

強弾性を示す金属錯体の半合理的な分子設計

(北大院工¹・北大 WPI-ICReDD²・静大院理³・横市大院生命ナノ⁴) ○馮 馳¹・陳 旻究²・関 朋宏³・高見澤 聡⁴・伊藤 肇^{1,2}

Semi-Rational Molecular Design for Achieving Ferroelastic Properties (¹Graduate School of Engineering, Hokkaido University, ²WPI-ICReDD, Hokkaido University, ³Faculty of Science, Shizuoka University, ⁴Graduate School of Nanobioscience, Yokohama City University) ○Chi Feng,¹ Mingoo Jin,² Tomohiro Seki,³ Satoshi Takamizawa,⁴ Hajime Ito^{1,2}

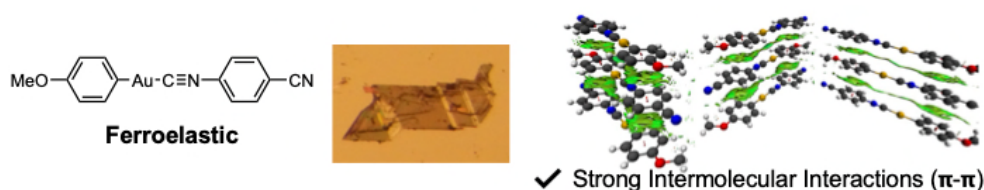
Ferroelasticity is the phenomenon where crystal samples show plastic bending with a spontaneous strain upon application of mechanical stress. This phenomenon has been applied to switches, pressure sensors, etc. In the past, this phenomenon has been observed only in inorganic materials. There have been very few reports of organic ferroelasticity.¹⁾ Here, we have found the structural features of the crystals with ferroelasticity and succeeded in designing the organometallic complexes with ferroelasticity.

The mechanical properties of isocyanide gold(I) complex crystals were investigated. It was found that two gold(I) complexes exhibit ferroelasticity. The crystal structures of the crystals were also evaluated, and the structural features of the ferroelastic crystals were clarified. The gold(I) complexes of ferroelastic crystal adopt a flat molecular conformation and form stacked columns in a head-to-tail arrangement. The presence or absence of the ferroelastic behavior and the crystal structure change were evaluated, and the necessary conditions for the discovery of ferroelasticity were clarified.

Keywords: *Ferroelasticity; Gold Complex*

強弾性とは、ある材料が力学的に変形し自発的なひずみを示す現象である。この現象はスイッチ、圧力センサーなどに応用されている。従来は、無機・合金材料でのみ見られる特異な現象であり、有機分子材料においては、その報告例は極めて少なかった¹⁾。本研究では、強弾性を示す結晶の構造特徴を見出し、強弾性を示す金属錯体の半合理的なデザインに成功した。

複数イソシアニド金(I)錯体からなる結晶の機械的特性を調査した結果、2つの金(I)錯体が強弾性を示すことを見出した。また、強弾性金(I)錯体の結晶構造を評価し、強弾性結晶の構造的特徴を明らかにした。すべての強弾性金(I)錯体の結晶では、分子はフラットなコンホメーションをとり、**head-to-tailed** スタッキング構造が観察された。さらに、強弾性挙動の有無や結晶構造変化などの結果から、強弾性の発見に必要な条件を明らかにした。



1) Seki, T.; Feng, C.; Kashiya, K.; Sakamoto, S.; Takasaki, Y.; Sasaki, T.; Takamizawa, S.; Ito, H. *Angew. Chem. Int. Ed.* **2020**, 59, 8839.