Secondary Structure of Hair Protein Studied by Non-Negative Matrix Factorization and Raman Imaging

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During perm treatments, the chemical reagents and the heating can cause damages to the hair. Raman spectroscopy and Raman imaging technique have been frequently applied to study changes in properties of hair. ¹⁾ The Amide vibrational modes distinguish secondary structures of protein by the different peak positions. But the problem is that the components corresponding to different secondary structures are largely overlapped with one another. To solve this problem, non-negative matrix factorization (NMF) is applied.²⁾ NMF is also called multivariate curve resolution (MCR) or self-modeling curve resolution (SMCR).

In this research, we applied Raman imaging and NMF into the cross sections of strands of gray human hair, about (i) the untreated hair (UN), (ii) the curly perm hair (PE) and (iii) the straight perm hair (ST), for revealing the microscopic mechanism of damages of hair through the perm treatments. NMF was applied into the amide I region of protein, giving reasonable decompositions into the components corresponding to different secondary structures of protein and the scaling factors (that is, images). NMF suggested that the amount of α -helix species increased after the ST treatment.



Figure. (a) Visible images of the cross sections of the gray human hair fixed on the quartz substrates. (b)
Decomposed spectra *w*₁, *w*₂, and *w*₃ (at the left side) and NMF images of ST, UN1, UN2, and PE constructed by the corresponding scaling factors, *h*₁, *h*₂, and *h*₃ (at the right side). **Reference**: 1) G. J. Zhang, L. Senak, and D. J. Moore, J. *Biomed. Opt.* 16(5), 056009 (2011)
2) D. D. Lee, and H. S. Seung, *Nature* 401, 788 (1999).