

The effect of titanium in $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ /graphene composites as cathode material for high capacity Li-ion batteries

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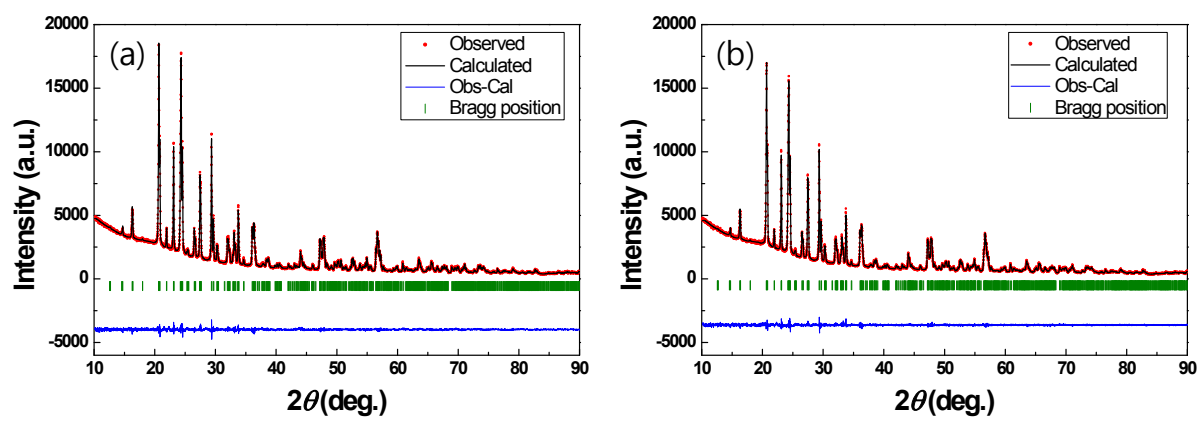


Fig S1 Refinement result of the (a) LVP-Ti1 and (b) LVP-Ti5 samples.

Table S1 Atomic sites and fractional coordinates of pristine LVP and LVP-Ti3.

Atom	<i>x</i>		<i>y</i>		<i>z</i>	
	LVP	LVP-Ti3	LVP	LVP-Ti3	LVP	LVP-Ti3
V1	0.2474(3)	0.2477(4)	0.4623(3)	0.4634(3)	0.1102(2)	0.1101(2)
V2	0.7533(4)	0.7527(4)	0.4711(3)	0.4706(3)	0.3898(2)	0.3896(2)
P1	0.1058(4)	0.1060(5)	0.1036(5)	0.1043(5)	0.1493(3)	0.1490(3)
P2	0.6041(5)	0.6043(5)	0.1141(5)	0.1153(5)	0.3523(3)	0.3519(3)
P3	0.0384(5)	0.0363(5)	0.2499(6)	0.2495(6)	0.4924(4)	0.4925(4)
O1	0.9269(10)	0.9273(10)	0.1129(9)	0.1130(10)	0.1469(6)	0.1454(7)
O2	0.1511(9)	0.1536(9)	0.9820(9)	0.9813(10)	0.2382(6)	0.2372(6)
O3	0.1750(8)	0.1750(8)	0.0437(8)	0.0427(9)	0.0415(6)	0.0419(6)
O4	0.1653(9)	0.1625(9)	0.2664(10)	0.2671(11)	0.1876(6)	0.1866(7)
O5	0.4324(10)	0.4335(10)	0.0915(9)	0.0917(10)	0.3290(5)	0.3293(6)
O6	0.6960(8)	0.6964(8)	-0.0016(9)	0.0053(10)	0.2789(6)	0.2788(6)
O7	0.6505(9)	0.6493(10)	0.0830(8)	0.0852(9)	0.4708(6)	0.4701(6)
O8	0.6418(8)	0.6439(9)	0.2834(10)	0.2820(11)	0.3187(6)	0.3187(6)
O9	0.9511(9)	0.9524(9)	0.1329(9)	0.1344(9)	0.5683(6)	0.5685(6)
O10	0.9350(9)	0.9338(10)	0.3187(8)	0.3196(9)	0.4036(6)	0.4047(7)
O11	0.1706(9)	0.1707(10)	0.1738(9)	0.1754(9)	0.4324(6)	0.4329(6)
O12	0.1096(9)	0.1112(9)	0.3624(10)	0.3561(10)	0.5731(6)	0.5737(6)
Li1	0.217(3)	0.225(4)	0.782(3)	0.774(3)	0.172(2)	0.173(2)
Li2	0.921(3)	0.902(3)	0.299(3)	0.289(3)	0.237(2)	0.226(2)
Li3	0.573(3)	0.570(3)	0.403(3)	0.407(3)	0.1927(19)	0.198(2)

