MULTISCALE MODELING SCHEMES SPANNING A LARGE RANGE OF SCALES

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In this work, we present effective multiscale modeling schemes in the interdisciplinary field of solid mechanics and materials science for a large range of scales. The proposed multiscale modeling scheme should be able to carry out analyses spanning micro/meso/macroscopic scales of a continuum and be able to bridge atomistic and continuum scales so that variables such as stress, strain, electric field and electric displacement at different scales can be quantitatively correlated; thereby improving our understanding of the salient features that govern various types of material behavior over a large range of scales.

Though scientists and engineers have realized for a long time that the properties of materials follow from both their atomic and microscopic structures and that failure has its origins at the microscopic and atomistic scales, multiscale analysis remains in its infancy. The efforts so far have been mostly limited to describing relationships of variables at different scales qualitatively rather than quantitatively. The existing quantitative efforts have been limited to analyses that either span only two scales or require extremely intensive calculations due to a lack of effective methodology[1].

The proposed idea of multiscale analysis in the continuum realms is to use the medium of the intermediate scale as a means to connect variables at the lower scale with those at the upper scale through developing equivalent constitutive equations. These equations of the homogenized intermediate medium can be used to connect the variables between the intermediate scale and upper scale through a self-consistent scheme or mean field theory. These equations are developed based on microstructures of the lower scale through making the variables satisfy corresponding physical, chemical and mechanics principles. Therefore, there would be two features of the intermediate medium, with one being a homogenized feature that connects to the upper scale, and the other being a realistic feature, which connects to the lower scale, making quantitative connections of variables between the three scales possible.

Figure 1 shows the comparison between experiments and the simulation results for the size effects on cyclic creep (ratcheting) obtained by the multiscale modeling across micro/meso/macro scales in which specimens with layer thicknesses of 267, 287 and 319 nm of pearlitic high carbon steel were used. The different sizes were obtained by changing the cooling rate of heat-treatment temperature from 860 ^{0}C to room temperature. This success in incorporation of size effects in multiscale modeling has been obtained by introducing a dislocation model for developing size laws of material parameters. The dislocation model used is derived from the solution of Eshelby et al. [2]. From the size laws we found that the Hall-Petch relationship is valid, and most importantly that the kinematic hardening material parameters depend even more on the layer thickness.

In the realm of joint atomisticc and continuum scales, a mixed particle and molecular dynamics (MD) method will be coupled with quantum methods. The particle method is used to lump many atoms together as a molecular particle to reduce degrees of freedom in the low-stress gradient region which has been originally proposed in [3]. This lumped molecular particle can further connect to structure particles that are used in mesh-free finite element analysis to make the transition from the atomic scale to the continuum possible. For ferroelectric materials a polarized quasi-particle pair that forms a particle dipole should be used.

Figure 2 shows the simulated strain-electric field and electric displacement-electric field behavior of a single crystal of PLZT and the composite by the proposed micro/meso/macro/structural modeling schemes. Here micro corresponds to domain scale, meso to single crystal, macro to polycrystal, and structural to layered ferro-plastic composites. For single crystal ferroelectric material, the well-known nonlinear butterfly curve is successfully simulated and, the effect of volume fraction of ferroelectric

