ICCES, 2026, vol.36, no.1

Tech Science Press

DOI: 10.32604/icces.2026.014787

PROCEEDINGS

Molecular Dynamics Study on Gradient Stiffness and Vibration Modes of Poly(3-alkylthiophenes) Thin Films on Substrates

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ABSTRACT

In this study, we investigated the gradient stiffness and vibrational modes of poly(3-alkylthiophenes) (P3AT) thin film on a substrate. We investigated the distribution of stiffness of P3AT thin films on a substrate as a function of height, which was divided into 20 layers, and the stiffness of each layer was calculated. Based on the distribution of stiffness, it can be divided into three regions: the adsorbed region, the bulk region, and the free surface region. The results indicate that the degree of polymerization does not have a significant influence on the stiffness distribution of the thin films. When the number of side chain beads is equal to 2 or 3, there is no change in the stiffness distribution. However, when the number of beads is 4, the thickness of the adsorbed region and the free surface region increases. Temperature significantly impacts the stiffness distribution. At low temperatures, stiffness is higher, whereas above the glass transition temperature, the stiffness values are an order of magnitude lower compared to those at lower temperatures. The phonon modes of P3AT on the substrate exhibit an inverse correlation between polymerization degree and phonon frequency. Different side chain lengths have a minimal influence on the phonon modes of P3AT. On the other hand, temperature significantly affects phonon frequencies, displaying a negative correlation with temperature. Next, we investigated the similarity between the main chain and side chains. This coefficient is utilized to quantify the degree of similarity in phonon modes. The results indicate a high similarity index between the main chain and side chains under various conditions. Finally, we performed an energy decomposition analysis of the interfacial interaction. The decomposition results indicate that van der Waals forces play a dominant role in interfacial forces, and there is a distinct π-π stacking interaction between P3AT and the substrate. Our results have reference significance for interface regulation. Our findings hold implications for interface manipulation and provide insights into phonon vibrational modes and interfacial interactions at the microscale level.

KEYWORDS

P3AT; gradient stiffness; phonon vibrational modes; energy decomposition

Funding Statement: The Science and Technology Research Project of Jiangxi Provincial Department of Education (Grant No. GJJ2402615) sponsored this study.

Conflicts of Interest: The authors declare no conflicts of interest to report regarding the present study.

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