For pristine LVP, the reliable factors are $R_p = 2.85\%$, $R_{wp} = 3.87\%$, $R_I = 3.01$, $R_F = 2.41\%$ and $\chi^2 = 2.23$.

For pristine LVP-Ti3, the reliable factors are $R_p = 2.48\%$, $R_{wp} = 3.29\%$, $R_I = 2.45$, $R_F = 2.27\%$ and $\chi^2 = 1.68$.

Table S2 Atomic sites and fractional coordinates of LVP-Ti1 and LVP-Ti5.

Atom	<i>x</i>		<i>y</i>		<i>z</i>	
	LVP-Ti1	LVP-Ti5	LVP-Ti1	LVP-Ti5	LVP-Ti1	LVP-Ti5
V1	0.2476(4)	0.2473(4)	0.4630(3)	0.4635(3)	0.1095(2)	0.1105(2)
V2	0.7534(4)	0.7514(4)	0.4714(3)	0.4707(3)	0.3895(2)	0.3899(2)
P1	0.1065(5)	0.1052(5)	0.1049(5)	0.1044(5)	0.1490(3)	0.1490(3)
P2	0.6036(5)	0.6047(5)	0.1142(5)	0.1147(5)	0.3517(3)	0.3521(3)
P3	0.0375(5)	0.0369(5)	0.2495(6)	0.2504(6)	0.4926(4)	0.4931(4)
O1	0.9277(10)	0.9283(10)	0.1113(10)	0.1156(10)	0.1452(7)	0.1455(7)
O2	0.1516(9)	0.1534(9)	0.9821(10)	0.9828(10)	0.2379(6)	0.2362(6)
O3	0.1738(8)	0.1733(8)	0.0430(9)	0.0410(9)	0.0407(7)	0.0413(7)
O4	0.1641(9)	0.1638(10)	0.2660(11)	0.2667(11)	0.1875(7)	0.1865(7)
O5	0.4336(10)	0.4327(11)	0.0902(10)	0.0932(10)	0.3286(6)	0.3298(6)
O6	0.6963(8)	0.6970(8)	0.0027(10)	0.0038(10)	0.2787(6)	0.2795(6)
O7	0.6500(10)	0.6489(10)	0.0834(9)	0.0851(9)	0.4711(6)	0.4721(6)
O8	0.6405(9)	0.6459(9)	0.2831(11)	0.2792(11)	0.3194(6)	0.3172(6)
O9	0.9514(9)	0.9516(9)	0.1338(9)	0.1326(9)	0.5687(6)	0.5688(6)
O10	0.9358(10)	0.9351(10)	0.3173(9)	0.3213(9)	0.4056(7)	0.4045(7)
O11	0.1726(10)	0.1710(10)	0.1758(9)	0.1743(9)	0.4326(6)	0.4312(6)
O12	0.1116(9)	0.1126(10)	0.3587(10)	0.3537(10)	0.5744(6)	0.5752(6)
Li1	0.223(4)	0.216(4)	0.785(3)	0.777(3)	0.171(2)	0.170(2)
Li2	0.913(3)	0.920(3)	0.286(3)	0.301(3)	0.230(2)	0.229(2)
Li3	0.569(3)	0.572(3)	0.409(3)	0.412(3)	0.197(2)	0.196(2)

For pristine LVP-Ti1, the reliable factors are $R_p = 2.57\%$, $R_{wp} = 3.42\%$, $R_I = 2.70$, $R_F = 2.37\%$ and $\chi^2 = 1.87$.

For pristine LVP-Ti5, the reliable factors are $R_p = 2.41\%$, $R_{wp} = 3.21\%$, $R_I = 2.27$, $R_F = 1.92\%$ and $\chi^2 = 1.60$.

