Structural investigation of the quasi-one-dimensional topological insulator $\mathrm{Bi_4 I_4}$

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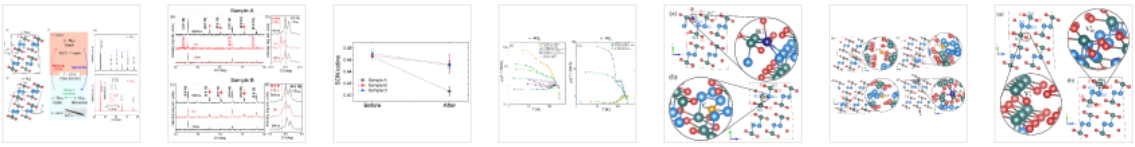
ABSTRACT

The bismuth halide $\mathrm{Bi_4 I_4}$ undergoes a structural transition around $T_P \sim 300$ K, which separates a high-temperature β phase ($T > T_P$) from a low-temperature α phase ($T < T_P$). α and β phases are suggested to host electronic band structures with distinct topological classifications. Rapid quenching was reported to stabilize a metastable $\beta-\mathrm{Bi_4 I_4}$ at $T < T_P$, making possible a comparative study of the physical properties of the two phases in the same low-temperature range. In this work, we present a structural investigation of $\mathrm{Bi_4 I_4}$ before and after quenching together with electrical resistivity measurements. We found that rapid cooling does not consistently lead to a metastable $\beta-\mathrm{Bi_4 I_4}$, and a quick transition to $\alpha-\mathrm{Bi_4 I_4}$ is observed. As a result, the comparison of putative signatures of different topologies attributed to a specific structural phase should be carefully considered. The observed phase instability is accompanied by an increase in iodine vacancies and by a change in the temperature dependence of electrical resistivity, pointing to native defects as a possible origin of our finding. Density functional theory (DFT) calculations support the scenario that iodine vacancies, together with bismuth antisites and interstitials are among the defects that are more likely to occur in $\mathrm{Bi_4 I_4}$ during the growth.



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Physics Subject Headings (PhySH)

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