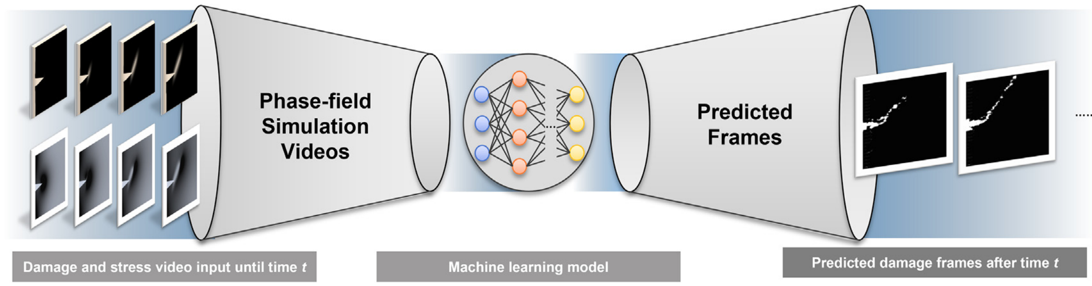

Figure 1. Overall workflow

The machine learning model replaces the simulation model by generating image frames after time t. A ConvLSTM neural network takes the damage and stress video frames simulated by a PF simulation as inputs and predicts damage progress in future video frames. The deep learning model provides a means of accelerated failure detection based on the previous sequence of dynamic time-correlated images.

et al.[22] proposed a surrogate model that learns the microstructural evolution of targeted systems by combining statistically representative, low-dimensional description of the PF data and history-dependent ML techniques. The high-dimensional microstructural representation given by the microstructure autocorrelations is simplified though principal component analysis and then modeled using a long short-term memory (LSTM) neural network to accelerate the PF framework. Alhada-Lahbabi et al.[23] presented a neural-network-trained model, which includes supervised and nonsupervised learning of Landau energy landscapes for ferroelectric PF modeling and predicts the polarization field evolution in the microstructure determining the electrostatic and mechanical equilibrium at each time step.

In this article, we create an ML video processing model to predict crack formation, gain a deeper understanding of the failure process, and provide a means of early failure detection through approximation of a segment of a multi-physics PF simulation video sequence. It is worth nothing that our purpose is not to build a computation-accelerating surrogate model to replace or complement the PF simulations, but instead to treat the PF output as realistic proxies of physical microscopy video data. In this context, the PF simulation introduces a pre-notch or pre-crack to emulate crack nucleation arising from the presence of surface defects. Our purpose is to develop a method that could be applicable, should the *operando* optical, scanning transmission X-ray, or electron microscopy video sequences that afford clear contrast mechanisms for imaging fracture become available such as to enable real-time battery control. The key findings reported in this paper thus correspond to video prediction rather than the improvement of surrogate models of PF simulations. The design of the model structure developed here does not explicitly encode any specific physics domain knowledge derived from partial differential equations used in the PF simulations nor does it adapt to the shape of any initial notch if there is one. The predictions of crack initiation and propagation are made based on the damage field and stress field simulation rather than a specific geometry. We instead examine the ability of the model to reveal the spatial-temporal evolution of inelastic deformation and fracture.

Our model is a deep learning (DL) model, which arguably is among the most common approaches for learning features directly from raw video/image data. Hochreiter and Schmidhuber[24] proposed a recurrent neural network with feedback connections—the LSTM network—which has been increasingly used to solve the time-series prediction problem. To learn good video representations, Srivastava et al.[25] used a composite model consisting of an autoencoder and a future predictor based on LSTMs. Lew et al.[26] applied a ConvLSTM-based model to physics-based molecular modeling (MD) simulations to learn the spatiotemporal relations of crack propagation. Wang et al.[27] developed a DL model, StressNet, to predict the sequence of maximum internal stress by combining a temporal-independent convolutional neural network and bi-directional LSTM. Despite recent advances, the use of DL models with multi-source data to predict the propagation of fracture patterns in materials remains limited. In this paper, we report our effort that builds a ConvLSTM neural network to predict damage initiation and propagation using the damage information along with internal stress information output from the PF simulations; see Figure 1.

RESULTS

Crack formation in lithiation process

Crack nucleation and growth phenomena can follow a wide variety of patterns, as exemplified by experimental data shown in Figure 2 for a single crystal of a canonical intercalation host, α-V_2O_5. Three lithiation/delithiation cycles led to crack expansion as well as new secondary crack formations branching from previously formed cracks present before lithiation in α-V_2O_5. Cracks present before lithiation provide a means for the Li-ion flux to engender local lattice expansion and contractions, which results in crack propagation and formation of secondary cracks, exposing new surfaces for interaction with the electrolyte (Figures 2A–2C). We note that crack propagation occurred perpendicular through stair-step layers due to increased flux during lithiation/delithiation processes (Figures 2D–2F) as seen before for another 2D-layered insertion host γ'-V_2O_5.[28] Similarly, lithiation-induced flux across crack formations formed from deintercalation processes can lead to crack formations post-lithiation perpendicular to the pre-lithiation crack (Figures 2G–2I). Such lithiation-induced cracks form due to the brittle nature of V_2O_5 where lattice expansion and contraction especially across phase boundaries lead to elastic misfit and crack formation/propagation.