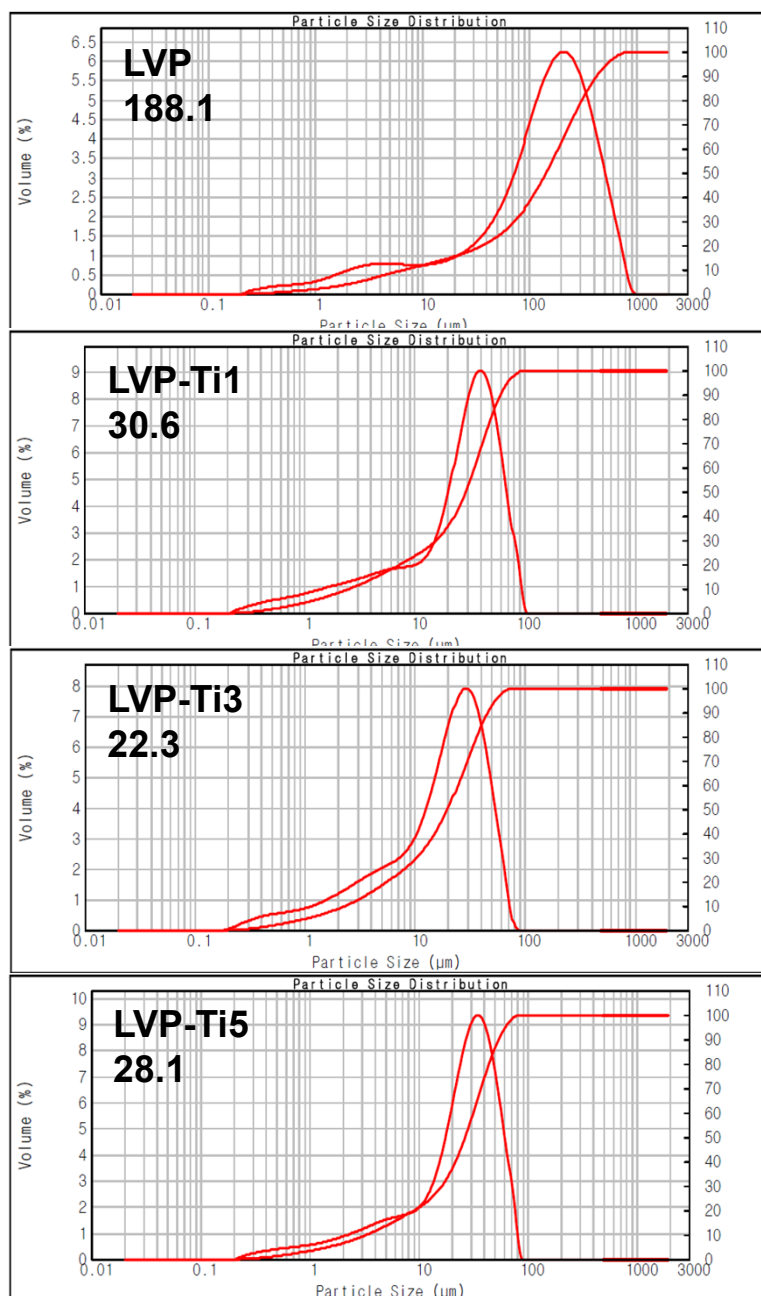


Fig. S2 Size-distribution diagram of the pristine LVP, LVP-Ti1, LVP-Ti3, and LVP-Ti5

