書類　その１概略情報　　尾崎幸洋

1.　　**専門分野**：「分子分光学」、「物理化学」、「分析化学」

2.　　**豊田理研での研究テーマ**：凝集体の遠紫外分光法の基礎と応用

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２．これまでの研究成果

私はこの約 45 年の間、**自ら新しい分子分光学の分野を開拓し、自ら独創的な分光システムを創案し、また自ら新規な応用分野を切り開き、**分子分光学のフロントランナーの一人として活躍してきた。その研究内容は、１）凝集相の新しい電子分光法・振動分光法の開拓（減衰全反射―遠紫外分光法など)、２）電子分光法・振動分光法の原理の探求（表面増強ラマン散乱の機構解明など)、３）スペクトル解析法の提案、４）電子分光法・振動分光法の物理化学、分析化学、ナノ物質化学、生物医学などへの応用など、極めて広範囲にわたる(1)。

私は遠紫外から遠赤外/テラヘルツに至るほとんど全ての領域の凝集体の分子分光学の研究を行っている世界的に見ても珍しい存在である。私の分子分光学研究における戦略の一つは、**未開拓、未踏峰の領域の研究に力を入れるという点である**(1)。例えば 140-200 nm の遠紫外領域における凝集相の分光はほとんど未開拓であったが、私はこの領域に減衰全反射（ATR）法を導入することにより、凝集相の遠紫外分光法を確立した。私はまた包括的に分子分光学（振動分光学と電子分光学）の研究を行い、スケールの大きな研究を発展させた。特に力を入れた分光法は、ラマン、遠紫外、近赤外、遠赤外/テラヘルツ分光法などであるが、ここでは、1）遠紫外～遠赤外/テラヘルツの全スペクトル領域とラマン分光法に共通する研究、2）凝集相における遠紫外分光法の創成―新しい σ 電子化学の構築をめざす、3）分子分光法としての近赤外分光法の確立―基礎、装置開発、量子化学の応用に関する研究、4）表面増強ラマン散乱（Surface-enhanced Raman Scattering; SERS)、チップ増強ラマン散乱（Tip-enhanced Raman Scattering; TERS)の機構解明とそれらの応用に関する研究、5）遠赤外/テラヘルツ、低波数ラマン、量子化学計算法を用いた高分子の高次構造、分子間相互作用の研究、6）ラマン分光法、近赤外分光法の生物医学への応用、の 6 項目に焦点を絞り研究成果を説明する(1)。

（1）遠紫外～遠赤外/テラヘルツの全領域とラマン分光法に共通する研究

全領域とラマン分光に共通する研究として、1）量子化学の分子分光学への応用に関する研究、2）全領域とラマン分光法に適用可能なスペクトル解析法の開発、3）異なる分光学領域間のスペクトルの比較の研究を行った。量子化学の研究では、**“「分子分光学」と「量子化学」に橋を架ける”**というビジョンを立てた（1- 7）。このテーマの目的は、量子化学の分子分光学研究における有用性を深めかつその応用範囲を広めるとともに、非調和性の考慮、巨大分子の取り扱い、分子間、分子内相互作用の取り扱いなどの幅広い分野に共通する課題の解決に努めることである。具体的な研究成果としては、(i)これまで赤外、ラマン中心であった非調和性を含む量子化学計算を近赤外まで拡げ、倍音、結合音によるバンドからなる近赤外スペクトルのシミュレーションに成功し、バンドの帰属や強度の研究を行った (4,5)。(ii) ポリマーの遠赤外/テラヘルツ、ラマン、赤外スペクトルにおける分子断片化法の適用（6,7)。この方法を用いることにより、巨大分子のスペクトル計算、分子間相互作用を含む分子の計算を幅広い領域で可能とした。(iii) 紫外、遠紫外領域のスペクトル解析に Symmetry

Adapted Cluster/Configuration Interaction (SAC-CI)法を適用し、Rydberg 状態を含む電子状態、電子遷移研究を発展させた（3)。

