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RECENT EFFORTS IN MODELLING COMBINED RATE, SIZE AND THERMAL EFFECTS ON SINGLE CRYSTAL STRENGTH

Zhen Chen[1], Luming Shen[2], Hui-Hui Dai[3] and Yong Gan[1]

[1]Department of Civil and Environmental Engineering,University of Missouri-Columbia, Columbia, MO 65211-2200, USA
[2]Department of Civil Engineering,Clayton Campus, Monash University, VIC 3800, Australia
[3]Department of Mathematics and Liu Bie Ju Centre for Mathematical Sciences,City University of Hong Kong, Kowloon Tong, Hong Kong, China

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Abstract. The understanding of structural responses at different sizes under various temperatures and loading rates is essential to evaluating the integrity and safety of MEMS/NEMS devices in an extreme environment. Based on the experimental and computational capabilities available, an effort has been made recently to formulate a hyper-surface in spatial, temporal and thermal domains to model combined rate, size and thermal effects on single crystal strength. 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 modelling framework at different temperatures. To further improve the proposed procedure, a mathematical analysis on the hyper-surface formulation, and the progress in investigating the effects of loading path and crystal orientation on the hyper-surface are presented, and future research tasks are discussed in this paper.

1. INTRODUCTION

As can be found from the open literature, much research has been conducted in the world to investigate the rate-dependence and size-dependence of material properties, respectively. However, the focus has been on the scale effect in the spatial domain with the loading rate being assumed to be quasi-static, as shown by the representative references [1-5]. The recent interests in developing multiscale model-based simulation procedures [6-8, among others] have brought about the challenging tasks of bridging different spatial and temporal scales within a unified framework. 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 [9].

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 investigating 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, as shown by the representative references [10-12]. 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. As can be found from the literature review related to the impact mechanics and shock physics [13-16, among others], 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

Corresponding author: Zhen Chen, e-mail: chenzh@missouri.edu

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 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 macroscopic experiments at various temperature levels.

Based on the previous research results [9,17-19], hence, an attempt has been made recently to formulate a hyper-surface in spatial, temporal and thermal domains to model combined size, rate and temperature effects on the material properties of single crystal tungsten (W), which has been verified by the available experimental data [20]. 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 modelling framework at different temperatures. To further improve the proposed procedure, a mathematical analysis on the hyper-surface formulation and the meaningful range of parameter values are presented in this paper. The remaining sections of the paper are organized as below. The hyper-surface formulation is briefly described in Section 2, followed by a mathematical analysis and discussion in Section 3. The recent progress in investigating the effects of loading path and crystal orientation on the hyper-surface is introduced in Section 4. Finally, concluding remarks and future research tasks are discussed.

2. FORMULATION OF A HYPER-SURFACE IN SPATIAL, TEMPORAL AND THERMAL DOMAINS

To better demonstrate the formulation of a hyper-surface in combined spatial, temporal and thermal domains, a brief description of the previously developed model with size and rate effects [9] is given first. Note that the material strength model in Subsection 2.1 is formulated at room temperature of T_0 = 298K without considering the thermal effect.

2.1. Combined rate and size effects

As shown in an asymptotic scaling analysis without considering the rate effect [1], the relationship between the nominal strength σ_N and different sizes D of geometrically similar structures exhibits a two-sided asymptotic support, namely, the small-size asymptotic limit and large-size asymptotic limit. Hence, a simple set of equations is chosen to represent the size effect on the quasi-static strength σ_0 in the spatial domain [9], as follows:

$$\begin{cases} \sigma_0 = \sigma_u & D \le D_u \\ \log\sigma_0 = \log\sigma_m + (\log\sigma_u - \log\sigma_m)\left[1 - \right. & \\ \left. -\sin\left(\dfrac{\pi(\log D - \log D_u)}{2(\log D_m - \log D_u)}\right)\right] & D_u < D < D_m, \\ \sigma_0 = \sigma_m & D \ge D_m \end{cases} \quad (1)$$

where D_u is the specimen size at which the ultimate strength (ideal strength) σ_u is reached, and D_m the minimum macro-scale size beyond which the strength σ_m becomes size-independent.

