

[Electronic Supplementary Information]

Mechano-chemical activation of the (3LiBH₄+TiF₃) system, its dehydrogenation behavior and the effects of ultrafine filamentary Ni and graphene additives

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Table 1S. Summary of hydrogen quantities desorbed due to mechanical and thermal dehydrogenation. The numbers in parenthesis indicate the time for thermal dehydrogenation in hours (h).

Sample	H ₂ desorbed during BM (wt.%)	H ₂ desorbed at 60°C (wt.%(h))	H ₂ desorbed at 85°C (wt.%(h))	H ₂ desorbed at 100°C (wt.%(h))	H ₂ desorbed at 120°C (wt.%(h))	H ₂ desorbed at 200°C (wt.%(h))	Total H ₂ desorbed during BM and at 200°C (wt.%)
(3LiBH₄+TiF₃)-1h BM	1.35	4.52 (93.2)	4.85 (23.6)	5.30 (25)	5.52 (23.15)	5.81 (21.3)	7.16
(3LiBH₄+TiF₃)-5h BM	1.58	4.73 (44)	4.83 (24.6)	5.04 (65)	5.29 (23.5)	5.58 (19.5)	7.16
(3LiBH₄+TiF₃)+5 wt.% Ni-1h BM	1.42	4.42 (44.7)	5.18 (96.2)	5.01 (24.8)	5.05 (20.3)	5.62 (23.5)	7.04
(3LiBH₄+TiF₃)+5 wt.% Ni-5h BM	1.97	3.92 (49.5)	4.52 (41)	4.82 (22.8)	5.27 (29.2)	5.39 (21.7)	7.36
(3LiBH₄+TiF₃)+5 wt.% graphene- 1h BM	0.87	3.62 (47)	4.78 (93.5)	4.87 (26.2)	5.08 (18.9)	6.02 (22)	6.89
(3LiBH₄+TiF₃)+5 wt.% graphene- 5h BM	2.38	2.98 (39.3)	2.96 (90.9)	2.45 (22.8)	2.86 (25.1)	2.84 (24)	5.22

