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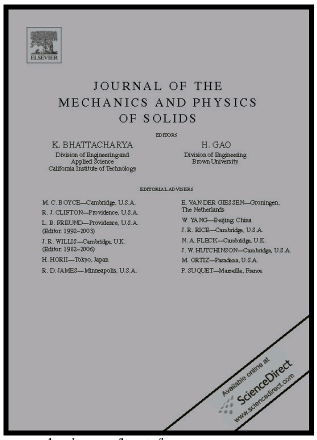

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Model for Charge/Discharge-Rate-Dependent Plastic Flow in Amorphous Battery Materials

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Abstract

Plastic flow is an important mechanism for relaxing stresses that develop due to swelling/shrinkage during charging/discharging of battery materials. Amorphous high-storage-capacity Li-Si has lower flow stresses than crystalline materials but there is evidence that the plastic flow stress depends on the conditions of charging and discharging, indicating important non-equilibrium aspects to the flow behavior. Here, a mechanistically-based constitutive model for rate-dependent plastic flow in amorphous materials, such as Li_xSi alloys, during charging and discharging is developed based on two physical concepts: (i) excess energy is stored in the material during electrochemical charging and discharging due to the inability of the amorphous material to fully relax during the charging/discharging process and (ii) this excess energy reduces the barriers for plastic flow processes and thus reduces the applied stresses necessary to cause plastic flow. The plastic flow stress is thus a competition between the time scales of charging/discharging and the time scales of glassy relaxation. The two concepts, as well as other aspects of the model, are validated using molecular simulations on a model Li-Si system. The model is applied to examine the plastic flow behavior of typical specimen geometries due to combined charging/discharging and stress history, and the results generally rationalize experimental observations.

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