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The Influence of Increased Temperature on the Miscibility and Mechanical Properties of poly(2,5-benzimidazole) and polytetrafluoroethylene

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Abstract content
   (Max 300 words)
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In this work molecular dynamics was used to study the effects of temperature on the miscibility and mechanical properties of two polymers found within the membrane electrode assembly (MEA) of a high temperature polymer electrolyte fuel cell. The polymers, poly(2.5-benzimidazole), (ABPBI), and polytetrafluoroethylene, (PTFE), are respectively, used as constituents of the membrane and ionomeric layers of the membrane electrode assembly. The temperature range considered is 298K to 383K. Of the two polymers, PTFE has the lower solubility parameter, which from the results, decreases by 6% as temperature increases. ABPBI solubility parameter decreases by 1% as temperature increases. The greater difference between these two values indicates that at elevated temperatures these two polymers are even more unlikely to mix. For the mechanical properties calculation, the molecular dynamics approach implements a constant strain algorithm. Polymers are subjected to a stress up to and including 2.0 GPa. The significance of this work is that it gives insight on the mechanical robustness of materials found within the MEA and confirms that unfavourable changes, such as miscibility, is unlikely to occur as temperature increases. The effect of elevated temperature on either property for ABPBI, using molecular dynamics, has not been reported before.

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