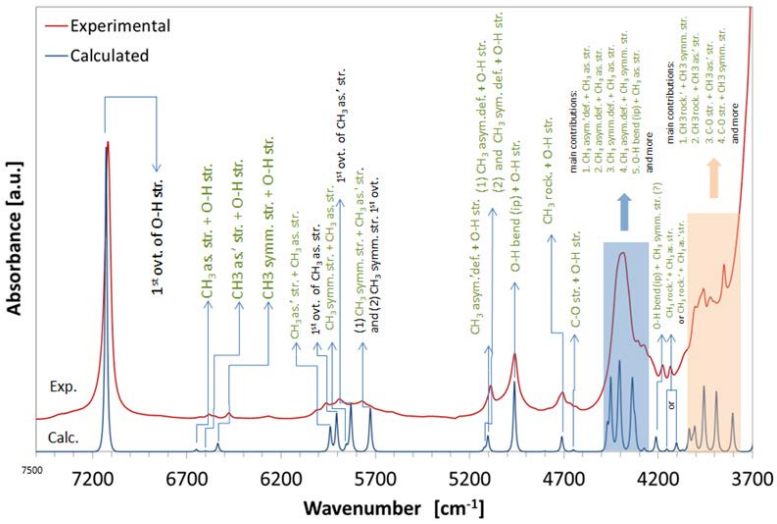

図１　メタノールの近赤外スペクトルー実験スペクトル(0.005M の四塩化炭素溶液)と計算スペクトルの比較(4)。

図１は量子化学計算の近赤外分光法への応用例で、メタノールの実験スペクトルと計算スペクトルの結果を比較したものである。非調和性を考慮した量子化学計算により倍音、結合音からなるメタノールの近赤外スペクトルが見事に再現され、バンドの帰属も明らかになった(4)。

2) の全領域とラマン分光法に適用可能なスペクトル解析法の開発の研究では、ケモメトリックス法と二次元相関分光法の研究で大きな成果を得た。前者ではスペクトルデータの２方向、すなわち波長方向、サンプル方向において有効な情報の選択・抽出を行い高精度の検量線を実現することを目指した。その中で最も注目を集めているのは、我々（Jiang ら）が提案した Moving Window Partial Least Squares Regression (MWPLSR)法である(8)。この方法は、赤外、ラマン、近赤外スペクトル等においてケモメトリックスを適用するときの波長選択法として非常によく用いられている。

(2)　凝集相における遠紫外分光法の創成―新しい σ 電子化学を目指して

遠紫外領域には数々の電子許容遷移が観測される。しかし遠紫外域ではモル吸光係数が非常に大きいため、これまで大方、気相でスペクトル測定が行われてきた。凝集相にとっては分子分光学の未踏領域となっていた(9)。

我々は減衰全反射（Attenuated Total Reflection; ATR)法を基本原理とする遠紫外分光器を開発し、通常の紫外スペクトルでは吸収バンドを示さない水、アルカン、アルコールなど

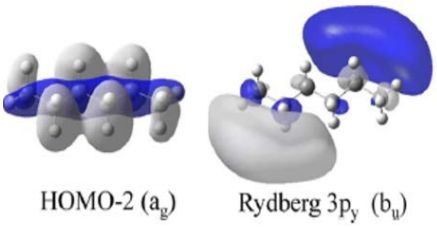

図 2　ATR-遠紫外スペクトルを再現する量子化学計算により得られた *n*-ヘキサンの電子遷移にかかわる占有軌道および非占有軌道 (2)。

ありとあらゆる分子の遠紫外スペクトルを凝集状態で測定できるようにした(3,9,10)。**このようにして分子分光学の新しい分野の開拓に成功した**（9）。さらに量子化学計算を用いて、種々の有機化合物の電子状態の研究を実験と理論の両面から進めた。

我々は遠紫外分光法の研究で、６つの顕著な成果を挙げた(9)。**1）凝縮相における Rydberg 軌道が関与する電子状態の実験的・理論的研究(3)、 2）分子間相互作用が分子の単結合骨格の価電子（σ電子）に与える影響の研究(10)、 3）遠紫外分光法を用いた水、水溶液、表面吸着水の研究(11,12)、4）遠紫外分光法を用いた金属ナノ粒子修飾酸化チタンの電子状態と光触媒活性の研究(13)、5）遠紫外分光法の材料化学（高分子、カーボンナノ材料、イオン液体）への応用(3,14)、6）遠紫外/深紫外―表面プラズモン法の開発(15)。**

