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Lattice elastic and plastic deformation restoring stability in silicon carbide film anode of secondary lithium battery

Zhang Hongtao[1], **Pan Jian**[1], **Liuxin**[1], **Xu Hui**[1] and **Zhang Zesen**[2]
[1]Hubei University of Technology, China
[2]Wuhan Chuneng electron Co. Ltd., China

In charge and discharge process of lithium ion battery special elastic and plastic deformation could be experienced with lithium intercalation and extraction in anode, which is a mechanical behavior. Silicon carbide has many polytypes, such as cubic symmetry, four hetero-structure, six hetero-structure, fifteen hetero-structure, etc., which is a solid with a compact structure. Normally, the lithium ion migration in its crystal could be impeded because of its strong covalent bond. Bulk silicon carbide is unable to store up lithium ion. Nanosized crystalline of silicon carbide could alternatively be a different situation. There could be a lot of surface defects and inner defects, the silicon carbide nanomaterials would produce the lithium ion migrating path. In nanocrystalline films of silicon carbide the nanocolumnar silicon carbide would be a dangling bond nanocrystal on surface with a great deal of defects, in which they are discrete distribution in the film of anode surrounded by the amorphous crystalline silicon carbide. The nanocrystalline columnar silicon carbide in film could supply the conducting pass due to its crystal structure defects. But its conductivity will not be large enough to make the lithium ion effectively move. It needs doping, especially nitrogen doping, which was in favor of forming high concentration nitrogen vacancy, to enhance its conductivity. The lithium ion migration in silicon carbide nanocrystalline would put up its lattice structure and configure six lithium atoms per silicon, which could realize the non-stoichiometric proportions of lithium ion. The crystal lattice would recovery its previous state while lithium ion extraction. The transversion of charge and discharge in lithium ion battery will repeat. The crystal lattice would attempt to recovery its original state, and the process would cycle repeatedly, and so on. It could need a proper indicator to describe the phenomena; we will use a word, which is the stability of elastic and plastic deformation restoring force. It would be related to the lithium ion diffusion, electron conduct, spatial distribution of lithium alloy, nanocrystalline size, and its dimension, diffusion coefficient. We could reduce a formula of the stability of elastic and plastic deformation restoring force

$$H = \frac{M}{R\Delta V}\left[\frac{I}{E}\right]^{n} \qquad (1)$$

R- the ratio of minimum and maximum value of nanocrystalline size, I-the strength of chemical bond, which could be computed by the bond breaking, E- lattice energy, ΔV-volume change ration , n-dimension, which would take the value 1 while zero dimension, the value 2 while one dimension, 1.5 while 2 dimension, and 0.5 while 3 dimension. The anode materials would divide into three types, i.e., stable, meta-stable, and unstable type. H could take the value $H \geq 15$, $1 \leq H < 15$, $H < 1$. The H of silicon carbide would be 20, it is stable.

Biography

Zhang Hongtao is a Professor in the Department of Communication Engineering, Hubei University of Technology, China. He is mainly engaged in quantum computing and quantum information, embedded systems development research and also have interest in battery and electric vehicles.

zhanght@mail.hbut.edu.cn

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