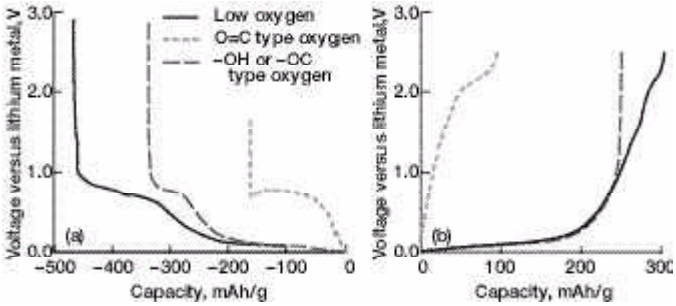
Chemical State of Surface Oxygen on Carbon and Its Effects on the Capacity of the Carbon Anode in a Lithium-Ion Battery Investigated

In a lithium-ion battery, the lithium-storage capacity of the carbon anode is greatly affected by a surface layer formed during the first half cycle of lithium insertion and release into and out of the carbon anode. The formation of this solid-electrolyte interface, in turn, is affected by the chemistry of the carbon surface. A study at the NASA Glenn Research Center examined the cause-and-effect relations. Information obtained from this research could contribute in designing a high-capacity lithium-ion battery and, therefore, small, powerful spacecraft.

In one test, three types of surfaces were examined: (1) a surface with low oxygen content (1.5 at.%) and a high concentration of active sites, (2) a surface with 4.5 at.% -OH or -OC type oxygen, and (3) a surface with 6.5 at.% O=C type oxygen. The samples were made from the same precursor and had similar bulk properties. They were tested under a constant current of 10 mA/g in half cells that used lithium metal as the counter electrode and 0.5 M lithium iodide in 50/50 (vol %) ethylene carbonate and dimethyl carbonate as the electrolyte.



Voltage of carbon anodes (with different surfaces) versus lithium metal. Left: During the first half cycle of lithium insertion. Right: During the first half cycle of lithium release.

For the first cycle of the electrochemical test, the graph describes the voltage of the carbon anode versus the lithium metal as a function of the capacity (amount of lithium insertion or release). From these data, it can be observed that the surface with low oxygen and a high concentration of active sites could result in a high irreversible capacity. Such a high irreversible capacity could be prevented if the active sites were allowed to react with oxygen in air, producing -OH or -OC type oxygen. The O=C type oxygen, on the other hand, could greatly reduce the capacity of lithium intercalation and, therefore, needs to be avoided during battery fabrication.

TABLE I.--CAPACITIES OF LITHIUM INSERTION AND RELEASE FOR CARBON WITH DIFFERENT SURFACES AND SIMILAR BULK STRUCTURE

Sample	Surface oxygen		Active sites concentration	Irreversible capacity, mAh/g	Reversible capacity, mAh/g	
	Chemical state	Content, at.%			Capacity contributed by intercalation, *I*	Capacity not contributed by intercalation, *NI*
A	-OH or -OC	1.5	High	163	169	135
B	-OH or -OC	4.5	Low	85	174	78
C	O=C	6.5	Low	66	0	95

Glenn contact: Dr. Ching-cheh Hung, 216-433-2302, Ching-Cheh.Hung@grc.nasa.gov
Author: Dr. Ching-cheh Hung
Headquarter program office: OSS (ATMS)
Programs/Projects: Space Power Technology