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ELECTRONIC TRANSPORT PROPERTIES OF $FePS_3$

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Abstract: a.c. and d.c. conductivity and photoconductivity measurements on $FePS_3$ compound have been carried out as a function of both temperature and frequency. The results, showing a semiconductor-like behaviour, have been interpreted on the basis of the so-called transition metal ion weakly interacting model.

1.-Introduction

$FePS_3$ belongs to the transition metal thiophosphates MPS_3 family, whose characteristic layered structure allows the intercalation of alkali ions or organic molecules in its Van der Waals gap. Due to its complex crystalline structure a complete band structure calculation is still lacking, although some semi-empirical models have been proposed. We have successfully interpreted the $NiPS_3$ and $MnPS_3$ electrical transport properties using a model in which the M-S interaction is weak and ionic in nature [1]. The aim of the present work is to obtain more detailed information on the electronic states energy distribution, through the interpretation, on the basis of the above model, of the d.c. and a.c conductivity and photonductivity measurements.

2.-Results and discussion

ac and dc conductivity and photoconductivity measurements as a function of both temperature and frequency have been carried out in a cryostat under high vacuum, using a phase detection technique.

Fig.1 shows the temperature dependence of both dark and photo conductivities. The σ_d curve is temperature activated with two different activation temperature energy values: 0.58 eV in the high

temperature range and 0.09 eV in the low temperature one. For Fe^{2+} ion the d^6 ground state configuration is $(t_{2g})^4(e_g)^2$ corresponding to a $^5T_{2g}$ state. On the basis of the M weakly interacting model [1] and not considering the d level substructure, we set the Fermi level on the Fe^{2+} d^6 ground state. As reported in the literature, $FePS_3$ behaves as a p-type material, just like $NiPS_3$ and $MnPS_3$ compounds [2,3]. Considering the 0.58 eV σ_d activation energy value we suggest, in analogy, that the conduction process is by holes and takes place in the $3p_z$ valence band. The small σ_d activation energy value, calculated in the low temperature region, may be due to a hopping conduction mechanism involving the 3d localized states. As shown in fig.1, the σ_p curve is temperature activated only in the high temperature region. On the basis of the selection rules for electric and magnetic dipole induced transitions and considering the 1.59 eV fundamental absorption edge value detected in $FePS_3$ [4], the 0.49 eV σ_p activation energy represents the energy separation between the $3p_xp_y$ and $3p_z$ bands, involving a recombination process, just like in $NiPS_3$ and $MnPS_3$ [2,3].

As shown in Fig. 2 ac conductivity σ_{ac} is almost linear dependent on frequency (s=0.89 in $\sigma_{ac}=A\omega^s$) and independent on temperature below about 400K. At higher temperatures a progressively stronger temperature dependence is observed. Such results are consistent with a semiconductor-like behaviour, supporting the conclusions drawn above for dc measurements.

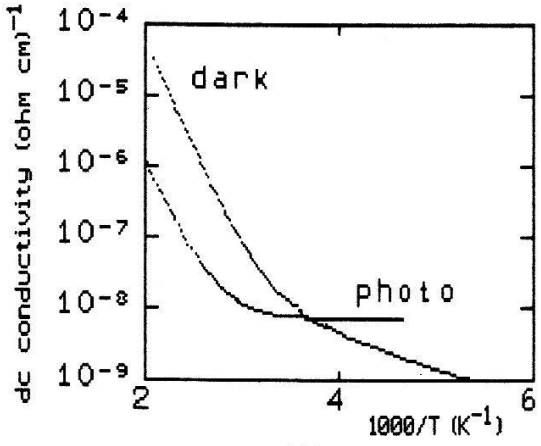

Fig. 1

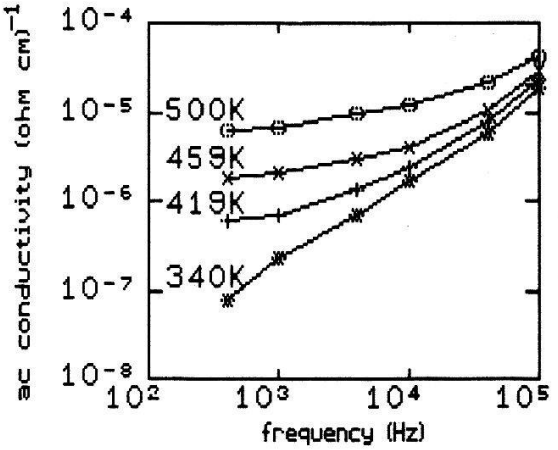

Fig. 2

3.- References

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