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Supporting Online Information

In situ study on charge/discharge of nanocrystalline Li_2C_2 as a new cathode material

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Series title:

A. Alloy microstructure characterization

B. Movie of in situ TEM observations of discharge/charge processes

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D. Morphology images of the electrode after different cycles

A. Alloy microstructure characterization

After the nanocrystalline Li_2C_2 alloy bulk was prepared at College of Materials Science and Engineering, Beijing University of Technology, China, the preparation of the TEM film and microstructure characterization of the nanocrystalline Li_2C_2 alloy were then performed at Friedrich Schiller University, Otto Schott Institute of Materials Research, Germany. As the high resolution TEM image shown in Fig. S1, the prepared nanocrystalline Li_2C_2 alloy has a nanograin structure. The main phase is Li_2C_2, as indicated by the SAED pattern. It is seen that some amorphous structure is coexisting with the nanograins, which is caused in the process of TEM film preparation using the FIB technique.

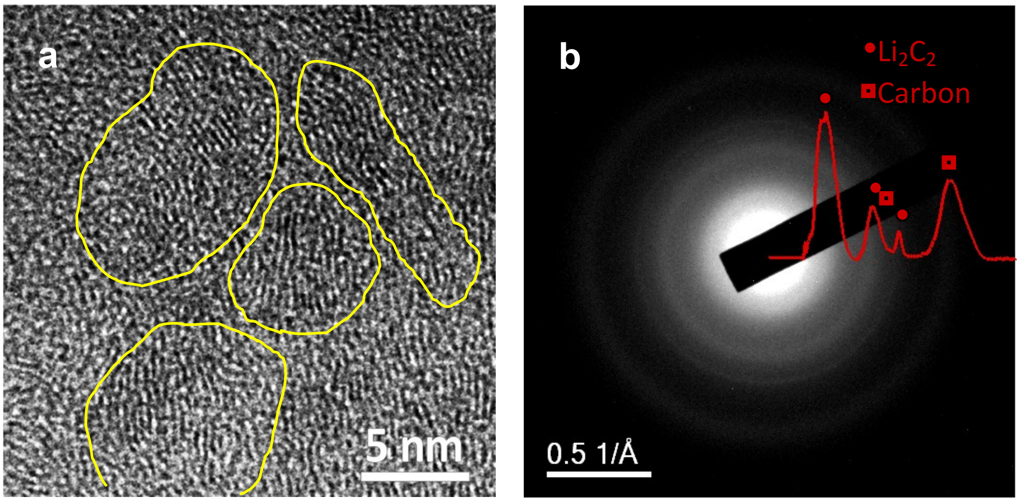

Fig. S1. (a) high resolution TEM image of the prepared nanocrystalline Li_2C_2 alloy, (b) the selected area electron diffraction pattern and indexing.

B. Movie of in situ TEM observations of discharge/charge processes

The movie recording the dynamic observations of discharge/charge processes is uploaded with our manuscript. It shows the details of the changes in the nanocrystalline Li_2C_2 cathode during the cycling of discharge and charge processes, using the in situ TEM observations.

To reduce the document size of the movie, the rate for playing was sped up for 13 times.

C. SAED analysis of the microstructure after first charge

To investigate the change of the Li_2C_2 structure after the first delithiation, we made the SAED pattern of the microstructure, as shown in Fig. S2. Based on the lattice structure (as shown in Figure 5 in our manuscript), we simulated the XRD patterns of LiC_2 and $Li_{0.5}C_2$, as shown in Fig. S3. The indexing of the SAED pattern shows that the diffraction planes are consistent with those in the XRD pattern of LiC_2. It is confirmed that in the in situ TEM test after the first charge the phase is still LiC_2. This result also agrees with the first-principle calculations in Section 3.2 of our manuscript.

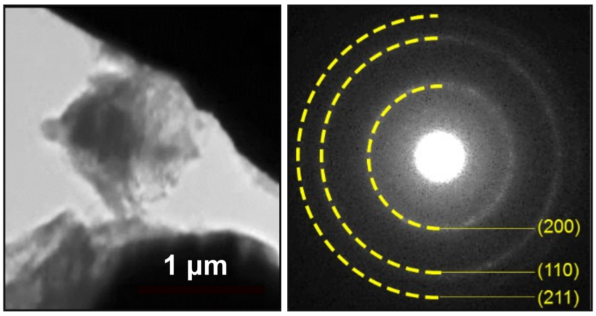

Fig. S2 The microstructure and SAED pattern of the nanocrystalline Li_2C_2 particle after first charge process.