我々（森澤ら）は開発した ATR 遠紫外分光器を用いてアルコール、アルカン、ケトン等の有機液体の遠紫外スペクトルを系統的に研究した(3,9,10)。液相と気相のスペクトルの比較や量子化学計算で求めた電子励起エネルギーなどから、遠紫外スペクトルの帰属法を確立した。アルカンの電子励起状態研究では 153 nm 付近に観測される吸収を HOMO-2 または HOMO-1 から 3p Rydberg（Ryd.と略す）への遷移であると帰属し、この遷移がアルカンのσ電子の状態を反映していることを示した（図 2)。この例のように遠紫外域における凝集相の Ryd.遷移の研究を精力的に行った（3,9,10)。

分子間相互作用が分子の単結合骨格の価電子（σ電子）に与える影響 に関する研究では、常温で液体のテトラデカン（$C_{14}H_{30}$）の温度依存遠紫外スペクトルを固体の-80℃まで測定した(10)。この測定で温度変化に伴い、153 nm の遷移がなくなり、202、208 nm に新たな吸収が現れるという変化を観測した。この変化の原因を探るために、アルカン 2 分子を並べたものの電子遷移計算を行った。そして分子間距離を近づけたときに、実験で見られたような大きな長波長シフトが観測されることを示した。このことから、シフトの原因は、外側に張り出したσ軌道である HOMO-1 および HOMO-2 軌道が固体中の分子間相互作用により不安定化軌道と安定化軌道を作り、この二つの軌道間の遷移が低エネルギー側に観測されることによると結論した。**このように遠紫外分光法でσ軌道の変化による遷移の変化を観測した例はこれまでにない。これはまさに新しいσ電子化学を開拓する第一歩となる成果である。**

アルカンに限らず、アルコール、ケトン、アミドなどほとんどの有機分子、高分子が遠紫外領域に重要な遷移を示す。森澤らはこれらの物質について遠紫外分光法を用いて電子状態の研究を行った(3,9,10)。ナイロンの研究ではナイロンの水素結合が遠紫外スペクトルに与える影響について調べた(3b)。 さらに遠紫外分光法を用いた水、水溶液、表面吸着水の

研究（12)や金属ナノ粒子修飾に伴う酸化チタンの電子状態変化と、それに対応した光触媒活性の増強についての研究も注目を集めている(13)。さらにイオン液体やカーボンナノ材料、カーボンナノコンポジットなどの材料研究に展開している(14)。

以上のようにアルカンの固体でのスペクトル変化から HOMO の反発からエネルギーが不安定化すること、金属担持 TiO_2でのスペクトル変化から金属ー触媒間の電子の流れを実測するなど、凝縮相で分子内の電子状態が変化し、電子の移動する様子を実験結果と量子化学計算から可視化することができた。**これらの研究は化学における新たな研究領域を拓いたと言える。**

(3) 近赤外分光法の確立―その基礎、装置開発、量子化学の応用に関する研究

私は倍音、結合音、非調和性、振動ポテンシャルなど近赤外分光法の基礎研究を進めるとともに(16)、水素結合研究や溶液化学への応用(16-18)、表面プラズモン共鳴―近赤外分光法の提案(19)、ポータブル近赤外イメージングなどの装置開発(20)、スペクトル解析法の研究(8,21)、生命科学、高分子分析、医薬品分析、オンライン分析への応用などを行った。これらにより、90 年代には十分に独立した分光法と言える状態になかった近赤外分光法を、独立した分子分光法として確立させた。

(3)-1　倍音、結合音、非調和性、振動ポテンシャルに関する研究およびそれらの応用　近赤外スペクトルには分子振動の倍音、結合音によるバンドが観測される。しかし倍音、結合音の帰属や強度の解析は非常に複雑であるため、これまで近赤外スペクトルに含まれる情報を的確に抽出することが難しかった。そこで我々は(Bec ら)非調和性を考慮した量子化学計算によって近赤外スペクトルの再現、バンドの帰属を行った(4-6)。近赤外スペクトルの再現は図 1 に示したメタノールのような比較的簡単な化合物だけでなく、核酸塩基、長鎖脂肪酸、天然物などかなり複雑なものも含まれる。量子化学の適用により、これまでバンドの帰属が非常に厄介であった近赤外スペクトルの解析に新しい道を切り開いた。

さらに量子化学計算を用いて水素結合の形成と溶媒効果の近赤外スペクトルに対する影響を解析した(22,23)。分子振動の非調和性や振動ポテンシャルには、分子への外的相互作用の影響が表れやすい。我々（二見ら）は基本音と倍音の吸収強度の変化を比較することにより、水素結合と溶媒効果との識別を明確にすることができることを示した（図 3)。