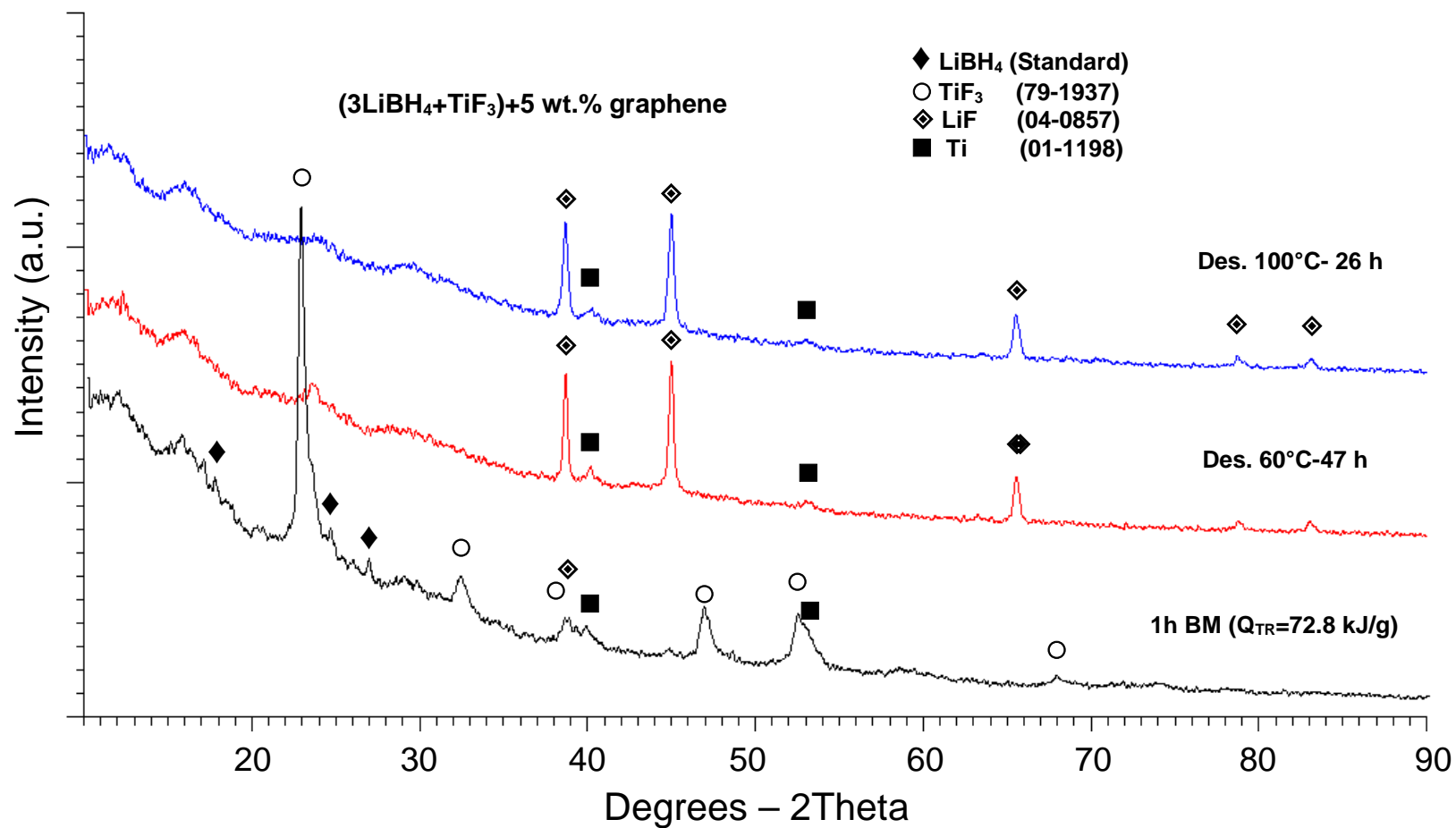


Fig. 1S. XRD patterns after ball milling (BM) and isothermal dehydrogenation at different temperatures for 3LiBH₄+TiF₃+5 wt.% graphene with an energy input, $Q_{TR}=72.8$ kJ/g (1h BM).