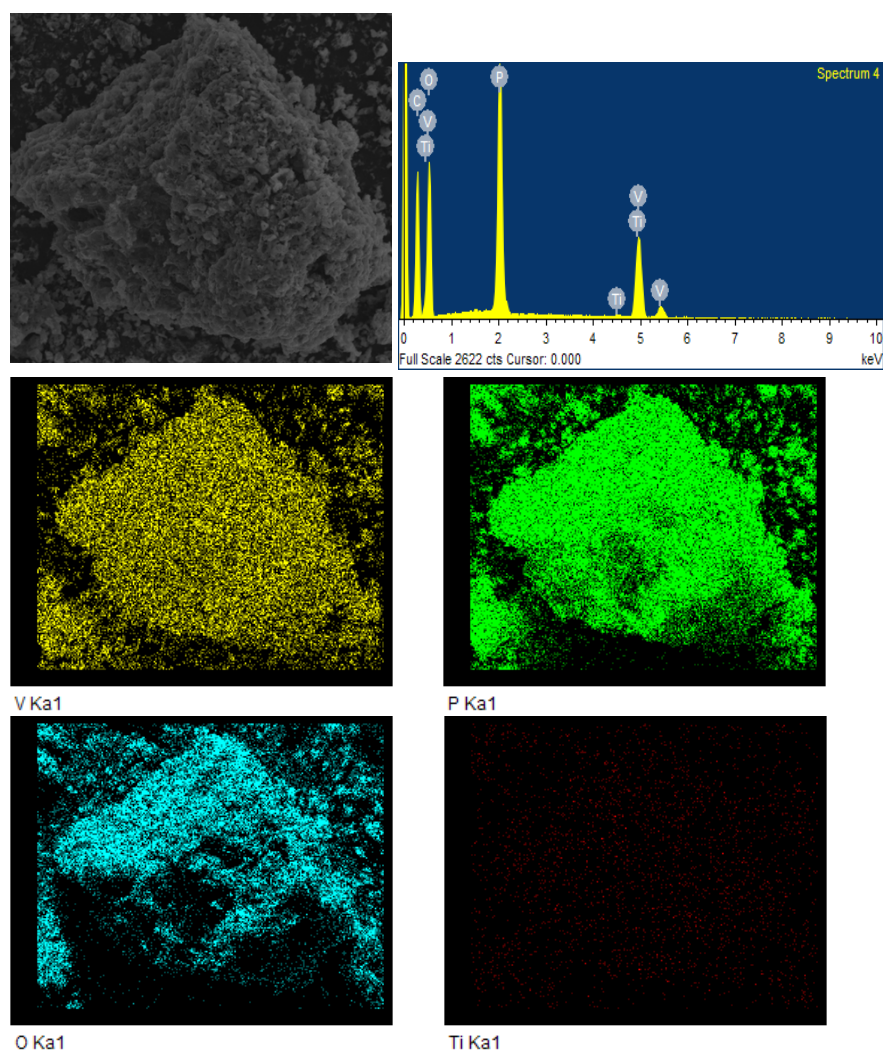


Fig. S3 EDX mapping of LVP-Ti3 sample.