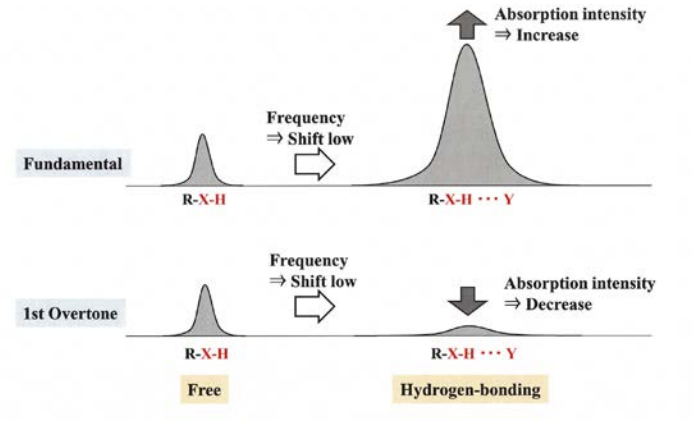

図 3 基本音と倍音の水素結合形成に対する吸収強度の変化

(3)-2 溶液化学への応用 我々（池羽田ら）は近赤外分光法の強みを生かし、液体分子の相溶性の研究を発展させた(18)。濃度差分スペクトルに基づく水素結合状態の解析や、疎水性部位の振動に注目する独自の視点によって、エタノールと水のように**相溶の溶液に関しても、微視的には相分離に近い状態にあることを示した。**

(3)-3 近赤外分光法の応用

応用面でも純水(24)や生体中の水の研究、表面プラズモン共鳴―近赤外分光法の創案(19)、ポータブル近赤外イメージング装置の開発とその応用(20)、近赤外イメージングによるメダカの卵の血流の非染色イメージング(25)などにおいて注目すべき成果を挙げている。これらにより、それ迄は十分に独立した分光法と言える状態になかった近赤外分光法を、独立した分子分光法として確立させたと言っても過言でない。

(4) 表面増強ラマン散乱(Surface-enhanced Raman Scattering; SERS)、チップ増強ラマン散乱(Tip-enhanced Raman Scattering; TERS)の機構解明とそれに基づく物理化学、分析化学、ナノ物質化学、生体関連化学等への応用に関する研究

(4)-1 表面増強ラマン散乱の機構解明 表面増強ラマン散乱（Surface-enhanced Raman Scattering; SERS)では、わずか分子 1 個からのラマン散乱の測定ができるので、SERS は基礎研究からも応用からも“夢の分光法”と言える。しかしこれまで SERS によるラマン散乱の増強のメカニズムが明らかでなかった。我々（伊藤ら）は、**分子種に依存しない普遍的な理論として電磁増強理論に着目し、その実証研究を行った**(26-28)。ラマン遷移は光励起遷移とラマン放射遷移の二つから構成される。それぞれの遷移では空間と分子は光子の受け渡しを行う。電磁増強とは空間の光子の状態密度を大きくしてこの受け渡しの効率を上げることである。金や銀ナノ粒子のプラズモン(伝導電子の集団振動)は高い伝導電子密度と長い集団振動時間のために、光子の非常に大きな状態密度向上効果をもたらし、その結果、ラマン遷移確率が増大する。これが電磁増強理論である。ところでプラズモン共鳴の波長、スペ

クトル形状、偏光特性などはナノ粒子のサイズや形状に依存して大きく変化する。したがって、従来の集団ナノ粒子系を用いた SERS の実験に基づく増強原理検証の研究では、増強の原因（プラズモン共鳴）が平均化され、増強の結果(SERS)との関係を直接捉えることができない。

伊藤らは、**プラズモン共鳴を平均化することなく、単一分子を用いて電磁増強理論の検証が可能だとの着想を得た。**そのため単一のナノ粒子 2 量体の電子顕微鏡測定、プラズモン共鳴測定、SERS 測定が可能な実験装置系を構築し、多くの 2 量体の SEM イメージ、プラズモン共鳴スペクトル、SERS スペクトルを測定した。つぎに実験結果を計算条件として SERS の再現を電磁解析計算（有限差分時間領域法(FDTD)法）で行った（図 4)。具体的には実験的に観測されたプラズモン共鳴を計算で再現し、再現したプラズモン共鳴から状態密度向上効果を導き、SERS スペクトルを算出した。この算出された SERS スペクトルと実験で得られた SERS スペクトルとを比較することで電磁増強効果の定量的検証を行った(26-28)。