To describe the dependence of the material strength on the strain rate $\dot{\varepsilon}$, a simple model proposed by Cowper and Symonds [21] is adopted as follows:

$$\frac{\sigma(\dot{\varepsilon})}{\sigma_0} = 1 + \left(\frac{\dot{\varepsilon}^p}{\dot{\varepsilon}_r}\right)^{1/q}, \quad (2)$$

in which $\dot{\varepsilon}^p$ denotes the plastic strain rate, and $\dot{\varepsilon}_r$ and q are two model parameters that can be determined with two experimental data points of $\sigma(\dot{\varepsilon})$. As compared with the plastic strain, the elastic strain can be neglected so that $\dot{\varepsilon}^p = \dot{\varepsilon}$ could be assumed. To include the size effect into Eq. (2), the model parameters $\dot{\varepsilon}_r$ and q are considered to be functions of size D. A two-sided asymptotic support from both continuum and atomic level studies is used to derive functions $\dot{\varepsilon}_r(D)$ and $q(D)$, namely,

$$\frac{\log\dot{\varepsilon}_r - \log\dot{\varepsilon}_{rl}}{\log\dot{\varepsilon}_{rs} - \log\dot{\varepsilon}_{rl}} = 1 - \sin\left(\frac{\pi(\log D - \log D_{rs})}{2(\log D_{rl} - \log D_{rs})}\right), \quad (3.1)$$

$$\frac{q - q_l}{q_s - q_l} = 1 - \sin\left(\frac{\pi(\log D - \log D_{rs})}{2(\log D_{rl} - \log D_{rs})}\right), \quad (3.2)$$

for $D_{rs} < D < D_{rl}$ with D_{rs} and D_{rl} being the specimen sizes at the small-size asymptotic limit and large-size asymptotic limit, respectively. For $D \ge D_{rl}$, one has $\dot{\varepsilon}_r = \dot{\varepsilon}_{rl}$ and $q = q_l$, while for $D \le D_{rs}$, one has $\dot{\varepsilon}_r = \dot{\varepsilon}_{rs}$ and $q = q_s$. It follows from Eqs. (1) - (3) that the model with combined size and rate effects takes the form of

$$\sigma(\dot{\varepsilon}, D) = \sigma_0(D)\left[1 + 10^{\left(\frac{1}{q(D)}(\log\dot{\varepsilon} - \log\dot{\varepsilon}_r(D))\right)}\right] \quad (4)$$

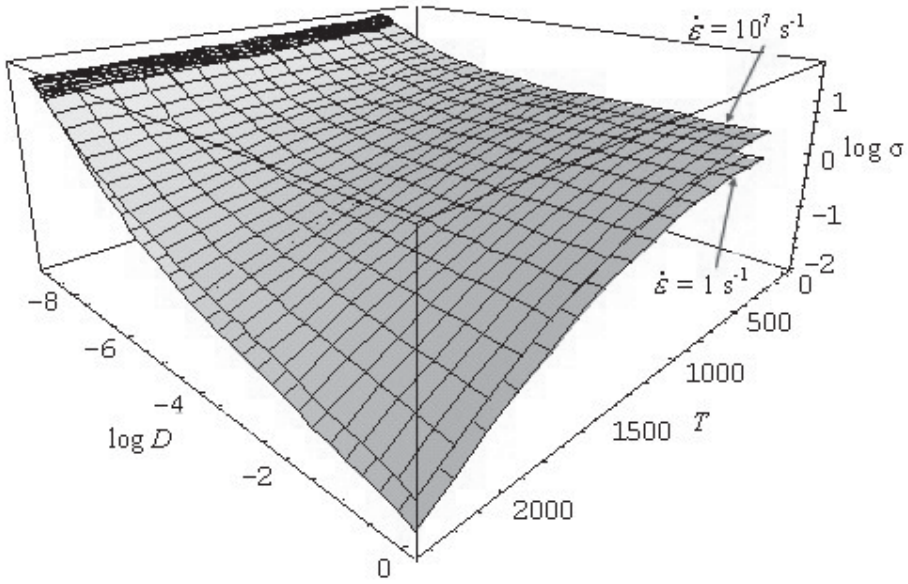

Fig. 1. Surfaces in log$D$ (m)-T(K)-logσ (GPa) space at strain rates of $\dot{\varepsilon}$ = 1 s^{-1} and 10^7 s^{-1}, respectively.

in the $\dot{\varepsilon}$ - D - σ space. In Eq. (4), parameters $\dot{\varepsilon}_r(D)$ and $q(D)$ are determined from Eq. (3), and quasi-static strength $\sigma_0(D)$ is defined by Eq. (1).

