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Microcrystalline Properties of PVA/Co3O4 Nanocomposites

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ABSTRACT

The whole pattern fitting was used to compute microcrystalline properties of Cobalt Oxide nanoparticles blended PVA/Co_3O_4/NaCl nanocomposite thin films of different weight percentage concentration.

Keywords : Solution Combustion, Cobalt Oxide nanoparticles, XRD

I. INTRODUCTION

Solution combustion synthesis (SCS) is a an effective, and expeditious method for the synthesis of scalable, highly pure, ordered crystalline metal oxide nanoparticles. Solution combustion synthesis has been widely explored as a flexible, straightforward and expeditious method for the metal oxide nanoparticles synthesis. Combustion synthesis provides equivalent molecular amalgamation, large extent of homogeneity and curtailed reaction time that prompts decreased crystallization temperature hindering aggregation [1,2]The pronounced properties of materials are vigorously affected by the microstructure. Moreover, microstructure is an intricate aspect with very different features which regularly depend on the method of investigation. The different properties of nanostructured materials are attributed to the structural imperfections of these materials. The methodical evolution of nanostructured materials rely upon the elucidation of material disposition in terms of detailed study of lattice imperfections. Enhanced conductivity of intrinsic semiconductors, strength of crystals, crystal growth, elastic properties and luminescence properties are attributed to the defects in crystals. In essence the real crystal is always idealistic and crystal imperfections are pragmatic. Basically there are three kinds of imperfections that can materialize in crystals: point defects, line defects, and plane defects.

Conventional line profile analysis methods [3-5] are based on approximate equations to relate line broadening to lattice distortions and diffraction domain size with simplifying assumptions. In recent times, a reasonable improvement has been the prelude of analytical functions to fit diffraction profiles, leading to the development of the defect characterization methods [6-7]. WPPF technique allows a simultaneous processing of the entire XRD profiles using established models of domain size/shape and defects, rather than hypothetical models .

The formation of high performance Nano composite materials based on a polymeric matrix with some inorganic salt spacers and nano fillers results in a new functional material which exhibits significant improvement in material properties [8-9]

Here we report the computation of microcrystalline properties of PVA/NaCl/Co_3O_4 nanocomposites using Line profile analysis

II. EXPERIMENTAL

A. Synthesis of Cobalt Oxide nanoparticles

Low temperature solution combustion synthesis [10] was employed to obtain Co_3O_4 nanoparticles and using solution casting polymer nanocomposites of varying concentration of nanoparticles were fabricated [10]

B. Charecterization of the synthesized polymer nanocomposite films

XRD profiles of the polymer nanocomposite films were obtained using Rigaku Miniflex II Diffractometer at 1.542 Å of CuKα radiation with a scanning range of 6^0 to 80^0 by an incremental 0.02^0

III. RESULTS AND DISCUSSION

Figure.1 represents the crystallite shape ellipsoid for pristine polymer and polymer matrix blended with metal oxide nanoparticles. Figure. 2 depict the XRD profiles obtained experimentally and also the profiles which were simulated using whole pattern fitting method. The analysis of the profiles reveals that there is a close match between the XRD profiles with a standard deviation close to 5%. The resulting microcrystalline parameters computed through exponential column length distribution are notified in Table 1 for pristine PVA and metal oxide nanoparticles blended nanocomposites. With the increase in nanoparticle concentration average crystallite area increases which is evident from Table 1.

X-ray diffraction studies were carried out from PEAK – FIT software [10], the line profile analysis were performed deploying Gaussian deconvolution method. The reflection profiles considered for evaluation were subjected to instrumental broadening correction [10].

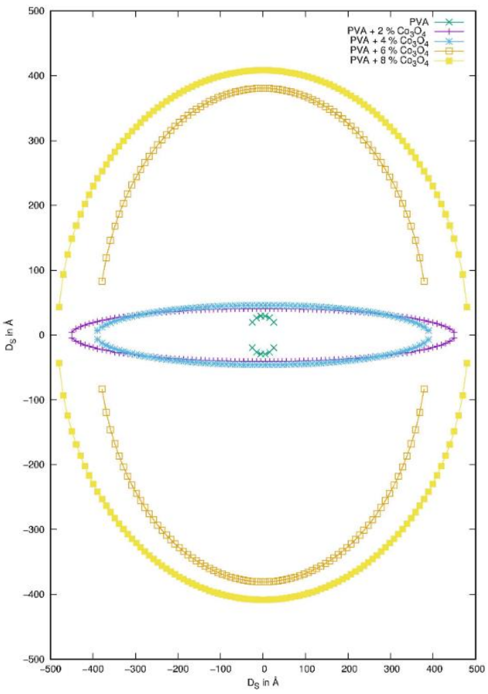

Fig 1. Crystallite shape ellipsoid for pristine polymer and polymer nanocomposites