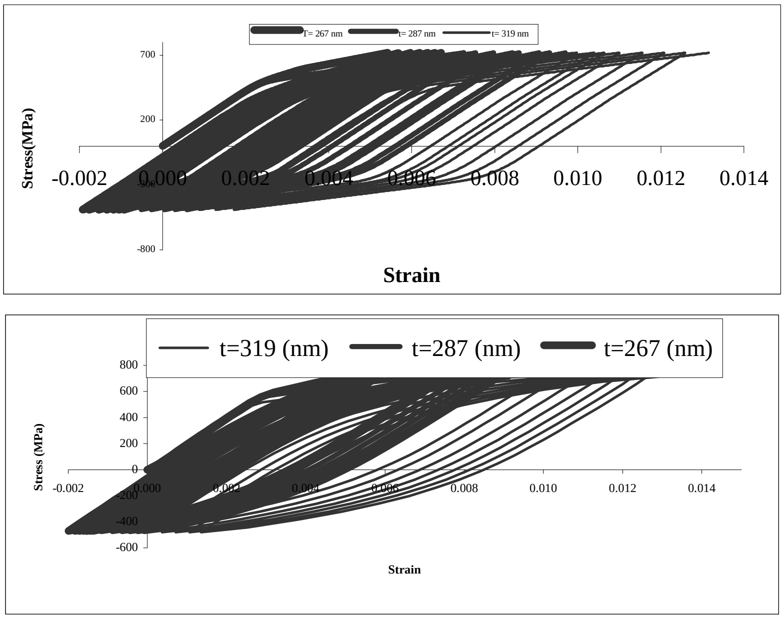

Figure 1: A Comparison between calculated results of three-scale simulation for cyclic creep (ratcheting) of high carbon rail steel specimens of layer thickness t= 319, 287 and 267 nm: (a) Experimental results; (b) Three-scale simulation

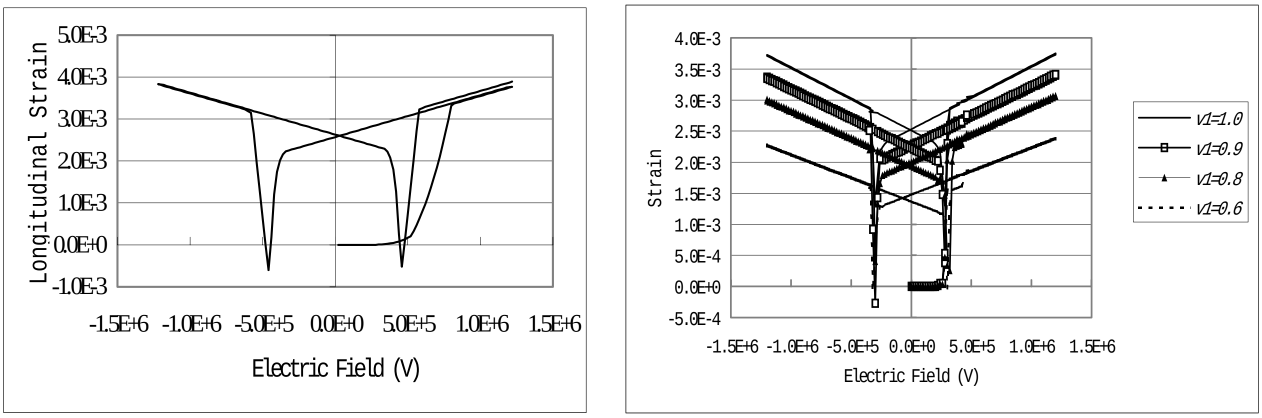

Figure 2: Curves of strain versus electric field: (a) single crystal; (b) ferroelectric-polymer layer composites where v1 indicates the volume fraction of ferroelectric ceramics

ceramics to performance of ferroelectric-polymer layer composites is well described.

Several significant findings resulted. These findings offer additional knowledge to both material behavior and failure mechanisms, proving the value of the proposed methodology and size laws.

Reference

[1]. R. E. Rudd and J. Q. Broughton (2000), Concurrent coupling of length scales in solid state systems, *Phys. Stat. Sol.* (b) **217**, 251-291.

[2].Eshelby, J. D., Frank, F. C. and Nabarro, F. R. N. 1951 The equilibrium of linear arrays of dislocations. *Philosophical Magazine* **42**, 351-364.

[3]. S. Hao, W. K. Liu, G. B. Olson, B. Moran, (2003) " Multi-Scale Constitutive Model and Computational Framework for the Design of Ultra-High Strength, High Toughness Steels", Presented in Plasticity-2003, Quebec; accepted by "Computer Method in Applied Mechanics and Engineering".