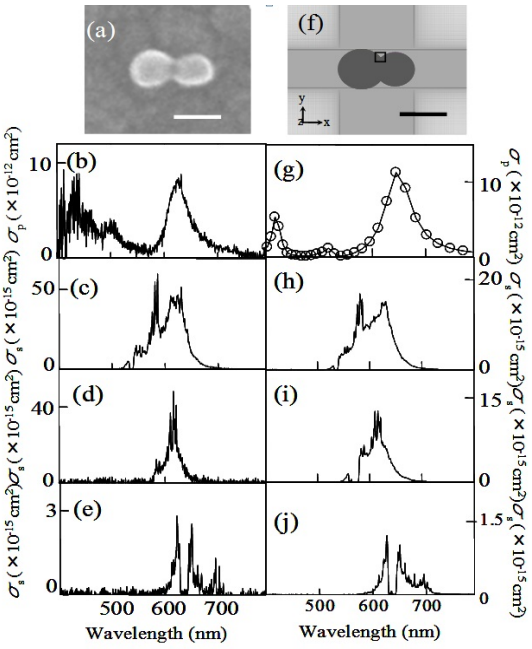

図 4 を用いて検証結果を説明する。実験と計算に用いた銀ナノ粒子 2 量体をそれぞれ図 4(a)と 4(f)に示す。SERS を引き起こしているプラズモン共鳴は、実験と計算（図 4(b)と 4(g)）とでよく一致した。図 4(c)-4(e)は、1 つの 2 量体について 3 つの励起

図 4(a) 銀ナノ粒子 2 量体の SEM イメージ、(b)実験的に測定されたプラズモン共鳴スペクトル、(c)–(e), 一個の 2 量体について三つの励起波長（532, 561, 633 nm）で測定したローダミンの SERS スペクトル、(f) 計算に用いた銀ナノ粒子 2 量体、(g) 計算されたプラズモン共鳴スペクトル、(h)–(j) 計算で再現された SERS スペクトル(28)

波長（532, 561, 633nm）で測定したローダミンの SERS スペクトルである。図 4(h)-4(j)は計算で再現された SERS スペクトルである。実験の SERS スペクトルの励起波長依存性が計算によって見事に再現されているのが分かる。たとえば、532nm 励起においては SERS の基本音（～560 nm)と禁制である倍音（～630 nm)が似た強度となっている興味深い現象を再現している（図 4(c)と 4(h))。さらに 633 nm 励起においては、アンチストークス側の SERS バンド強度がストークス側の SERS バンド強度を超えるという異常現象を再現している（図 4(e)と 4(j))。以上のように我々は**電磁増強効果が SERS 発現において支配的であることを実証した(31,32)**。以上の研究結果は、プラズモンを利用することで金属ナノ構造近傍の分子を孤立状態の時と比べて最大で 10 桁程度効率的に光と相互作用させることができることを意味する。したがって**本研究は、適切なプラズモン共鳴条件を設定すれば、光の回折限界を超えた普遍的な超高感度測定ツールや超高効率光反応場を創生できることを示した。**この研究は 1970 年代から 40 年あまり続いた SERS の増強メカニズムの研究を飛躍的に発展させたものとして国際的に非常に高く評価されている。またこの分野の基礎研究のみならず、応用に大きなインパクトを与えた(26-28)。

我々は電磁場増強理論のみならず化学増強機構や半導体励起ラマン散乱の機構と応用の研究でも注目すべき業績を挙げている(29,30)。半導体励起ラマン散乱は半導体を基板とした SERS で、感度は通常の SERS に比べれば低いが、再現性などについては優れている。SERS の機構を電磁場増強理論と化学増強理論の両面から研究しているグループは世界的に見ても珍しい。

(4)-2 表面増強ラマン散乱の応用　我々は すでに 1990 年代に ”indirect SERS” 法を用いた酵素イムノアッセイの研究で注目を集めた(31)。1998 年に発表した PCR によって増幅された二本鎖 DNA の定量分析の研究も高い評価を受けた。その後、SERS を用いたラベルフリー間接イムノアッセイやラベルフリータンパク質検出で大きな成果を挙げた(32)。最近は、SERS を用いたラベルフリーの光学異性体判別法を提案し注目を集めている(33)。この SERS による光学異性体判別を可能とするのは、電荷移動に基づく化学増強機構による。さらに我々は世界で初めて 3 次元 SERS イメージングに成功した(34)。