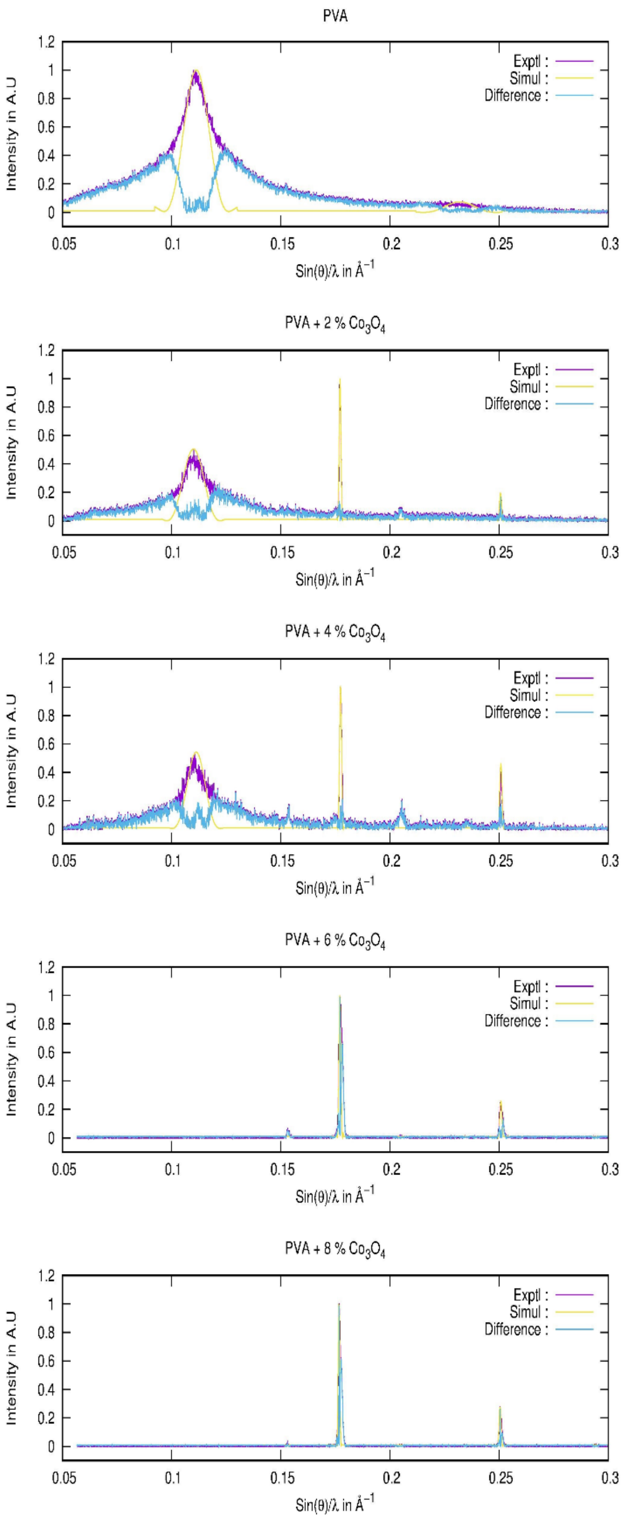

Fig.2. XRD profiles of PVA and PVA/NaCl/ Co_3O_4 nanocomposites

TABLE 1. Computed MICRO crystalline parameters

Samples	Peaks	2θ (deg)	α	g (%) Lattice strain	d_{hkl} (Å)	<N> Crystallite size	D_s (Å)	α^d Stacking faults	β twin faults	delta (E-03)	Crystallite area (Å²)
PVA	1 2	19.70 41.91	2.30 3.41	0.5 0.5	4.50 2.15	7.50 13.8	33.7 29.7	0.33E-6 3.10E-5	7.21E-5 8.54E-5	3.00	1000
PVA + 2 % Co_3O_4	1 2 3	19.53 31.67 45.42	4.89 0.42 0.03	0.5 0 0.5	4.54 2.82 1.99	9.03 160.5 210.0	40.99 452.6 417.9	1.55E-5 2.60E-6 4.57E-9	2.31E-5 2.35E-6 9.38E-9	0.88	18552
PVA + 4 % Co_3O_4	1 2 3	19.57 31.71 45.45	0.78 1.65 0.17	0 0 0	4.49 2.81 1.99	10.26 140.0 175.3	46.06 393.4 348.8	1.94E-5 5.71E-6 1.75E-6	3.79E-5 9.06E-6 3.53E-6	0.89	18120
PVA + 6 % Co_3O_4	1 2	31.66 45.42	1.55 1.04	0 0	2.82 1.99	135.0 195.1	380.7 388.2	6.49E-6 1.63E-6	5.04E-6 1.36E-6	0.87	147787
PVA + 8 % Co_3O_4	1 2	31.58 45.38	0.41 0.61	0 0	2.83 1.99	170.5 205.3	482.5 408.5	1.71E-6 5.62E-9	1.79E-6 2.63E-9	0.57	197101

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