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Study the optical properties of polymer material and its applications

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Abstract

PVC/PS (polyvinyl chloride/polystyrene) polymer blend embedded copper chloride ($CuCl_2$) with different wt.% were synthesized using the casting method solution technique. The prepared composite films were described by appropriate techniques such as X-ray diffraction and UV-visible spectrum. The amorphous nature of the structure for the composites was confirmed by X-ray spectra. In the UV/Vis. spectrum of PVC/PS showed CUT-OFF range that was largely increased after the filler addition, where there is a significant decrease in the transmittance values of filled films from 80% for pure PVC/PS blend to 1% for the sample (8 wt% $CuCl_2$). This result mean that, the prepared composite film can be used as a promising material for excellent UV-Vis optical limiting and UV-protector. Add to that, doping PVC/PS polymeric blend with different concentration of $CuCl_2$ leads to a strong decrease in the band gap from 4.38 eV for PVC/PS polymeric blend till it becomes very close to 2.61 eV for PVC/PS – 8 wt % $CuCl_2$.

Key Words:

PVC/PS; $CuCl_2$; UV/V

1. Introduction:

The PVC polymer is one of the most extensive thermoplastic materials in the world due to its valuable properties, wide applications, high chemical resistance, barrier properties and low cost (El-Bashir ,2017 ; Al-Muntaser,2020). This thermoplastic-hydrophobic polymer is extensively used in various industrial applications due to its low cost, good flexibility, high electrical insulation and excellent chemical/mechanical stability as a result from the dipole-dipole interaction between the Cl and H atoms (A. Abdelghany, 2019;A. Abdelghany,2018). Further, this resin is a suitable candidate in the biomedical applications such as surgical dressings, tubes oxygenators and blood bags since the effect of ascertained stabilizing that exerted on red blood cells by this material (S. El-Bashir 2017;A. Abdelghany, 2019;A. Al-Muntaser, 2020). But, the heat-softening temperature and poor thermal stability in processing and low toughness are obstacles for PVC to increase its application. Thus, this polymer is blended with other polymers (S. El-Bashir 2017).The blending process for polymers has a significant attention since it allows one to prepare new polymeric materials having some of the required properties of each component for specific applications (M. Morsi, 2019).This process is an effective method for the preparation of flexible polymeric matrix with a high degree of miscibility instead of new polymer preparation. The transparent PS polymer is chosen as a partner in the blending process since it has different stereo regular configurations (C.I. Park, 2004;P. Slobodian, 2009).This vinyl polymer is low cost and is considered as significant materials because of its excellent mechanical and dielectric properties. Also, it has many excellent properties such as easy processing good chemical resistance, high dimensional stability. Thus, it has been widely utilized in food packing, kitchen appliances and electronic industry (O. Farag, 2018). The PVC and PS polymers are the most frequently used synthetic polymeric materials in engineering medical devices and food packaging (C.I. Park, 2004). Correspondingly, Farman et al investigated the optical properties of PVC/PS blends through terahertz time-domain spectroscopy (THz-TDS) and they found that these blends are miscible at various compositions and can be utilized in the THz technology. (Abdeleghany,2018) prepared a polymeric nanocomposite matrix of PVC/PS (50/50 wt.%) filled with various mass fractions of silica nanoparticles (S. El-Bashir, 2017).Also, the various physical properties of these blends have been studied.(M.Rao, 1984).These studies indicated that the PVC/PS blends are molecularly miscible over all compositions of either PVC or PS. Thus, these blends exhibit a broad range of outstanding properties for applications in business equipment and computers, the automotive industry, electrical insulation, electronics, telecommunications, and many other industries.

Inorganic-organic-polymer composites have attracted great important because they frequently exhibit unexpected hybrid properties synergistically derived from the main components (M.Rao,1984).The addition of transition metal halides (TMH) within the polymeric matrix has a significant effect on its physical properties because of the variance of the filling mode of TMH for various filling levels. The paramagnetic- $CuCl_2.2H_2O$ is one of the important classes of inorganic fillers because it has been utilized as a pigment in dying and catalyst for organic reactions. It is also used in the preparation of battery electrolyte, supercapacitors, and optical (S. El-Bashir, 2017).Up to our knowledge, the PVC/PS blend containing TMH has been received very little attention in the literature. In the current work, the $CuCl_2$ effect as a potential filler for the PVC/PS blend was studied by XRD, UV/Vis. and SEM techniques.

