

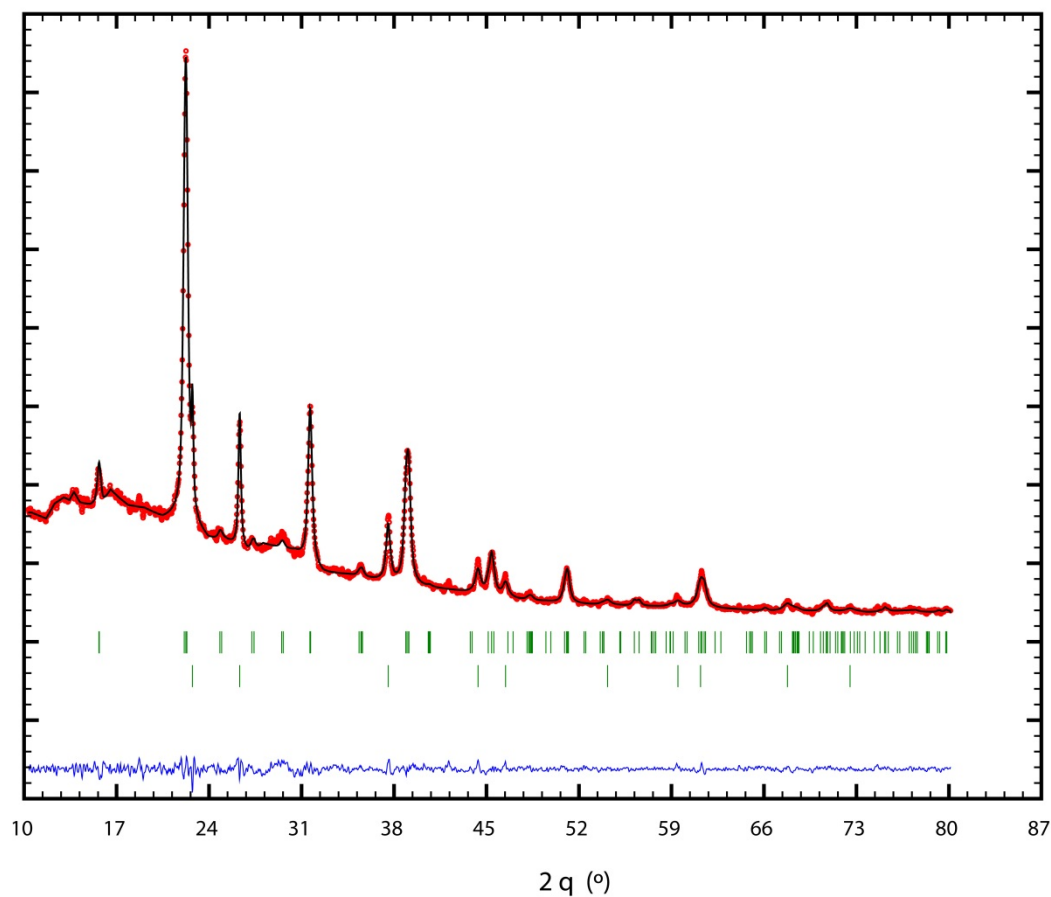
Flux-assisted single crystal growth and heteroepitaxy of perovskite-type mixed-metal borohydrides

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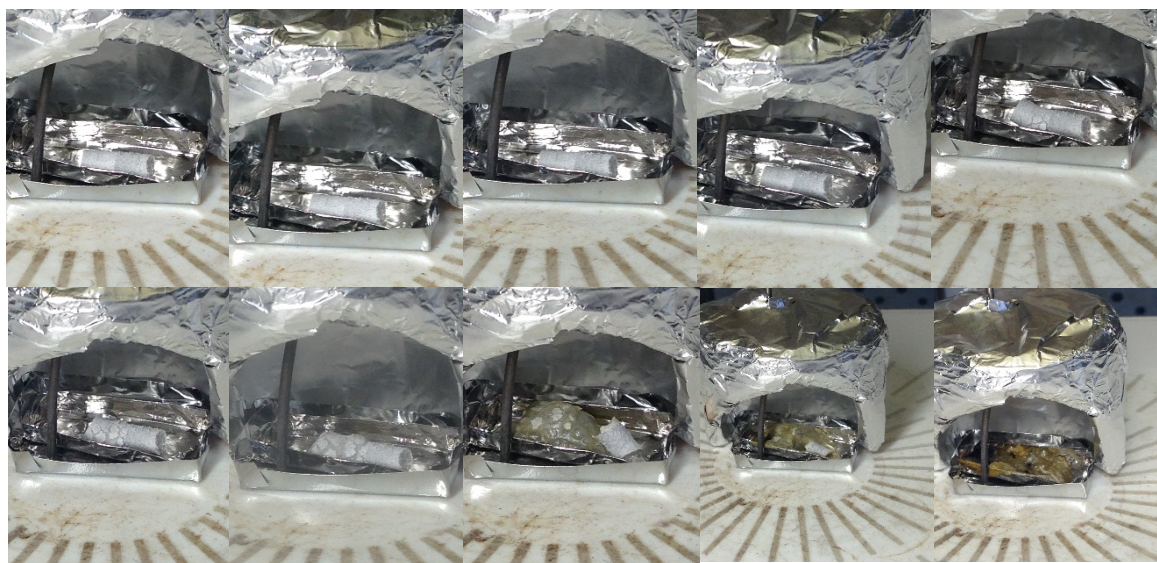
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Supplementary Information



Supplementary Fig. 1 Rietveld plot for ball milled sample $\text{LiBH}_4\text{-Ca}(\text{BH}_4)_2\text{-KBH}_4$, measured at room temperature. *hkl* ticks, from top to bottom: $\text{KCa}(\text{BH}_4)_3$, KBH_4 . The quantitative analysis yield 76 mol% $\text{KCa}(\text{BH}_4)_3$ and 24 mol% KBH_4 . The Gaussian profile parameters were refined per phase and one additional mixing parameter for $\text{KCa}(\text{BH}_4)_3$ to allow for Lorentzian lineshape.



Supplementary Fig. 2 Pellet composed of 50 vol% solvent (left half) and 50 vol% sample $\text{KCa}(\text{BH}_4)_3$ (right). From left to right, top to bottom: 298 K, 423 K, 473 K, 493 K, 503 K, 513 K, 523 K, 543 K, 553 K, 573 K.

Sample preparation for flux-melting

Three different compositional mixtures eutectic mixture : $\text{KCa}(\text{BH}_4)_3$ were prepared, to investigate the effect of volume and molar excess on the melting behaviour.

Molar ratio 1:1, excess sample volume of $\text{KCa}(\text{BH}_4)_3$:

The sample decomposed at 593 K. This means that the melting point of $\text{KCa}(\text{BH}_4)_3$ was lowered due to the eutectic with respect to 618 K, but decomposition still present. No single crystals were found in the molar mixture 1:1, also not at the final operating temperature of 513 K.

Molar ratio 8.6:1.4, same sample volumes:

Two pellets used, to study influence of solvent on the sample (Fig. 1 and Supplementary Fig. 2). Single crystals found at synthesis attempts at 513 K.

Molar ratio 9:1, excess sample volume of eutectic mixture:

Single crystals found at experiments run at 513 K.