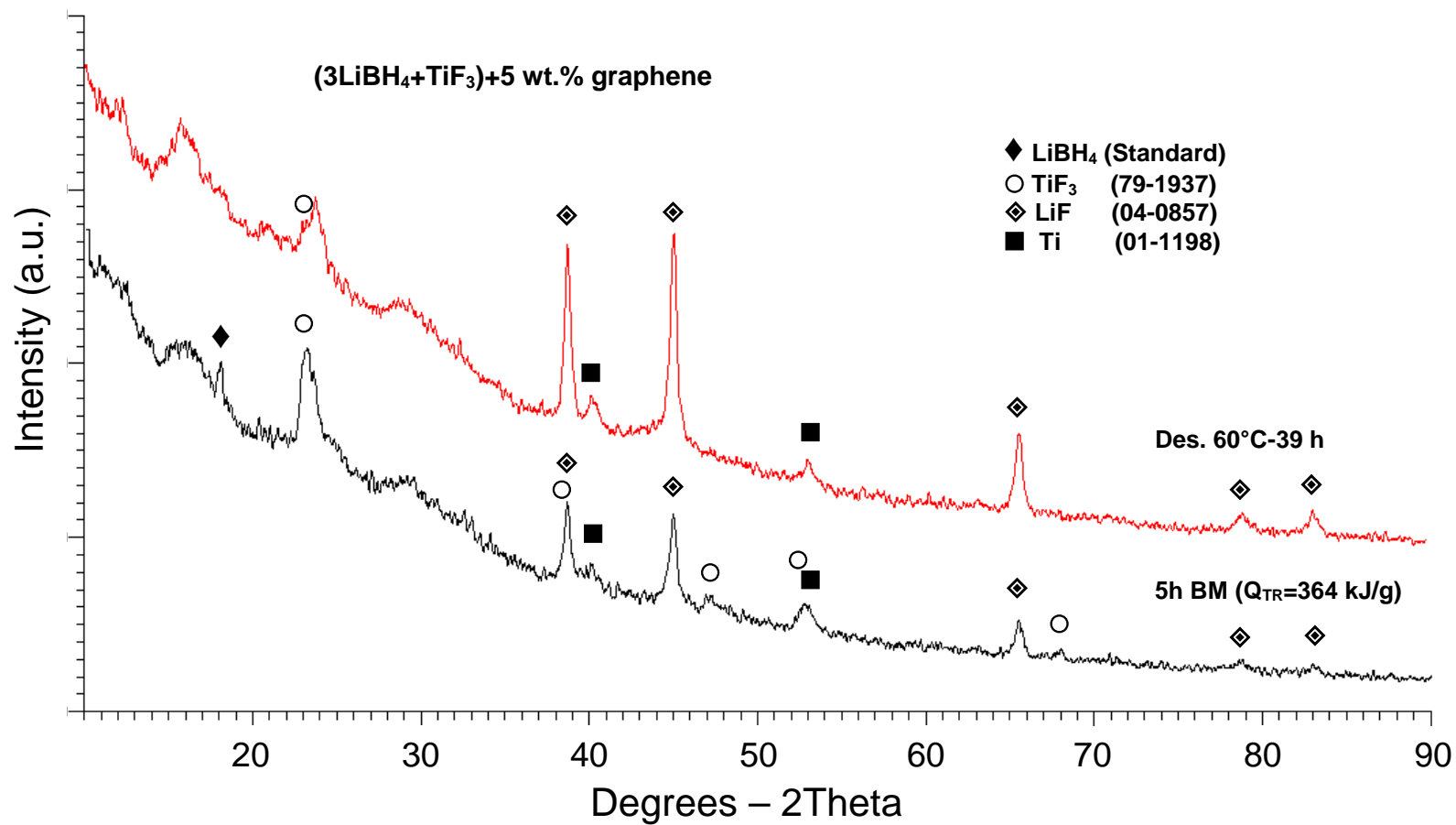


Fig. 2S. XRD patterns after ball milling (BM) and isothermal dehydrogenation at different temperatures for 3LiBH₄+TiF₃+5 wt.% graphene with an energy input, Q_{TR}=364 kJ/g (5h BM).

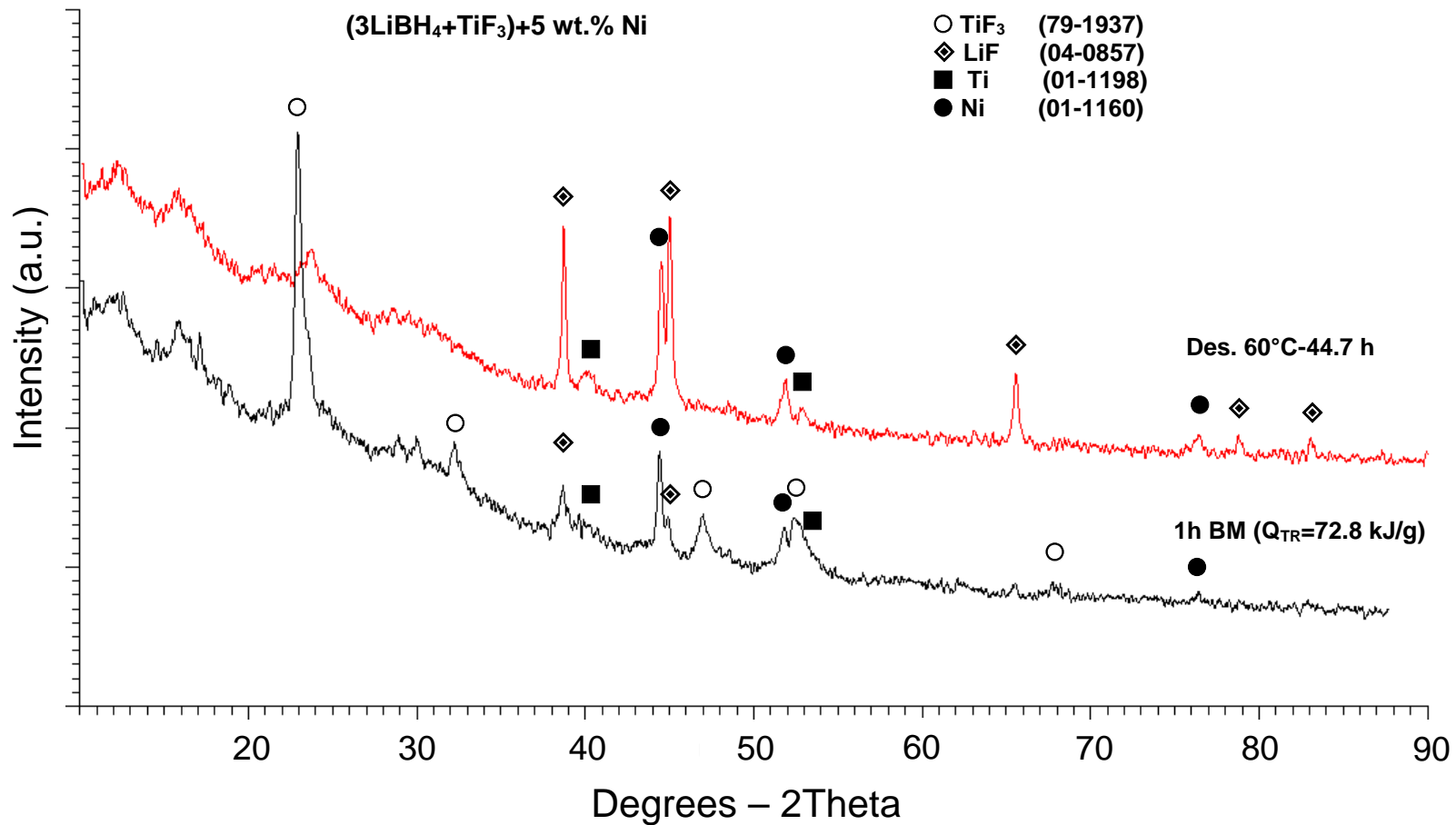


Fig. 3S. XRD patterns after ball milling (BM) and isothermal dehydrogenation at different temperatures for 3LiBH₄+TiF₃+5wt.% Ni with an energy input, $Q_{TR}=72.8$ kJ/g (1h BM)

