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RECENT ADVANCES IN DEVELOPING A UNIFIED MULTISCALE SIMULATION PROCEDURE FOR SINGLE CRYSTAL MATERIALS

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ABSTRACT

As can be found from the open literature, much research has been conducted worldwide to investigate the rate-dependence and size-dependence of material properties, respectively. However, the focus has usually been on the scale effect in the spatial domain with the loading rate being assumed to be quasi-static. Based on the experimental and computational capabilities available, an attempt has been made recently to formulate a hyper-surface in both spatial and temporal domains to predict combined specimen size and loading rate effects on the mechanical properties of single crystal materials [1-3].

To evaluate the integrity and safety of MEMS/NEMS devices under extreme loading conditions, it now becomes necessary to understand the structural responses at different sizes under various temperatures and loading rates. Although material properties are rate-, size- and temperature-dependent in nature, little has been done in exploring combined rate, size and thermal effects on the material responses, as can be seen from the open literature. For example, the research focus for blast, impact and penetration problems has been on the effects of strain rate and temperature with the size effect in the spatial domain being neglected. Atomistic simulations are an important part in studying multiscale structural responses. However, the length and time scales that can be probed by the atomic level simulations are still fairly limited due to the limitation of existing computational hardware and software. Not only the loading rate but also the specimen size used in the current molecular dynamics (MD) simulation can not be handled by the existing experimental techniques. With or without the consideration of thermal effects, a specimen of finite size is usually employed in the bar and plate impact experiments to investigate the rate-dependent mechanical properties under the loading rate which is

way below what is used in the MD simulation as reported so far. Hence, there exists an urgent need for developing a multi-scale model that could bridge the different spatial and temporal scales between atomistic simulations and available experiments at various temperature levels.

Based on the previous research results, hence, efforts have been made recently to establish a hyper-surface to model combined size, rate and temperature effects on the material properties of single crystal specimens [4]. It appears from the preliminary results that the proposed procedure might provide an effective means to bridge different spatial and temporal scales in a unified multiscale modeling framework at different temperatures. Since the loading path and crystal orientation also play a very important role in characterizing the size effect [5], further research is required to improve the formulation of hyper-surface for general applications.

In this conference, recent advances in developing a unified approach for multiscale model-based simulation of MEMS/NEMS responses under extreme loading conditions will be presented, based on available computational and experimental capabilities. Especially, the effects of loading path and history on material properties will be explored. Since the size effect is the key component in developing nano technologies, the recent investigations on the size effect in bio-nano interaction [6] and energy generation [7] will also be introduced. Although the physical, chemical and biological phenomena involved appear to be different, there might be a correlation among these seemingly different problems from the viewpoint of the interactions across various scales.

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