Physicists detect elusive 'Bragg glass' phase with machine learning tool

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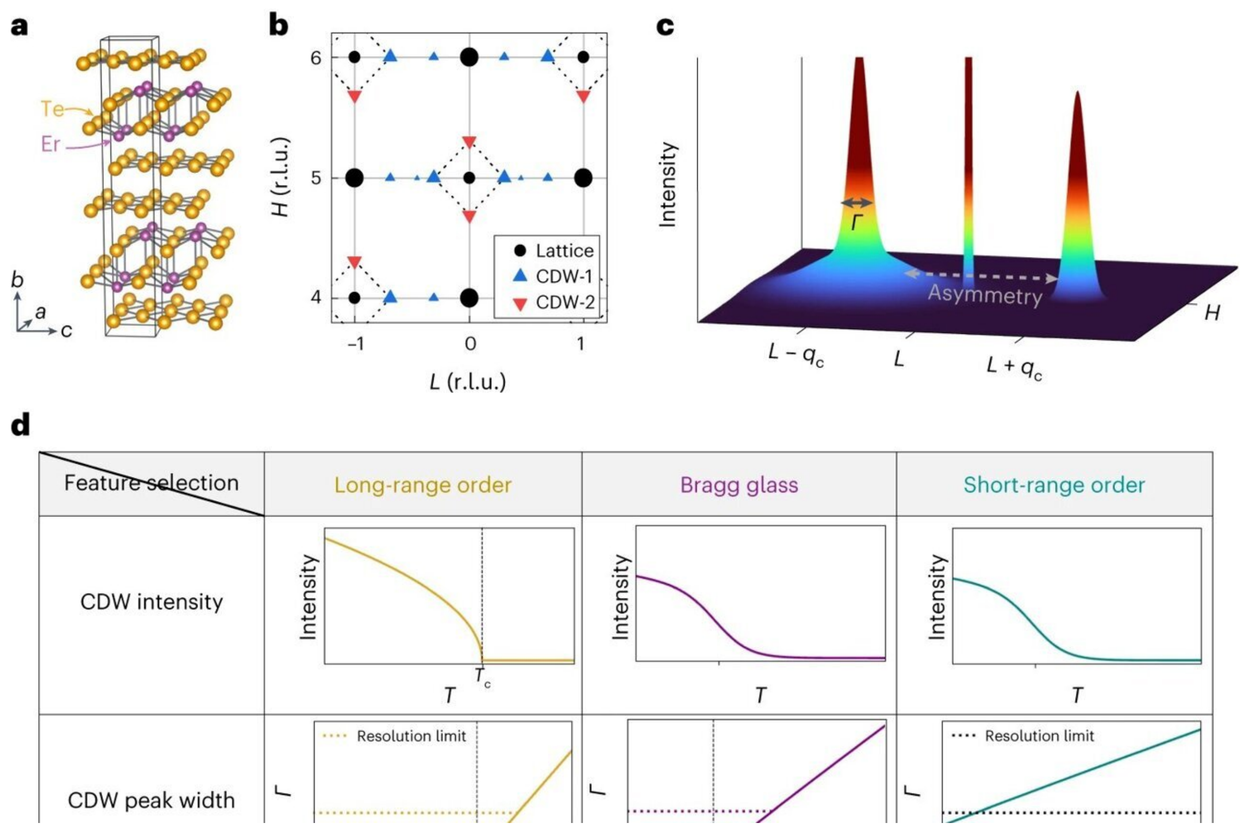

