ABSTRACT

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TITLE OF THE THESIS: EFFECT OF GAMMA IRRADIATION ON SOLID POLYMER ELECTROLYTES USING DETERMINISTIC FRACTAL MODEL.

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The present thesis is aimed at a detailed theoretical investigation regarding the effect of gamma irradiation on solid polymer electrolytes with the help of deterministic Vicsek fractal. The research study was carried out at the Condensed Matter Physics Center, Department of Physics, Jadavpur University, under the supervision of Prof. Sujata Tarafder (presently retd.) and Prof. Tapas Ranjan Middya (presently retd.). The thesis comprises five chapters which will be discussed below:

Chapter-1: consists of a general introduction with a brief review regarding polymer, polymer electrolyte and their classification. Different chemical, as well as physical techniques are discussed here including the external irradiation and their effect on polymer electrolytes. The last part of this chapter contains a brief overview of the ion conduction mechanism, a short discussion on different theoretical models regarding the ion conduction mechanism and application of solid polymer electrolytes (SPEs) in different electrochemical devices.

Chapter-2: contains a brief overview of the concept of fractals, their classification and their intrinsic characteristics. Later, a short literature review has been given regarding the experimental studies about the fractal analogies of polymer electrolyte samples. The second part of this chapter deals with the detailed mathematical analysis regarding diffusion. Initially, the theory of diffusion and its classifications has been discussed briefly. Later the nature of diffusion inside the fractal has been analyzed. The computer simulation of the diffusion process inside the fractal object has also been discussed here.

Chapter-3: deals with the detailed theoretical investigation regarding the effect of gamma irradiation on the molecular distribution pattern of the SPE. Initially, a host polymer sample has been constructed mathematically with the help of Vicsek fractal based on certain assumptions. The radiation-induced scission and cross-linking process have been incorporated mathematically. The effect of gamma irradiation on molecular distribution has been extensively evaluated based on a Master equation. The variation of molecular distribution in both scission, as well as, cross-linking dominating region has been extensively studied in this chapter for both mono-disperse as well as poly-disperse samples.

Chapter-4: consists of the computer simulation study regarding the variation of different molecular weight averages of the solid polymer electrolyte sample due to the application of gamma irradiation. Four different types of molar mass averages have been considered for the investigation: number average molecular weight $\langle M_n \rangle$, weight average molecular weight $\langle M_w \rangle$, viscosity average molecular weight $\langle M_v \rangle$ and z-average molecular weight $\langle M_z \rangle$. We have used the molecular distribution of the sample that has been calculated from the master equation, mentioned in chapter-3. The simulated results have been extensively discussed for both mono-disperse and poly-disperse systems in four different cases: 1. pure scission and pure crosslinking cases, 2. Scission dominating region, 3. Cross-linking dominating region, 4. The intermediate case where scission and cross-linking occur with equal probabilities.

Chapter-5: deals with the theoretical study regarding the radiation-induced variation in ionic conductivity inside the host SPE. The single ionic motion inside the host SPE is assumed to be controlled by two factors: 1. Intramolecular trapping of ions and 2. The segmental motion of the polymer chain segments. We have taken two mathematical functions: $\tau_2(s) = (exp(-bs^c))$ empirically and $\tau_1(s) = (3^s)^{d_w}$ to incorporate the effect of segmental motion of polymer branches and ion trapping inside the molecules respectively. The whole simulation has been performed for both mono-disperse and poly-disperse samples. Significant enhancement in ionic conductivity has been observed when the scission process occurs with greater probability. Whereas the enhancement in ionic conductivity is reduced in the cross-linking dominating cases. Moreover, the enhancement is more pronounced in the case of the mono-dispersed sample rather than the poly-disperse one. The outcome of the simulation has been elaborately discussed in this chapter on the basis of radiation-induced scission and cross-linking process for different cases same as in chapter-4. The simulation outcomes of all chapters (from chapter-3 to chapter-5) have been analyzed in detail and compared with different experimentally observed facts in the discussion section of each chapter.

Finally, a summary of the entire thesis work has been given in a separate section on the basis of the results obtained from the computer simulation and the future direction of the research work has been provided in the last section of the thesis.

All the results incorporated in the thesis have been published in different journals of international repute. A list of publications in peer-reviewed journals along with the reprints and a list of papers presented in national, international conferences are included at the end of this chapter.

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