

Atomistic insights into the conversion reaction in iron fluoride: A dynamically adaptive force field approach

Scientific Achievement

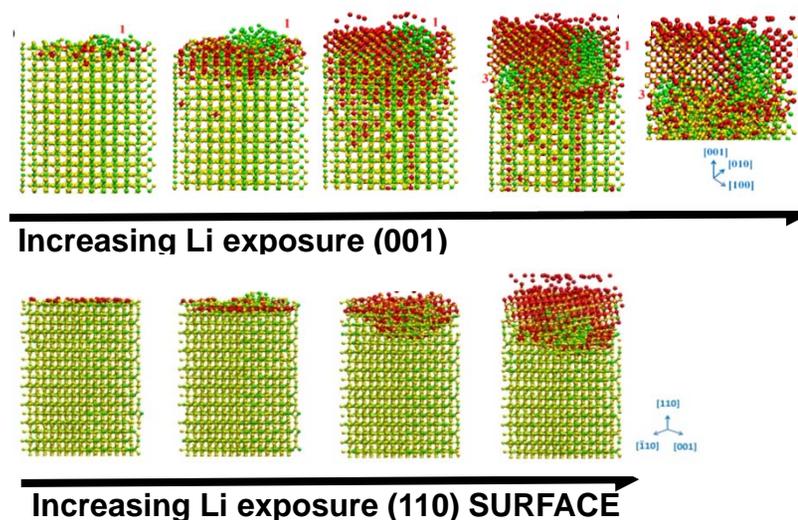
By developing and applying a dynamically adaptive force field, the local structures and phase growth mechanism on two different low-energy FeF_2 surfaces exposed to Li have been identified in molecular simulations. The different reaction pathways are observed, with the reaction on the (110) surface being significantly more self-limiting.

Significance and Impact

The simulations allow for the change in the valence of the Fe from the +2 state in the FeF_2 crystal to the metallic state in the metal particles during the reaction. The resultant structures are similar to the TEM data, but provide atomistic details that offer the explanation for the observed need for nanoparticle starting sizes and slow rates.

Research Details

Local Li concentration plays a key role in driving the conversion reaction through amorphous reaction products to the final crystalline product phases of LiF and Fe^0 . The amorphous phases predicted in these simulations were corroborated in experiments by partners in this EFRC. Rapid transport paths along the [001] direction, but not the [110] (nor [100]), provide differences in the extent of reaction.



FeF_2 crystal surfaces ((001) and (110)) (green, yellow) exposed to Li^+ ions (red) as a function of exposure time showing the conversion reactions and crystalline products of Fe metal and LiF via an amorphous phase.

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