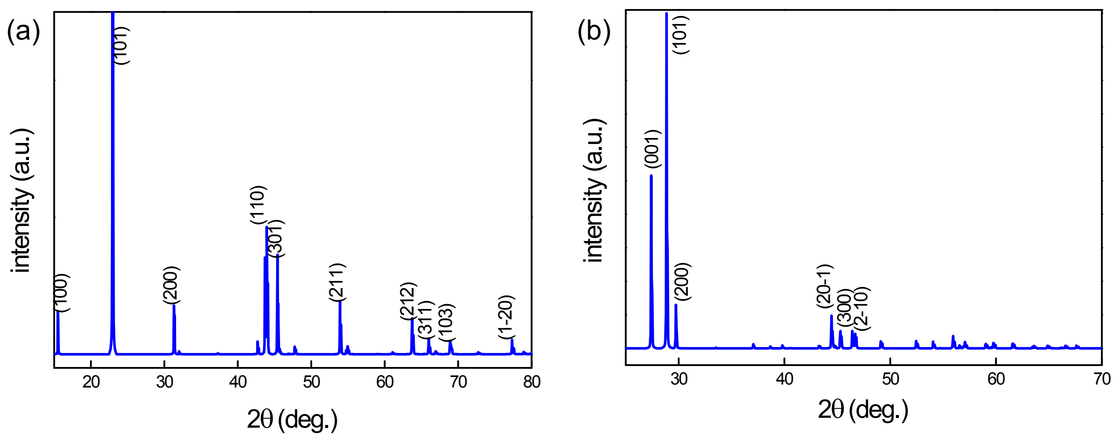

Fig. S3 The simulated XRD patterns of LiC_2 (a) and $Li_{0.5}C_2$ (b).

D. Morphology images of the electrode after different cycles

The Scan electron microscope images of the electrodes after different cycles are shown in Fig. S4. After 10 cycles (Fig. S4 (b)), holes appear in the electrode, as indicated by the arrows. The capacity of the nanocrystalline Li_2C_2 decreases by 2.8% of the initial capacity, and there is slight change in the structure. After 20 cycles, there is a little increase of the holes in the electrode, as shown in Fig. S4 (c). As a result, there is a quick decrease of the capacity of the nanocrystalline Li_2C_2. After 50 cycles, some cracks and holes can be clearly seen at the surface of the electrode (Fig. S4 (d)), which causes further decrease of the lithium storage capacity. These results are consistent with the electrochemical tests. The discharge capacity of 172 $mAhg^{-1}$ after 50 cycles indicates that the nanocrystalline Li_2C_2 has important potential as a cathode material for lithium ion batteries.

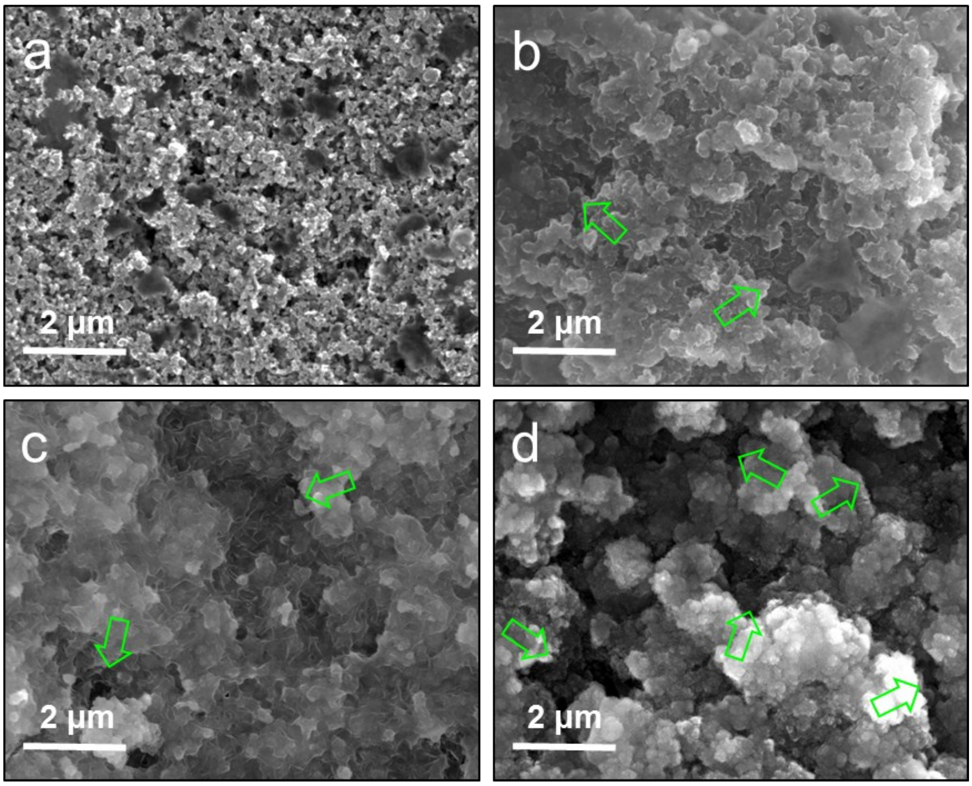

Fig. S4 SEM images of the nanocrystalline Li_2C_2 electrodes after different cycles: (a) 0 cycle, (b) 10 cycles, (c) 20 cycles, (d) 50 cycles.