materials. The lack of experimental details has urged us to investigate in depth of its as prepared and intercalated compound) electrical properties which can lead to better device performance in future [9–11].

In our paper, we have discussed the synthesis and the dielectric property of as grown bulk

$MnPSe_3$ and its intercalated systems. Bulk $MnPSe_3$ has a stacking of many atomic layers with a weak inter layer Van der Waals interaction. Similar to most other transitional metal dichalcogenides, 2D$MnPSe_3$ crystal has a similar hexagonal honey comb lattice structure. Furthermore, due to its ability to accommodate different extrinsic

atoms in the van der Waals gap, drastic modification of electrical, chemical and optical properties in $MnPSe_3$ is expected which needs thorough investigation. Most importantly, due to the crystal structure, this system has no inversion symmetry and has a broken time reversal symmetry which may result in interesting magneto -electric applications [10].

2. Experimental details

$MnPSe_3$ crystals are grown using chemical vapor transport in sealed silica tubes consisting of polycrystalline powders and iodine as a transport agent. The tube is placed in a tube furnace with 50°C temperature gradient from the hotter end of the tube containing the charge(1000°C) to the colder end where growth occurs(950°C). Crystals in the form of shiny green colored plates with typical size $6\times5\times0.1mm^3$grew over the course of 5 days. Elemental analysis was performed using energy dispersive x-rays (EDX) and wavelength dispersive spectrometry (WDS) on a CamecSX100 electron microprobe. An accelerating voltage of 20kV and beam current of 40 nA were used in as pot size of 10 microns. The complex dielectric permittivity and a.c. conductivity are measured using a precision LCR meter (Agilent4282A) at temperatures between 100K and 380K and at frequencies between 20HZ to 2MHz. Oscillating voltage of 1V was applied throughout the dielectric measurement.

3. Results and discussions

Fig.1shows variation of dielectric constant (K) of vanadium intercalated $MnPSe_3$ as a function of frequency at 380K. The static value of dielectric constant for pure $MnPSe_3$ ($x = 0$) is found to be ~ 10^3 whereas at high

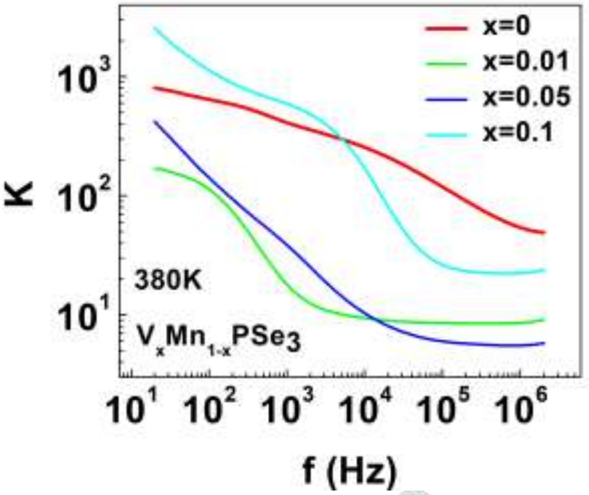

Figure 1: Dielectric constant as a function of oscillating frequencies for various concentration of intercalated $MnPSe_3$ at 380 K.

frequency it drops by one order of magnitude. The higher value of K in pure $MnPSe_3$ is due to presence of dipolar polarization (permanent dipole moment) as a result of broken inversion symmetry. On addition, the weak dependence of dielectric constant especially on low frequency regime also suggests absence of space charge polarization which is also known as Maxwell-Wagner effect [12, 13]. On the other hand, at higher frequency ($10^5 - 10^6$ Hz) the dielectric constant reduces slowly with frequency suggesting weak dipolar interaction. But when vanadium is intercalated between the range $0<x<0.05$, lowering of dielectric constant at low frequency is observed. This is due to redistribution of vanadium 3d electrons around Mn ion in honey comb lattice[14]. But further intercalation ($x > 0.1$) leads to space charge effect which results in strong frequency dependent dielectric constant as shown in the picture.