2. Experimental Techniques

2.1. Materials

The PVC powder, Fluka Co., Romania, and PS grains of molecular weight 100,000 g/mol, BDH Co., were used in the preparation of polymeric blend. A cupric chloride anhydrous ($CuCl_2.2H_2O$) of purity 99.5%, Merck company, Germany were used as inorganic fillers. All materials were dissolved in Tetrahydrofuran(THF),Aldrich, Fisher scie ntific for chemicals, UK.

2.2. Preparation of polymeric composite films

The composite samples were prepared through the solution casting method. The solution of PVC/PS blend (50/50 wt.%) was prepared through mixing (0.5 g PVC + 0.5 g PS) in the THF solvent (50 ml) for 3 h on the magnetic stirrer. Then, 1, 2, 4, 8 wt.% of filler were weighted and added to the homogenous solution of prepared blend under stirring at room temperature for 1 h to ensure the dissolution of filler within the polymeric matrix of blend. These mixtures were cast into glass Petri dishes and put in the air at room temperature for the evaporation of solvent. The obtained polymeric films were dried in a vacuum at 40 °C oven for 1 h to remove the residual solvent and moisture.

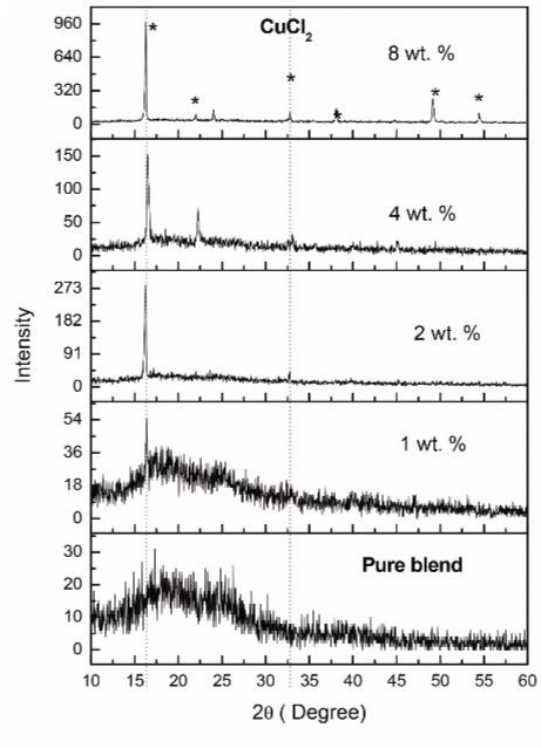
2.3. Characterization techniques and devices.

The X-ray diffraction (XRD) patterns were recorded in the Bragg's angle (2θ) range (10-60°) by XRD-6000 Shimadzu with Cu-Kα radiation (λ = 1.5406 Å and operating voltage of tube 30kV).In the wavelength range 200-2000 nm, the optical spectra were recorded by the ultraviolet spectrophotometer (UV/Vis.) (JASCO V-570) with an accuracy of $\pm$0.2 nm

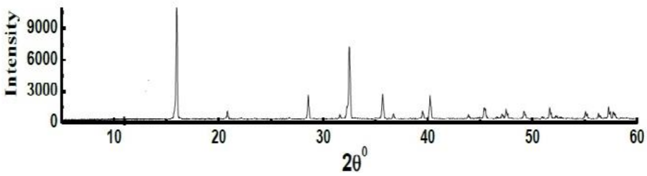
3. Results and Discussion

3.1. XRD analysis

Fig 1a shows the XRD patterns of pure PVC/PS blend and its composite samples. The pattern of blend shows two halo peaks at 18.35 and 24.5° and broad peak at 38.78° reflecting the amorphous nature of the blend component. (Abdelghany, 2018) reported that the diffractogram of PVC polymer exhibits at least three halos at about 17.7°, 24.7° and 40.6° (O. Farag, 2018; M. Morsi, 2019). While, both (Elashmawi, 2017;Abdelghany ,2018) found that the XRD pattern of pure PS polymer shows halo peak at ~ 24.50°.