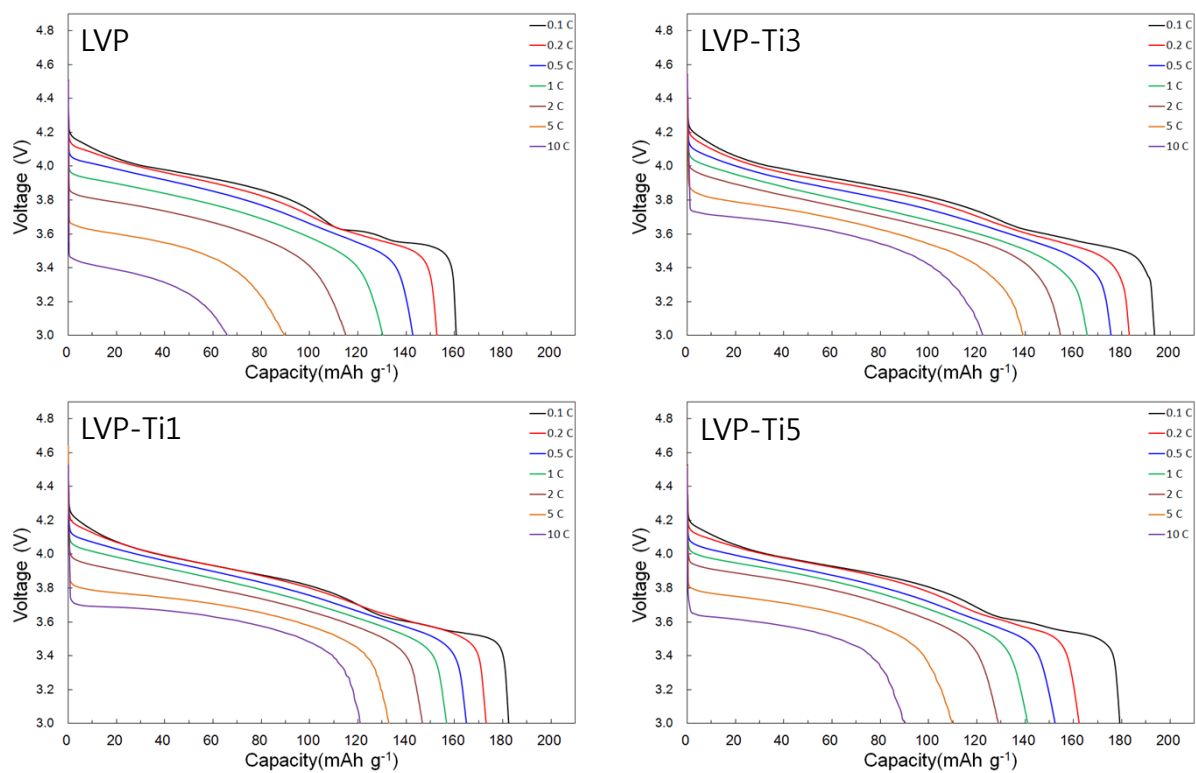


Fig. S4 Rate capabilities of the pristine LVP, LVP-Ti1, LVP-Ti3 and LVP-Ti5 in the potential range of 3.0-4.8 V.

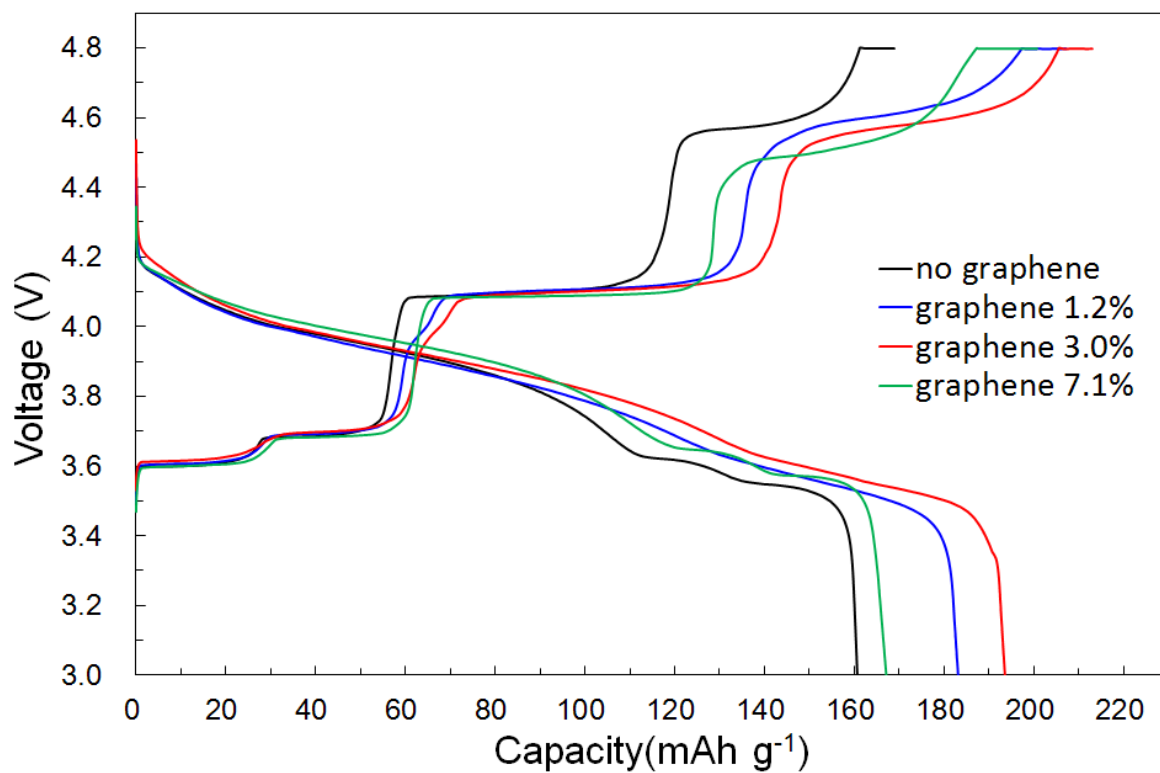


Fig. S5 First charge-discharge profiles of the LVP-Ti3 with 0, 1.2, 3.0 and 7.1 wt% graphene in the potential range of 3.0-4.8 V.