2.2 Formulation of the hyper-surface

From the preliminary MD simulation results, it seems that the temperature and rate effects are co-related since the critical strain rate decreases with the increase of temperature [20]. As adopted in the previous work [10,11,22], however, it is assumed here that the effect of temperature on material strength is not coupled with that of strain rate, although it is size-dependent.

Following the format of Johnson-Cook's thermal softening model [22], a constitutive equation that could effectively predict the strength-temperature relationship of nano-scale specimens is proposed as follows:

$$\log Y(T) = \log Y_0 + \\ +\left(\log Y_{\max} - \log Y_0\right) \times \left(\frac{T - T_0}{T_{\max} - T_0}\right)^{\beta}, \qquad (5)$$

where $Y(T)$ is the material strength at temperature T ($T_0 \le T \le T_{max}$), Y_0 is the strength at room temperature T_0, Y_{max} is the strength at temperature T_{max}, and β is a model parameter. Note that the current model does not consider the temperature effect on the material strength near the melting point. The hyper-surface for material strength as a function of loading rate ($\dot{\varepsilon}$), size (D) and temperature (T) can then be formulated as

$$\log\sigma\left(\dot{\varepsilon}, D, T\right) = \log\sigma\left(\dot{\varepsilon}, D, T_0\right) + \\ +A(D) \times \left(\frac{T - T_0}{T_{\max} - T_0}\right)^{\beta(D)}, \qquad (6)$$

where $\sigma(\dot{\varepsilon}, D, T_0)$, the material strength with given size and rate at room temperature, is calculated by using Eq. (4), and both $A(D)$ and $\beta(D)$ are functions of specimen size D. Similar to the way establishing the size effect on the rate-dependence, a two-sided asymptotic support can also be adopted to develop a size-dependent model for the temperature effect [20]. The thermal-dependent model as defined by Eq. (5) is regarded as the small-size asymptotic limit at atomic-scale, which can be determined via molecular level simulations. At the macroscopic scale, experiments could be performed to find the large-size asymptotic limit.

To demonstrate the proposed 4-dimensional hyper-surface for tungsten material strength in a 3-dimensional space, surfaces in log$D$-T-logσ, log$D$-

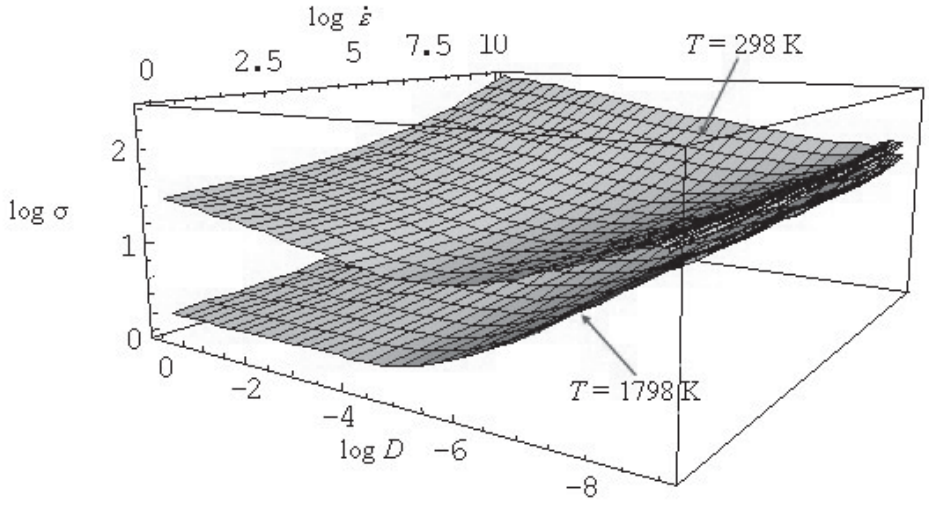

Fig. 2. Surfaces in log$D$ (m)-log$\dot{\varepsilon}$ (s^{-1})-logσ (GPa) space at temperatures of T = 298K and 1798K, respectively.

