The study of segregation of impurities on grain boundaries of lithium metal anodes

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Due to its high specific capacity and low electrode potential, lithium metal is considered the best anode material in chemical current sources, e.g. in lithium-oxygen or sulfur-oxygen batteries. The key issue of lithium metal anode is its tendency to non-uniform morphology during the charge process: metal needle-like structures called ‘whiskers’ are forming on the negative electrode surface. Their formation leads to a significant loss of battery capacity after several charge-discharge cycles, meanwhile creating the risk of a short circuit. [1] The problem of lithium uneven deposition hinders the commercialization of rechargeable batteries with lithium metal anode.

According to the scientific literature, one of the key factors affecting the morphology of lithium during electroplating is the residual mechanical stress generated in bulk metal due to the deposition of lithium under the passivation layer (SEI) on the electrode surface. [2] The resulting mechanical stress enhances the diffusion of lithium atoms to the bases of some grains that grow in form of whiskers.

To suppress the growth of needle-like structures, we have proposed to limit the diffusion along the grain boundary and on the electrode surface by adding sodium as an impurity that should be segregated at the grain boundaries and on the lithium metal surface.

Sodium-lithium mixtures with different sodium content were obtained via alloying these metals in inert argon atmosphere. Using scanning electron microscopy, we investigated the distribution of sodium in lithium-sodium mixtures, and studied the influence of sodium adding on the morphology of electrodeposited lithium. It was noted that the minimum on the voltage curve of lithium galvanostatic electrodeposition on pure lithium metal refers to the beginning of secondary nucleation that is followed by whisker growth. In the time before the minimum, the bulging of some surface grains is observed, which is the result of diffusion of lithium atoms to the bases of these grains. We have discovered that the increases in sodium concentration in mixtures leads to the reduction of time before the beginning of whisker growth, which may indicate the blocking of grain-boundary diffusion.

References

1. Liu, He, et al. // EnergyChem. 2019. 1. 1. 100003.
2. He, Yang, et al. // Nature nanotechnology. 2019. 14. 11. 1042-1047.