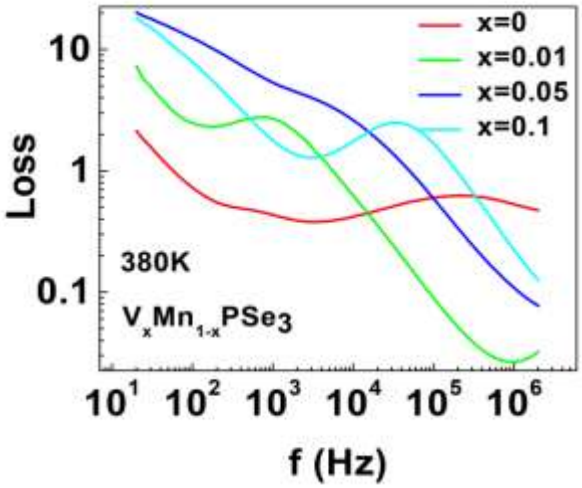

Figure 2: Imaginary part of dielectric permittivity or the loss is plotted as a function of input frequencies for the same set of intercalated compounds.

But for all the compositions the dielectric constant in high frequency regime falls sharply followed by a flat platue. Fig.2 shows the imaginary part of the dielectric permittivity or the dielectric loss as a function of oscillating frequency at 380K. At low frequency all the intercalating compounds including x=0 shows a loss greater than 1 followed by a peak at higher frequency regime. At low frequency, the loss increases as x increases indicating hopping type of conduction behavior. To shed more light into this behavior, we have plotted ac conductivity as a function (f) frequency at elevated temperature (380 K) as shown in Fig. 3. This ac measurement is effective on investigating frequency dependent conductivity which is also known as polarization conduction [11,14]. At low frequency regime, ac conductivity of as prepared $MnPSe_3$ shows a strong frequency dependent behavior which indicates presence of long range hopping process i.e. dc conductivity process which is more likely to be influenced by strong charge coupling interaction.

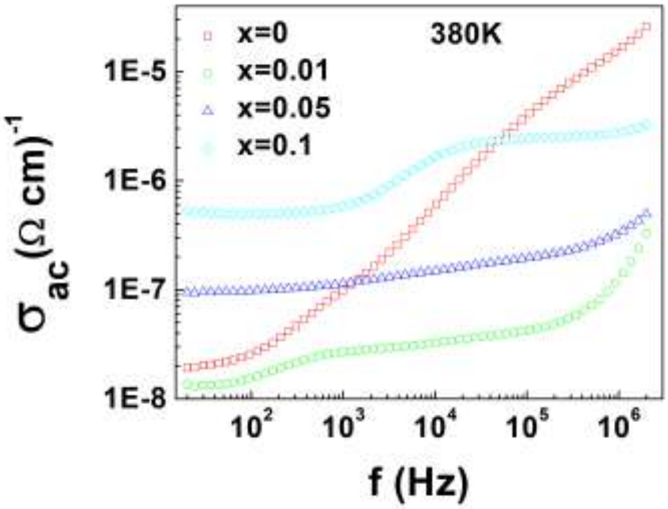

Figure 3: Ac conductivity as a function of frequency at 380 K for increasing concentration of intercalated vanadium atom.

Whereas for intercalated $MnPSe_3$ compounds, a flat frequency independent ac conductivity is observed at low frequency regime. This may be due to breaking of long-range interaction by vanadium ion which results in more localization of charge carriers. At high frequency the carriers find sufficient energy to hop owing to increase in ac conductivity with increasing frequency.

4. Conclusion

We have synthesized vanadium intercalated $MnPSe_3$ compounds using chemical vapor transport technique. By incorporating vanadium in between the layers we found the magnitude of dielectric constant decreases for low concentration of vanadium. For concentration x > 0.1 the dielectric constant shows strong frequency dependence. Moreover, the ac conductivity shows presence of long-range hopping interaction in pure $MnPSe_3$ which weakens upon intercalation of vanadium.

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