(a)



(b)

Fig.1.a–b: The XRD patterns of the PVC/PS blend, filled samples and pure $CuCl_2$

With the $CuCl_2$ addition within the PVC/PS matrix, the intensity of main halos is significantly decreased and become more broadness. This reveals the increase of amorphous phases within the filled samples and may be due to the variation of chelation mode of the $CuCl_2$ filler (M. Rao,1984;A. Abdelghany,2018). Also, this depicts the variation in filler–polymer interaction within the polymer composite films. These amorphous phases increase the flexibility of polymeric chains and hence improving the transportation of ions, which is more useful in the preparation of solid polymer electrolyte since the increase of amorphous phases is needed for the improvement of electrical conductivity within solid ion–dipolar complexes (M. Antsotegi,2017;L. Levinskaite, 2001). From the XRD patterns of filled samples, new crystalline peaks are existed, which are attributed the $CuCl_2$ phases (L. Levinskaite, 2001) (Fig.1.b), and their intensities increase with the increase of $CuCl_2$ concentration within the PVC/PS matrix. This appearance of new peaks depicts the presence of $CuCl_2$ phases within the composite matrix.

Using Scherrer's formula (C. Luna, 2015), the average size of $CuCl_2$ crystallites is determined at 2θ~16.3° (Table 1).

The calculated values are increased with increasing the concentration of $CuCl_2$, which reveals that there is significant improvement in the sizes of $CuCl_2$ crystallites and the formation of filler aggregations within the composite films as will be indicated in the SEM micrographs. All these findings depict the $CuCl_2$ presence within the PVC/PS structures.

Table 1: The crystallite size, CUT–OFF range, transmittance at λ = 600 nm, E_g, n, σ_{DC} and S for the prepared films.

Samples	Crystallite size (nm)	CUT-OFF range (nm)	Transmittance (%)	E_g (eV)	*n*
Pure blend	-	-	80	4.38	2.49
1 wt.% $CuCl_2$	48	190-272	26	3.95	2.56
2 wt.% $CuCl_2$	57	190-320	17	3.54	2.64
4 wt.% $CuCl_2$	70	190-326	8	3.35	2.68
8 wt.% $CuCl_2$	149	190-850	1	2.61	2.88

3.2UV/Vis. spectra .

From Fig. 2. the transmittance spectra of prepared films increase with increasing the wavelength. In the wavelength range (215–320 nm), this increase is sharp for the spectrum of pure blend due to the high energy of the incident photons that can excite more electrons from the valence band to the conduction band. The $CuCl_2$ addition results in a significant decrease in the transmittance values of filled films, at λ = 600 nm, the transmittance values reduce from 80 % for pure PVC/PS blend to 1 % for the sample (8 wt.% $CuCl_2$) as listed in Table 1. Further, the transmittance values of composite films with high content of $CuCl_2$ reach almost zero and the light was fully absorbed in the wavelength range (190–850 nm). This significant reduction is a legal result since the $CuCl_2$ filler behave as scattering centers for the incident light due to the complexation/interaction formation between the filler and the polymeric chains of $CuCl_2$ (M. Antsotegi, 2017;L. Levinskaite, 2001;K.A. Mosa, 2018)

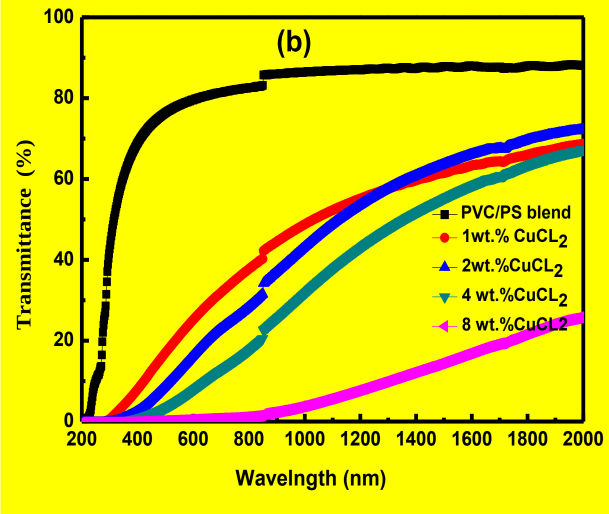


Fig. 2. depicts transmission of pure PVC/PS blend and the blend filled with different concentrations of $CuCl_2$.

