Oral presentation

Exploring structure–property interplay – thermally and mechanically stimulated crystal's dynamic properties

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Highly ordered structural arrangement in crystalline solids, which can be modified in a controlled manner, has proven to be an exceptionally useful feature in achieving and adjusting a specific material property, such as electric or magnetic [1]. Relatively recently, it has been demonstrated that the introduction of slight changes in the structure of 1-D crystalline coordination polymers on a molecular level allows a precise and controlled tuning of their mechanically stimulated flexible responses [2–6]. While in some cases the modification of a single atom in a molecule had no effect on the overall arrangement of building units in crystal structure, but only the importance of intermolecular interactions in the supramolecular network, the response of crystals to mechanically induced stress ranged from exceptional plastic to highly elastic bending or even brittleness.

To investigate in greater depth the correlation of structural features of crystalline materials and the observed properties, we opted for crystals of one-dimensional coordination polymer of cadmium(II) with bromide and 3,5-dichloropyridine ligands. In addition to mechanically stimulated, direction-dependent elastic and plastic flexible responses at a room temperature, these plate-like crystals displayed also a reversible thermosalient phenomena at elevated temperatures. While the reason for the thermally induced crystal's jumping has been unambiguously determined as the consequence of the stress release during the single-crystal-to-single-crystal phase transformation, the origin of the mechanically stimulated response was not straightforward. To determine the structural changes which allow elastic response of a crystal, μ-SCXRD experiments were performed where the structural features throughout the cross-section of elastically bent crystal were mapped out. Further three-point bending experiments were conducted at several different temperatures higher than room temperature and were correlated with structural changes observed from variable-temperature single-crystal diffraction experiments on undeformed crystals to explore the influence of subtle temperature changes to crystal's mechanical output. The results obtained demonstrate that the properties of a material can be fine-tuned by introducing slight structural modifications, either thermally or mechanically, and shed light on the origin and mechanism of stimuli initiated dynamic response, while opening a new direction for research into dynamic materials.

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