

“Twisting Layers” in Solid State: A Breakthrough in conversion of waste heat to electricity

Researchers have developed a new material with potential for highly efficient conversion of waste heat to energy by introducing twisted layers in ferecrystals, a distinctive class of misfit layered compounds. The material which has exceptionally high thermoelectric figure of merit (measure of thermoelectric performance of a material) exceeding the value two can act as tremendous heat blockers and has significant implications for thermoelectric energy conversion, a process that captures and converts waste heat from sources like industrial processes in chemical, thermal, steel plants, petroleum refineries and vehicle exhaust into electricity.

Two-dimensional (2D) superlattice materials, composed of alternating layers of two or more different structures are engineered at the atomic level, with each layer typically just a few atoms thick. The periodic stacking of different 2D materials creates a new material with unique electronic properties that are not present in the individual layers.

Misfit Layered Compounds (MLCs), an interesting example of 2D natural superlattice structured materials, consist of at least two or more periodically stacked independent layers wherein the difference in the repeating patterns of the two layers in MLCs causes a misalignment along one direction.

This misalignment results cause a ‘misfit’ between the layers. Despite exhibiting weaker bonding along the stacking direction, the presence of twisting between the layers (rotational disorder) in a unique class of MLCs known as *ferecrystals*, can hamper the heat transport tremendously,

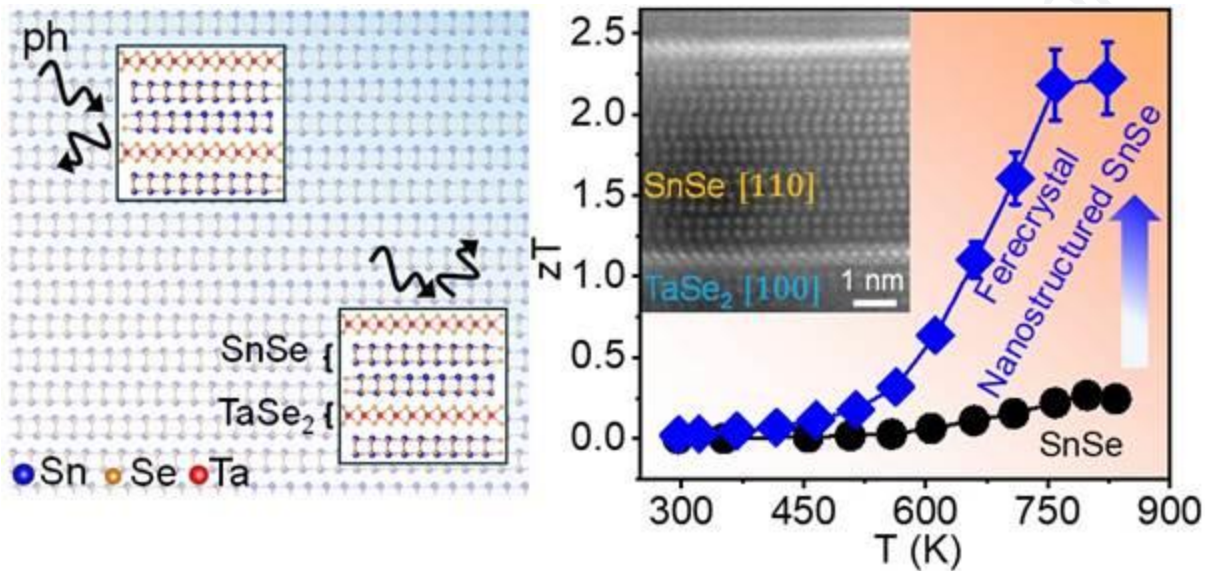
effectively blocking heat waves in any material. This property of ferecrystals makes them particularly interesting for thermoelectric energy conversion, which can convert waste heat into electricity.

However, imbibing these ferecrystals as nanostructures in a solid-state matrix can be a daunting task and grand challenge in synthetic chemistry and materials science, but it could lead to significant advancements in thermoelectric technology and push the boundaries of current material synthesis techniques.