Using the Davis and Mott formula (J. Mackie, 2016), the value of optical energy (E_g) for the direct transition is calculated according to the following eq.:

$$(\alpha h\upsilon)^2 = B(h\upsilon - E_g) \quad (1)$$

where, α is the absorption coefficient, $h\nu$ is the photon energy and B is a constant. Fig. 3 shows the $(\alpha h\nu)^2$ dependence on the photon energy for the prepared films and the calculated E_g values are listed in Table 1. The E_g values decrease gradually with increasing the $CuCl_2$ content since the filler induces local crosslinking structures within the amorphous phase of PVC/PS matrix that increase the charge carrier ttransportatio(A. Shoaib, 2015; A.T. Jan, 2015)

J. Mackie, 2016). The E_g results are the best compared with that reported for PVC/PS (50/50 wt.%), where its E_g just decreased from 4.37 to 4.30 eV after embedding silica nanoparticles (10 wt.%) (M. Antsotegi, 2017). Thus, these filled films have a significant importance in the development of many potential optical devices and solid polymer electrolytes.

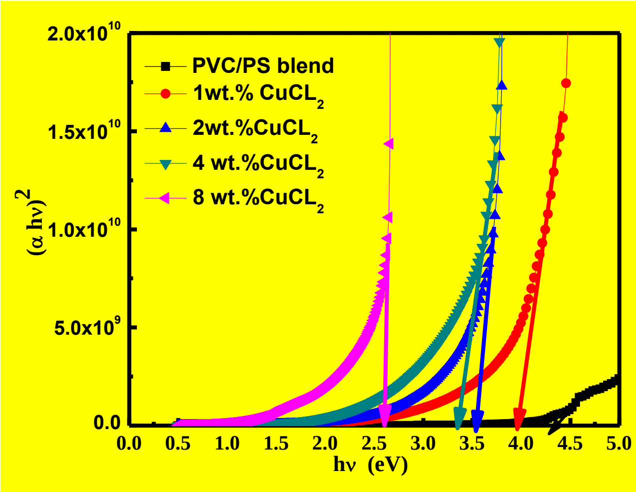


Fig. 3. Plots of $(\alpha h\nu)^2$ versus hν for pure PVC/PS blend and the blend filled with different concentrations of $CuCl_2$

Due to the importance role of refractive index (n) in the design of optical device, the n value of prepared samples is calculated in terms of the E_g value according to the emperical relation that was introduced by Reddy and Ahammed (M. Antsotegi, 2017; K.A. Mosa, 2018):

$$n = \sqrt{\frac{12.417}{\sqrt{E_g - 0.365}}} \quad (2)$$

From Table 1, the high value of n of the composite samples indicates more scattering for the incident light and so on more loss in its transparency. Further, this increase for the n values implies that the Cu^{2+} ions form more localized electronic states within the band gap which behave as trapping/recombination centers (M. Antsotegi, 2017;A.T. Jan, 2015). Thus, these composite samples are a candidate in the preparation of high refractive index lenses and optical filters.

4. Conclusion

In the current work, composite films based on PVC/PS–wt.% $CuCl_2$ were prepared by the solution casting method. The XRD analysis provides an increase for the amorphousity degree with increasing the $CuCl_2$ salt. The absorbance/transmittance spectra of the composite films in the UV/Vis. range can be utilized as candidate materials for outstanding UV-protector and UV/Vis. optical limited

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References and Sources

S. El-Bashir, I. Yahia, M. Binhussain, M. AlSalhi,(2017). Designing of PVA/Rose Bengal long-pass optical window applications, Results in physics, 7, 1238-1244.

A. Al-Muntaser, A. Abdelghany, E. Abdelrazek, A. Elshahawy,(2020), Enhancement of optical and electrical properties of PVC/PMMA blend films doped with Li4Ti5O12 nanoparticles, Journal of Materials Research and Technology, 9 ,789-797.

A. Abdelghany, M. Meikhail, N. Asker, (2019),Synthesis and structural-biological correlation of PVC\PVAc polymer blends, Journal of Materials Research and Technology, 8 ,3908-3916.

A. Abdelghany, G. El-Damrawi, A. ELShahawy, N. Altomy, (2018),Structural Investigation of PVC/PS Polymer Blend Doped with Nanosilica from a Renewable Source, Silicon, 10 ,1013-1019.

A. Al-Muntaser, A. Abdelghany, E. Abdelrazek, A. Elshahawy,(2020), Enhancement of optical and electrical properties of PVC/PMMA blend films doped with $Li_4Ti_5O_{12}$ nanoparticles, Journal of Materials Research and Technology, 9 ,789-797.

A. Abdelghany, G. El-Damrawi, A. ELShahawy, N. Altomy, (2018),Structural Investigation of PVC/PS Polymer Blend Doped with Nanosilica from a Renewable Source, Silicon, 1013-1019.