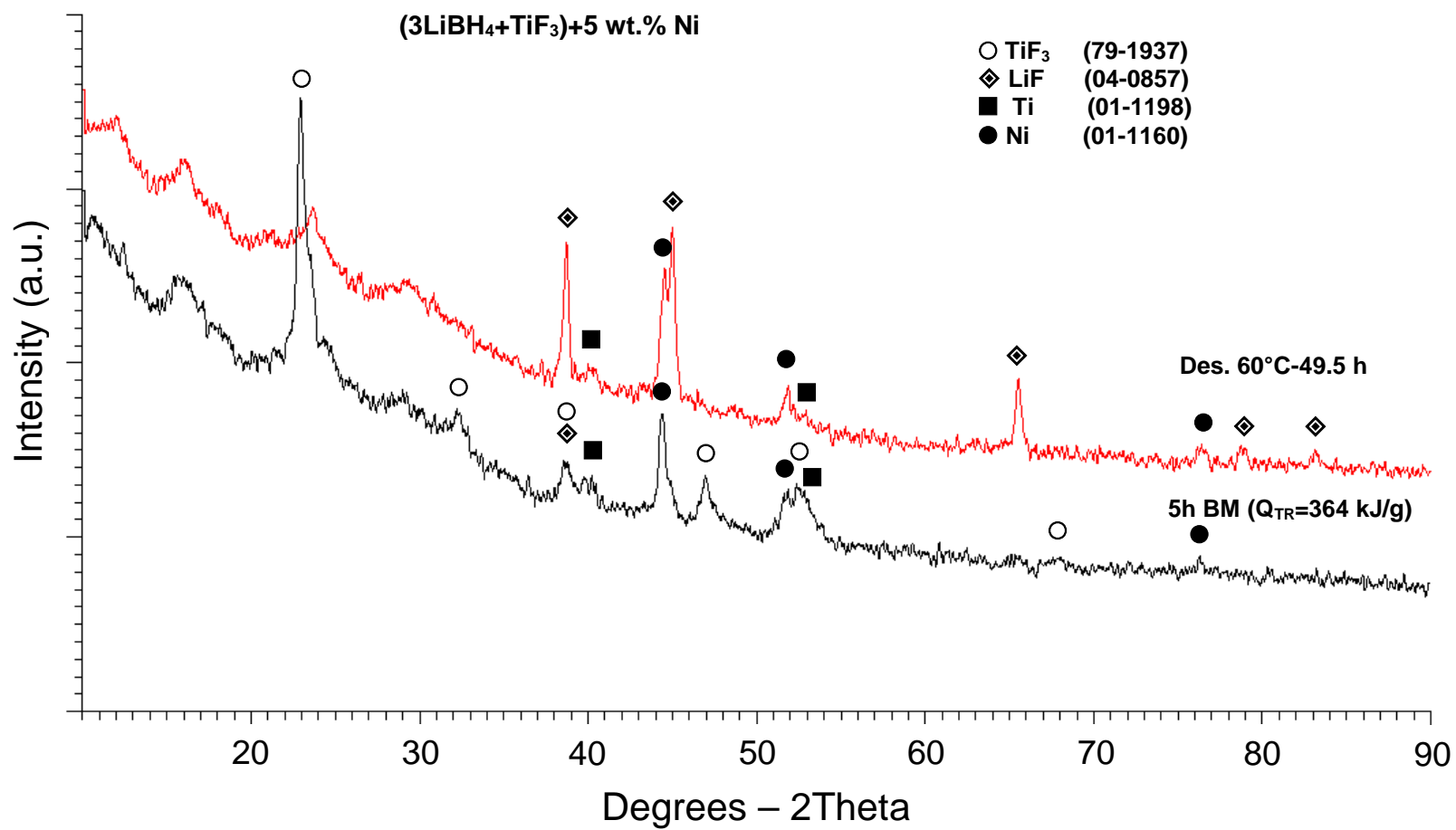


Fig. 4S. XRD patterns after ball milling (BM) and isothermal dehydrogenation at different temperatures for 3LiBH₄+TiF₃+5wt.% Ni with an energy input, $Q_{TR}=364$ kJ/g (5h BM).