(4)-3 チップ増強ラマン散乱の研究 我々はまた TERS の研究でも大きな貢献をしている。例えば、TERS を用いた固液界面におけるナノスケールでの pH プロファイル測定 (35)は非常に大きな反響を受けている。TERS を用いたグラフェンやポリマーナノコンポジットの研究も有名である(36)。さらに最近、TERS を用いた光学異性体判別にも成功した。また超高真空、極低温下での TERS 測定装置を開発し、それを用いてグラフェンの構造、物性研究を行いつつある。このように我々の SERS,TERS 研究は、物理化学、分析化学、応用物理学、ナノサイエンス/テクノロジー、生体関連化学などの幅広い分野に大きな波及効果を与えた。

(5) 遠赤外/テラヘルツ、低波数ラマン、量子化学計算法を用いた高分子の高次構造、分子間相互作用の研究

遠赤外分光法を用いた高分子の研究は長い歴史を有するが、低波数域のバンドの帰属はこれまで十分ではなかった。我々は、バンドの帰属を明らかにし、バンドの帰属と高次構造、物性との関係を明らかにすることを目指した(6,7)。我々が用いた戦略は、バンドの帰属のために、吸収分光法（遠赤外/テラヘルツ）とラマン散乱、さらに両者の量子化学計算を合わせ用いるということである。高分子の量子化学計算を行うときに問題となるのは、分子量の大きい試料をいかに扱うか、分子間、分子内相互作用をいかに計算に取り込むかということである。そのために我々（山本ら）は Bouř らによって提案された分子断片化法を用いた。

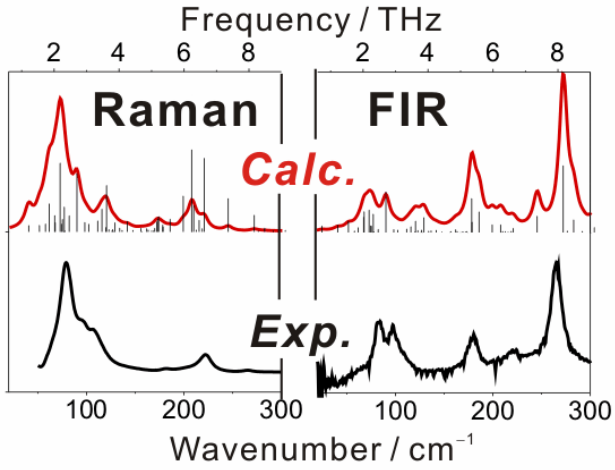

図 5 Poly-(*R*)-3-hydroxybutyrate)(PHB)の低波数ラマンスペクトルと遠赤外スペクトルー実験スペクトルと計算スペクトルの比較

図 5 は生分解性ポリマーの一つである Poly-(*R*)-3-hydroxybutyrate)(PHB)の低波数ラマンスペクトルと遠赤外スペクトルとそれぞれの計算スペクトルを比較したものである(6)。遠紫外、ラマンいずれの場合も実験スペクトルをよく再現している。この研究は-C=O…CH_3の弱い水素結合を計算にうまく取り込んだ点が評価される。

山本らは Poly(glycolic acid)(PGA)についても同様な研究を行い、実験スペクトルを分子断片化法により良く再現できることを示した。PGA と PHB のスペクトルの比較から、両者はいずれも C=O の面外変角振動を～70-～125 cm^{-1} に与えることが明らかになった。さらにこのバンドが、結晶格子の熱膨張とそれに伴う分子間相互作用の変化に敏感であることも分かった。このようにポリマーの熱膨張を直接的に見ることができるバンドは赤外、ラマンでは見出されておらず、低波数分光法で初めて見つけられたものである。

ナイロンの遠赤外スペクトルは 1960 年代から研究されている。モデル化合物の基準振動計算などを用いてバンドの帰属が試みられたが、100 cm^{-1}付近のブロードなバンドについては、アミド結合によるものか CH_2基によるものか議論があった。さらにアミド結合の面内振動なのか面外振動なのか分かっていなかった。我々の研究から、100 cm^{-1}付近のバンドの温度変化は、シフトによるものではなく、二本のバンドの強度比が温度とともに変化するこ