M. Morsi, A. Rajeh, A. Menazea,(2019), Nanosecond laser-irradiation assisted the improvement of structural, optical and thermal properties of polyvinyl pyrrolidone/carboxymethyl cellulose blend filled with gold nanoparticles, Journal of Materials Science: Materials in Electronics, 2693–2705.

M. Morsi, A. Oraby, A. Elshahawy, R.A. El-Hady, (2019),Preparation, structural analysis, morphological investigation and electrical properties of gold nanoparticles filled polyvinyl alcohol/carboxymethyl cellulose blend, Journal of Materials Research and Technology, 8, 5996-6010.

C.I. Park, W.M. Choi, M.H. Kim, O.O. Park, (2004),Thermal and mechanical properties of syndiotactic polystyrene/organoclay nanocomposites with different microstructures, Journal of Polymer Science Part B: Polymer Physics, 42 , 1685-1693.

P. Slobodian, V. Pavlínek, A. Lengálová, P. Sáha,(2009), Polystyrene/multi-wall carbon nanotube composites prepared by suspension polymerization and their electrorheological behavior, Current Applied Physics, 9 ,184-188.

O. Farag,(2018) Comparison of the effect of plasma treatment and gamma ray irradiation on PS-Cu nanocomposite films surface, Results in Physics, 9 ,91-99.

A. Abdelghany, M. Morsi, A. Abdelrazek, (2018),Structural, optical, morphological and electrical properties of CoCl 2-filled poly (vinyl chloride-co-vinyl acetate-co-2-hydroxypropyl acrylate) Terpolymer, Silicon, 10 ,1697-1704.

F. Gerwien, V. Skrahina, L. Kasper, B. Hube, S. Brunke,(2018), Metals in fungal virulence, FEMS microbiology reviews, 42 fux050.

M. Rao, C. Mishra,(1984), Properties and applications of Penicillium funiculosum cellulase immobilized on a soluble polymer, Biotechnology letters, 319-322.

S. El-Bashir, I. Yahia, M. Binhussain, M. AlSalhi,(2017), Designing of PVA/Rose Bengal long-pass optical window applications, Results in physics, 1238-1244.

E. Ozkazanc, S. Zor, H. Ozkazanc, (2013),Structural and dielectric properties of CuCl2 and ZnCl2 doped polyaniline, Polymer composites, 31 ,1862-1868.

M. Antsotegi-Uskola, A. Markina-Iñarrairaegui, U. Ugalde, (2017),Copper resistance in Aspergillus nidulans relies on the PI-type ATPase CrpA, regulated by the transcription factor AceA, Frontiers in Microbiology, 912.

L. Levinskaite,(2001), Effect of heavy metals on the individual development of two fungi from the genus Penicillium, Biologija, 25-30.

A. Al-Kadeeb,(2007), Effect of lead and copper on the growth of heavy metal resistance fungi isolated from second industrial city in Riyadh, Saudi Arabia, J Appl Sci, 1019-1024.

A. Shoaib, S. Akhtar, N. Akhtar, Copper tolerance,(2015), protein and catalytic activity in phytopathogenic fungus Alternaria alternata, Global NEST Journal, 17,664-672.

C. Luna, A. Marcos, E. Rodrigues Vieira, K. Okada, G.M. Campos-Takaki, A.E. do Nascimento ,(2015), Copper-induced adaptation, oxidative stress and its tolerance in Aspergillus niger UCP1261, Electronic journal of biotechnology, 18,418-427.

A.T. Jan, M. Azam, K. Siddiqui, A. Ali, I. Choi, Q.M. Haq, (2015),Heavy metals and human health: mechanistic insight into toxicity and counter defense system of antioxidants, International journal of molecular sciences, 16, 29592-29Feldman

J. Mackie, E.K. Szabo, D.S. Urgast, E.R. Ballou, D.S. Childers, D.M. MacCallum, J. Feldmann, A.J. Brown, (2016),Host-imposed copper poisoning impacts fungal micronutrient acquisition during systemic Candida albicans infections, PloS one, 40_48.

K.A. Mosa, M. El-Naggar, K. Ramamoorthy, H. Alawadhi, A. Elnaggar, S. Wartanian, E. Ibrahim, H. Hani,(2018), Copper nanoparticles induced genotoxicty, oxidative stress, and changes in Superoxide Dismutase (SOD) gene expression in cucumber (Cucumis sativus) plants, Frontiers in plant science, 872.