ADDITIONS AND CORRECTIONS

2007, Volume 111B

Seung Soon Jang, William A. Goddard, III*, M. Yashar S. Kalani, David Myung, and Curtis W. Frank: Mechanical and Transport Properties of the Poly(ethylene oxide)–Poly(acrylic acid) Double Network Hydrogel from Molecular Dynamic Simulations

Our recent paper[1] reported atomistic MD simulations to investigate the mechanical and transport properties of the PEO–PAA double network (DN) hydrogel. The effective mesh size of this DN hydrogel is 28 Å compared to mesh sizes of 30 Å for the PEO SN and 53 Å for the PAA SN.

We reported that with applied uniaxial extensions the stress–strain curves for the hydrogels show that the DN hydrogel has a sudden increase of stress above ~100% strain, much higher than the sum of the stresses of the two SN hydrogels at the same strain. This arises because PEO has smaller M_c (molecular weight between crosslinking points) than PAA so that the PEO in the DN reaches fully stretched out at 100% strain that corresponds to 260% strain in PEO SN (further stretching beyond this point causes significant strains in the bond lengths and bending angles bending, with concomitant increases in stress).

We reported that the solvation of polymer and ions in the DN hydrogel is enhanced by 1.5% and 4.9% with respect to the PEO and PAA single network (SN) hydrogels, respectively. This indicates that combining dissimilar materials in the double network can lead to nonadditive effects in binding to solutes.

We also calculated the diffusion coefficients of D-glucose and ascorbic acid solutes in these hydrogels, finding that the diffusion coefficients of both solutes in the DN hydrogel are 60% of that in PEO SN and 40% of that in PAA SN, probably because of the smaller effective mesh size of the DN.

As stated in this paper, we studied this particular DN because of several papers from the Curtis W. Frank group[2–4] of Stanford pointing out that PEO–PAA DN are potentially valuable for ophthalmic applications because of the transparency and biocompatibility of the these DNs. Unfortunately, the paper[1] did not acknowledge additional prior experimental data we had received on the mechanical properties and diffusion properties of PEO–PAA DNs measured by the Stanford group and co-workers, which were provided to us as part of an anticipated collaboration between our groups. This data was described in full in an unpublished manuscript[5] provided to the Caltech group by the Stanford group in July 2005 prior to our study of this system. A portion of this data was mentioned in a 2005 meeting abstract[6] that reported experimental results on a PEO–PAA DN, finding that the DN was 10 times stronger than PEG or PAA SN alone (based on the stress at the break point). Unfortunately, ref 1 did not acknowledge the data from the unpublished manuscript[5] or from the 2005 publication.[6]

The Caltech group did not calculate the break point specifically, but they found similar results to those obtained by the Stanford group. For example, the calculations found that the DN requires greatly increased stress above 100% strain, which at 250% strain is 10 times larger than for either of the two SNs. Also, the calculated Young' modulus for the DN (0.43 GPa) is the sum of that for the two SNs, 0.07 GPa for PEO and 0.36 GPa for PAA

In addition, this uncited reference[6] and manuscript[5] from the Stanford group reported diffusion data for glucose: the diffusion coefficient of glucose in the double network 0.9×10^{-6} cm^2/s, which is 50% of the value they measured for the PEO SN. This compares to the calculated result in ref 1 that predicted a diffusion of glucose in the DN of 1.1×10^{-6} cm^2/s, which is 60% of the value (1.8×10^{-6}) calculated for PEO SN. Thus, the calculations predict a diffusion constant ~20% larger than experiment (presumably because of the more uniform and homogeneous nature of the computational system) and the calculations predict nearly the same differential effect between the DN and SN (60% vs 50%). This suggests that such calculations could be useful in predicting the effects of various network structures on the diffusion of various molecules within the networks.

We want to acknowledge here that the suggestion that we study the diffusion of glucose and vitamin C in the DN was made by David Myung in a private communication to one of us (Y.K.) but not acknowledged in the paper.[1]

Jang, Kalani, and Goddard hereby apologize to David Myung, Jaan Noolandi, and Curtis W. Frank for our oversight in not acknowledging the important suggestions and experimental data they provided.

References and Notes

(1) Jang, S. S.; Goddard, W. A., III; Kalani, Y. *J. Phys. Chem. B* **2007**, *111*, 1729–1737.

(2) Farooqui, N.; Myung, D.; Masek, M.; Dalal, R.; Koh, W.; Gupta, S.; Noolandi, J.; Frank, C.; Ta, C. N. *Invest. Ophthalmol. Vis. Sci.* **2005**, *46*, 873.

(3) Koh, W.-G.; Myung, D.; Ko, J.; Noolandi, J.; Frank, C. W.; Ta, C. N. *Invest. Ophthalmol. Vis. Sci.* **2005**, *46*, 4994.

(4) Bakri, A.; Farooqui, N.; Myung, D.; Koh, W. G.; Noolandi, J.; Carrasco, M.; Frank, C.; Ta, C. N. *Invest. Ophthalmol. Vis. Sci.* **2006**, *47*, 3592.

(5) Myung, D.; Koh, W.-G.; Ko, J.; Noolandi, J.; Ta, C. N.; Frank, C. W. Synthesis and Characterization of Double Network Hydrogels Designed for Corneal Implant Applications. Communicated to Goddard group in July 2005 but never published.

(6) Myung, D.; Koh, W.; Ko, J.; Noolandi, J.; Carrasco, M.; Smith, A.; Frank, C. W.; Ta, C. *Invest. Ophthalmol. Vis. Sci.* **2005**, *46*, 5003.

10.1021/jp079537q
Published on Web 11/30/2007