とによるものであることが分かった(7)。量子化学計算の結果からこれら二本のバンドはアミドの面外振動と CH_2 の振動の両方が関与していると帰属された。

(6) ラマン分光法、近赤外分光法の医学、生物学への応用

私は水野らとともに 40 年近く前に世界で初めて病気の発症メカニズム(ラットの白内障)の研究にラマン分光法を用いた (37,38)。その研究に関連してラットの水晶体の老化の研究も行い、白内障形成のメカニズムと老化のメカニズムの違いを明らかにした。加齢の場合は、水晶体の中の水の量が減少して行くのに対し、白内障形成の場合は、逆に水の量が増えていくことを非破壊でとらえることができた。また白内障形成の場合は、水晶体タンパク質のチロシン残基のいくつかがタンパク質に埋まった状態から露出した状態に変化することも明らかにした (図 6)。40 年も前に生体組織中の水の変動やタンパク質残基の微環境変化を非破壊でラマン分光法で捉えることができたというで、非常に注目を集めた。

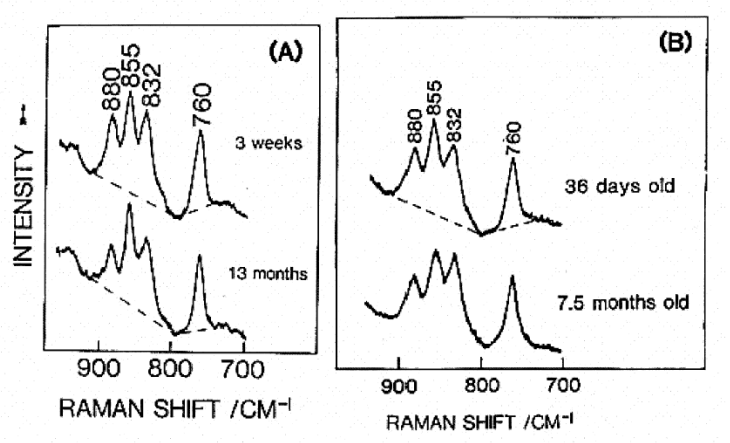

図 6 (A) 正常水晶体と (B) 白内障の水晶体の加齢に伴うラマンスペクトルの変化 (チロシンダブレットの領域)

その後 1990 年代前半に水野らとともに近赤外励起ラマン分光法をいち早くがん組織の研究に応用し、蛍光の妨害のほとんどないがん組織 (脳腫瘍) のスペクトル測定に成功した (39)。グリア細胞腫のスペクトルでは多糖類によるバンドがかなり強くなっているが見られた。また神経細胞腫のスペクトルではヒドロキシアパタイトのバンドが 960 cm^{-1} に強く観測され、石灰化物質の沈着が確認された。これらの研究は、ラマン分光法を用いたがん組織の研究の先駆けの一つである。

最近は、石垣らとともにラマン分光法の食道がんの早期発見に関係したがん診断への応用で注目を集める研究成果を発表した (40)。がんの早期発見では、形態学的変化が現れる前の異常な分子組成変化を検出することが非常に重要に重要である。食道がんのステージ 0,1 のがん組織のスペクトルでは、グリコーゲン、コラーゲン、トリプトファンによるバンドの減少が見られた。スペクトルの解析には、通常のケモメトリックス法のほかにニューラ

ルネットワークなども用いられ、ラマン分光法が初期食道がんの検出に有用であることが示された（40)。このほかに佐藤（英）らとともにラマンイメージングを用いたがん組織の研究を行っている（41)。また石垣らとともにラマン分光法の基礎生物学への応用研究に力を入れており、例えばラマン分光法を用いてマウス胚の成長の過程を非破壊、非ラベル標識で分子レベルで研究することに成功した（42)。

私は近赤外分光法の医学応用でもパイオニア的研究成果を挙げた。1989年に近赤外分光法を用いて手の甲の血中ヘモグロビンの動態を非破壊、非侵襲で測定した(43)。この研究は、その後の医学分野の研究に大きな影響を与えた。さらに丸尾らの1990年代後半に手の腕の血糖値の非侵襲モニタリングの研究へとつながった。

以上のように私は未開拓、未発達な分子分光学分野に独創的なアイデア、研究手法で挑戦し、それを大きく発展させた。それにより幅広い学界あるいは社会へ一定の貢献をしたと言える。

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