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Atomistic mechanism of lithiation of nanomaterials as Li-ion battery anodes studied by *in-situ* TEM

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The weak van der Waals interaction between the MoS_2 layers allows alkali ions to intercalate without a significant volume expansion, which enables MoS_2 to be an alternative as an electrode material for high capacity lithium ion batteries. Research on the electrochemical lithiation mechanism of MoS_2 has important significance, both in fundamental studies and practical applications. We recently studied the dynamic electrochemical lithiation process of MoS_2 nanosheets by construction of an *in-situ* TEM electrochemical cell. It is found that MoS_2 undergoes a trigonal prismatic (2H)-octahedral (1T) phase transition upon lithium intercalation. The *in-situ* characterization at atomic scale provides a great leap forward in the fundamental understanding of the lithium ion storage mechanism in MoS_2. MoS_2 by its nature is a semiconductor with trigonal (2H) structure, where the S atoms locate in the lattice position of a hexagonal close-packed structure. Planes of Mo atoms are sandwiched between two atomic layers of S, such that each Mo is coordinated to six S atoms in a trigonal prismatic geometry (2H). Another MoS_2 polytype based on tetragonal symmetry is the octahedral phase (1T) with one MoS_2 layer per repeat unit. A structural transformation of 2H-1T corresponds to the electronic structure change from semiconducting to metallic. In our work, a systematical study has been performed on the structural properties of MoS_2 nanosheets during the lithiation process using an *in-situ* electrochemical TEM holder. The results demonstrate the existence of a phase transition of 2H-MoS_2 to 1T-$LiMoS_2$ and structural modulation in the 1T-$LiMoS_2$ in the first lithiation process. The time-lapse migration of lithiation reaction boundary is shown in the figure below. Furthermore, utilizing the *in-situ* measurements, the electrochemical reaction in each stage has been studied, which can also be correlated with the ex-situ performance of MoS_2 coin-type cells. After the phase transition of 2H-MoS_2 to 1T-$LiMoS_2$, there follows a conversion reaction during the lithiation of MoS_2. So the structural mechanism corresponding to the electrochemical property of MoS_2 during lithiation can be clearly understood. In this talk, our studies on the dynamic lithiation processes of SnO_2 nanowires and silicon nanowires will be also included.

Biography

Xuedong Bai received his PhD degree in 1999 from Institute of Metal Research, Chinese Academy of Sciences (CAS), and then joined Institute of Physics, CAS. He is a Professor of physics. He ever spent two years as a Postdoc in Georgia Institute of Technology, USA, and one year in National Institute for Materials Science, Japan. His research interest is focused on *in-situ* TEM technique and its applications on nano research. He has co-authored over 130 publications, and given over 20 invited talks in international conference. His papers have been cited more than 6000 times and H-factor is 41.

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