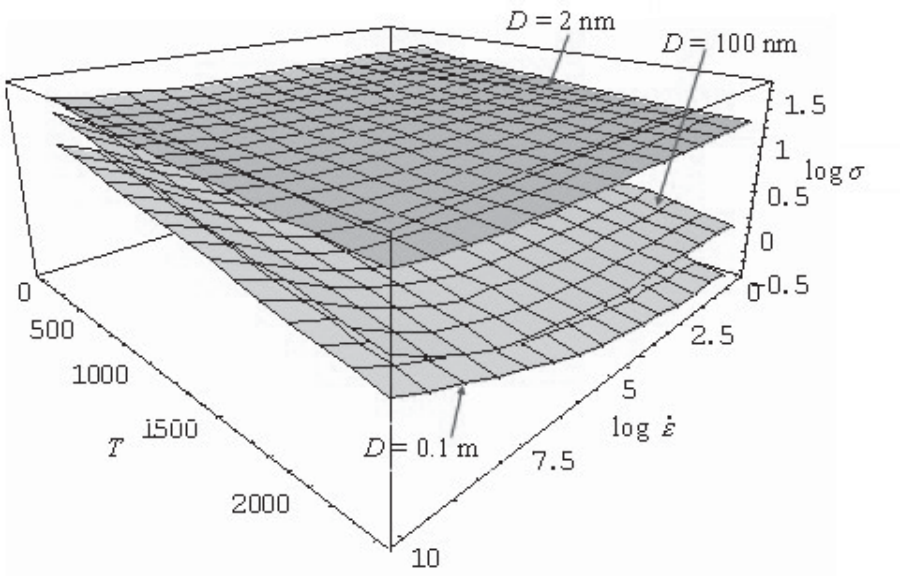

Fig. 3. Surfaces in log$\dot{\varepsilon}$ (s^{-1})-T (K)-logσ (GPa) space at specimen sizes of D = 2 nm, 100 nm and 0.1 m, respectively.

log$\dot{\varepsilon}$-logσ and log$\dot{\varepsilon}$-T-logσ spaces are presented, respectively, in Figs. 1-3. Fig. 1 shows two W strength surfaces as a function of D and T in log$D$-T-logσ space at strain rates of $\dot{\varepsilon}$ = 1 s^{-1} and 10^7 s^{-1}, respectively. Two W strength surfaces as a function of D and $\dot{\varepsilon}$ in log$D$-log$\dot{\varepsilon}$-logσ space at temperatures of T = 298K and 1798K, respectively, are given in Fig. 2. To demonstrate the size effect on the hyper-surface, three W strength surfaces as a function of $\dot{\varepsilon}$ and T in log$\dot{\varepsilon}$-T-logσ space with specimen sizes of D = 2 nm, 100 nm and 0.1 m, respectively, are shown in Fig. 3. As can be seen, the effect of loading rate on W strength is not as significant as those of specimen size and temperature.

3. MATHEMATICAL ANALYSIS OF THE HYPER-SURFACE FORMULATION

It appears from the hyper-surface formulation described above that the hyper-surface could be

uniquely determined via the boundary data, namely, two-sided asymptotic supports in different domains. Also, Figs. 1-3 for tungsten strength demonstrate that the hype-surface is monotonic. As shown below, the proposed hyper-surface is consistent mathematically in the sense that there is neither a maximum nor a minimum in the interior.

