Revealing the Metal-Ligand Coordination effects on the

Structure modifications for Balanced Tensile Modulus and

Self-Healing of Polyurethane Films

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Abstract

Polyurethane (PU) films are potential candidate substrate for current and future stretchable electron devices that attract much attention. Both tensile modulus and selfhealing of PU films are anticipated yet seemingly mutual excluded properties. Here, metal-ligand coordination is proposed to modify the crystalline and nanostructural features of PU films for balanced tensile modulus and self-healing. PU films of bpyPTD are prepared from reaction of bpy with PTD of different molar masses in mixed solvent of DMF/THF for linear products of $[bpy(PTN)_n bpy]_m$ with n =19, 34, and 64, and $m \sim 6$. Metal precursors solutions of Zn, Ni, or Cu, were selectively mixed into the [bpy(PTN)_nbpy]_m solution for cast of the final product films of M-bpyPTD, with M = Ni, Zn, or Cu. X-ray absorption reveals formation of metal-ligand coordination in the PU film. Small-angle and wide-angle X-ray scattering results further indicate that the metal-ligand coordination could form crosslinking centers for locally enriched and partially ordered hard segment domains of a mean spacing of ~ 4nm, thereby resulting in increased Young's modulus. Density (or mean spacing) of the metal-ligand coordination cites could be enriched with reduced n value of [bpy(PTN)_nbpy]_m for improved tensile modulus; improvement of the self-healing capability is reached with enhanced metal-ligand coordination strength of bpy with Zn, compared to that with Cu and Ni.

References

[1] W. Z. Mostafa, R.A Hengazy, Journal of Advanced Research 2015, 6, 793-804

[2] G. A. Tabot, S.S. Kim, J. E. Winberry, S.J. Bensmaia, *Neurobiol Dis* **2015**,83, 191-198.

[3] D. Wang, J. H. Xu, Adv. Funct. Mater. 2020, 30, 1907109