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Lithiation of Li_2SnO_3 and Li_2SnS_3 in context of Li-ion battery materials[1] JASON HOWARD, N. A. W. HOLZWARTH, Wake Forest University — The closed pack layered crystal material (space group 15 ($C2/c$)) Li_2SnO_3 has been studied as a possible anode material since the late 1990s.[2,3,4] The material undergoes an irreversible decomposition to Li_2O and Li_XSn alloys during the first lithiation cycle. The crystal material Li_2SnS_3 of the same structure was recently proposed as an electrolyte material.[5] The question is posed whether Li_2SnS_3 would be a good electrolyte or whether it could function as an anode material similar to Li_2SnO_3. In this research a model is proposed for the lithiation process of Li_2SnO_3 and Li_2SnS_3; Li – Li_2SnS_3 interfaces are also examined. The results show Li_2SnO_3 begins to decompose at approximately $Li_{2+0.5}SnO_3$. In Li_2SnS_3 the lithiation process shows it can lithiate to $Li_{2+1}SnS_3$ without significant lattice distortion, volume expansion, or decomposition. Li – Li_2SnS_3 interfaces are shown to be unstable, showing the formation of Li_2S.

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[2]Courtney & Dahn, JES **144**, 2045(1997)
[3]Zhang et al., J. Alloy compd. **415**, 229(2006)
[4]Wang et al., Surf. Interface Anal. **45**, 1297(2013)
[5]Brant et al., Chem.Mater. **27**,189 (2015)

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