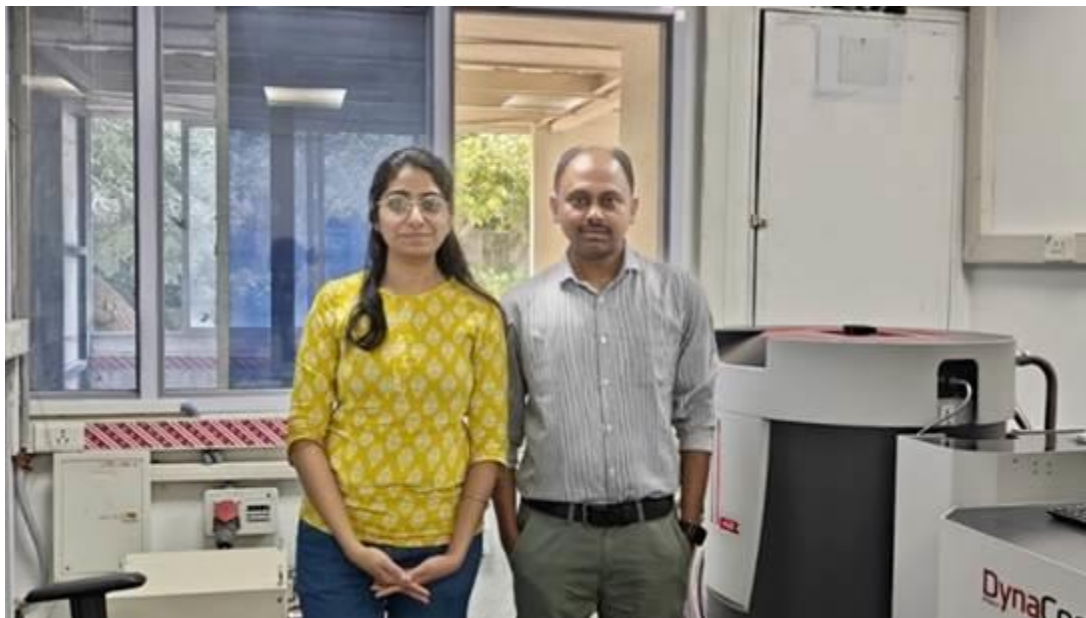
In a recent research paper, Professor Kanishka Biswas, his Ph.D student, Ms. Vaishali Taneja from New Chemistry Unit at Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) Bengaluru, an autonomous institution under the Department of Science & Technology, Govt. of India and other research team members has synthesized ferecrystalline intergrowths as nanoscale region inside bulk SnSe along with n -type halide doping, This has resulted in stabilization of SnSe-TaSe₂ ferecrystal in the form of nanostructures in a solid state SnSe matrix that act as tremendous heat blockers. The thermoelectric figure of merit is achieved to be 2.3.

This study, published in *Journal of the American Chemical Society*, would be the way forward for achieving high performance in n -type SnSe polycrystals. To confirm that the intended intergrowth nanostructures have actually been formed, the team collaborated with Prof N. Ravishankar from IISc, Bengaluru to perform high-resolution transmission electron microscopy (HRTEM) and high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) analysis which revealed the presence of TaSe₂ layers after every 7 bilayers of SnSe. Furthermore, they

have shown the presence of extensive rotational disorder present in the ferecrystals wherein SnSe and TaSe₂ sublattices are twisted (rotated) around the stacking direction (*c* axis) and are translated perpendicular to the stacking direction. The findings from this research could lead to substantial improvements in energy efficiency and contribute to greater sustainability.



A schematic and HAADF-STEM image illustrating the ferecrystalline intergrowths that result in ultrahigh thermoelectric performance in Ta and Br co-doped SnSe.



Vaishali Taneja (left) and Kanishka Biswas (right), JNCASR, Bangalore

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