CDWs in Pd_xErTe_3. **a**, Crystal structure of pure $ErTe_3$. The Te planes have approximately square geometry. The crystal belongs to the *Cmcm* space group, *b* denotes the out-of-plane axis, and *a* and *c* are the in-plane axes. **b**, Schematic[25] showing the Bragg peaks (circles) and CDW peaks (triangles) in the in-plane (a^*–c^*) reciprocal space. The satellite peaks of CDW-1 (up triangle) and CDW-2 (down triangle) are aligned along the c^* and a^* axes, respectively. **c**, Schematic for the in-plane (a^*–c^*) intensity distribution of the pair of CDW satellite peaks (at $(H, L \pm q_c)$) around a Bragg peak (at (H, L)), with the following three features of interest: the intensity of the peak, the width of the peak Γ (solid arrow) and the asymmetry in the diffuse scattering surrounding the satellite peaks (dashed arrow). **d**, Table summarizing the diagnostics for classifying the three phases. The first row describes the CDW intensity–temperature trajectory. Only the pristine sample with a long-range order exhibits a sharp onset, marking the transition temperature T_c. On the other hand, one cannot distinguish Bragg glass from short-range order as even after the breakdown of Bragg glass order with increasing temperature, short-ranged fluctuations persist (due to disorder pinning) and contribute to the CDW intensity. The second row illustrates a simplified temperature dependence of the CDW peak width Γ. Credit: *Nature Physics* (2024). DOI: 10.1038/s41567-023-02380-1

Cornell quantum researchers have detected an elusive phase of matter, called the Bragg glass phase, using large volumes of X-ray data and a new machine learning data analysis tool. The discovery settles a long-standing question of whether this almost–but not quite–ordered state of Bragg glass can exist in real materials.

The paper, "Bragg glass signatures in Pd_xErTe_3 with X-ray diffraction Temperature Clustering (X-TEC)," is published in *Nature Physics*. The lead author is Krishnanand Madhukar Mallayya, a postdoctoral researcher in the Department of Physics in the College of Arts and Sciences (A&S). Eun-Ah Kim, professor of physics (A&S), is the corresponding author. The research was conducted in collaboration with scientists at Argonne National Laboratory and at Stanford University.

The researchers present the first evidence of a Bragg glass phase as detected from X-ray scattering, which is a probe that accesses the entire bulk of a material, as opposed to just the surface of a material, in a systematically disordered charge density wave (CDW) material, Pd_xErTe_3. They used comprehensive X-ray data and a novel machine learning data analysis tool, X-ray Temperature Clustering (X-TEC).

"Despite its theoretical prediction three decades ago, concrete experimental evidence for CDW Bragg glass in the bulk of the crystal remained missing," Mallayya said.

Theoretically, there is a sharp distinction between three phases: long-range order, Bragg glass, and disordered state, Kim said. In the disordered state, the CDW correlation decays within a finite distance. In the long-range ordered state, the charge density wave correlation continues indefinitely.

In the Bragg glass phase, Kim went on, the CDW correlation decays so slowly that it will only completely vanish at infinite distances.

"The challenge is detecting these distinctions from experimental data that also reflects real-life issues like noise and finite resolution of the experimental setup," Kim said.

The researchers overcame key challenges through strategic synergy among materials, data, and machine-learning tools. On the materials front, they found, in collaboration with scientists at Stanford, a family of CDW materials that will allow a systematic study with control over dirt to use in the experiment—Pd_xErTe_3. On the data front, they took massive amounts of data at Argonne National Laboratory in collaboration with Argonne scientists.

On the machine learning front, they used X-TEC, a machine learning tool, to analyze the massive volume of data with a scalable and automated approach.

"An experimental detection of Bragg glass phase through X-ray diffraction has settled the open question regarding the fate of CDW order subject to dirt," Mallayya said.

Going beyond the specific scientific problem, the paper presents a new mode of research in the age of large data, Kim said, "Using machine learning tools and data-scientific perspectives, we can go after challenging questions and track down subtle signatures through a comprehensive data analysis."

The researchers wrote that this detection of Bragg glass order and the resulting phase diagram significantly advance our understanding of the complex interplay between disorder and fluctuations. Moreover, using X-TEC to target fluctuations through a high-throughput measure of "peak spread" can revolutionize how the fluctuations are studied in scattering experiments.

More information: Krishnanand Mallayya et al, Bragg glass signatures in Pd_xErTe_3 with X-ray diffraction temperature clustering, *Nature Physics* (2024). DOI: 10.1038/s41567-023-02380-1

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