Letting $\log\sigma=u$ and $\log D=V$, the use of Eqs. (1), (4) and (6) results in

$$u = u_m + (u_u - u_m)\left\{1 - \sin\left[\frac{\pi(V - V_u)}{2(V_m - V_u)}\right]\right\} + \\ + \log\left\{1 + 10^{\left[\frac{1}{q(D)}\log\frac{\dot{\varepsilon}}{\varepsilon_r(D)}\right]}\right\} + A(D)\left(\frac{T - T_0}{T_{\max} - T_0}\right)^{\beta(D)}, \quad (7)$$

where

$$u_m = \log\sigma_m,\ u_u = \log\sigma_u,\ V_u = \log D_u,\ V_m = \log V_m,$$
$$A(D) = -a_1 \log D - a_2 = -a_1 V - a_2,\ a_1 > 0,\ a_2 > 0,$$
$$\beta(D) = b_1 \log D + b_2 = b_1 V + b_2,\ b_1 > 0,\ b_2 > 0.$$

For a fixed strain rate, it follows that

$$\frac{\partial u}{\partial V} = -\frac{\pi(u_u - u_m)}{2(V_m - V_u)}\cos\left[\frac{\pi(V - V_u)}{2(V_m - V_u)}\right] - \\ -a_1\left[\frac{T - T_0}{T_{\max} - T_0}\right]^{b_1 V + b_2} \\ -(a_1 V + a_2)\left[\frac{T - T_0}{T_{\max} - T_0}\right]^{b_1 V + b_2} b_1 \log\left[\frac{T - T_0}{T_{\max} - T_0}\right], \text{ and}$$

$$\frac{\partial u}{\partial T} = -\frac{(a_1 V + a_2)(b_1 V + b_2)}{T_{\max} - T_0}\left[\frac{T - T_0}{T_{\max} - T_0}\right]^{b_1 V + b_2 - 1}.$$

It can be seen from the above equations that $\partial u/\partial T \neq 0$ if $V \neq -a_2/a_1$ or $-b_2/b_1$ (i.e., $A(D)\neq 0$ or $\beta(D)\neq 0$). On the other hand, a necessary condition for u to have a local maximum or minimum at a point is $\partial u/\partial T = \partial u/\partial V = 0$ at this point. However, it is required in physics that both $A(D)\neq 0$ and $\beta(D)\neq 0$ in the interior of the hyper-surface are satisfied (otherwise, the material strength is independent of the temperature). Thus, it can be concluded that u does not have a local maximum or minimum. In other words, the hyper-surface could be uniquely determined by the boundary data.

4. THE EFFECTS OF LOADING PATH AND CRYSTAL ORIENTATION

Due to the simple formulation of the hyper-surface, the effects of loading path and crystal orientation on the material strength can not be directly predicted. A numerical study is being performed to investigate the size, rate and crystal orientation effects on the mechanical properties along different loading paths. As a first example, mechanical responses of single crystal diamond (SCD) blocks with three different sizes under <100> and <110> tensions, and under {100}<010>, {100}<110> and {110}<001> shear slips at different loading rates have recently been investigated. Most of the simulated initial elastic moduli for SCD blocks decrease with the increase of specimen size due to the effect of the free surface, while all of them are almost rate-independent regardless of crystal orientation and loading path. The corresponding tensile and shear strengths of pristine diamond decrease as the specimen size increases, while the simulated strengths increase with loading rate.

It can be observed from the failure patterns under tensile loading, the failure might occur randomly within the active zone of the simulated SCD block. The specimen breaks almost at one flat surface under <100> tensile loading, while x-shape shear bands can be clearly observed from the SCD block under <110> tensile loading. On the other hand, the shear failure of diamond block mainly occurs in the region near to the boundary zone, and the dislocation initiates at the free surface and evolves into the centre of the SCD block under shear loading regardless of crystal orientation and shear slip system.

5. CONCLUDING REMARKS

The recent efforts in modelling combined rate, size, and thermal effects on single crystal strength are summarized in this paper. Based on the experimental and computational capabilities available, a hyper-surface in spatial, temporal and thermal domains could be formulated to predict combined rate, size and thermal effects on single crystal strength. The proposed hyper-surface is consistent mathematically in the sense that there is neither a maximum nor a minimum in the interior so that it could be uniquely determined with the use of boundary data. 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 modelling framework at different temperatures.

Due to the simple formulation, however, several important factors such as defects, loading path and crystal orientation are not considered in the current version of the hyper-surface. An integrated analytical, experimental and numerical effort is required to further improve the proposed procedure and to advance our knowledge in multiscale structural responses.

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