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Probabilistic Analysis and Design of HCP Nanowires: an Efficient Surrogate Based Molecular Dynamics Simulation Approach

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We investigate the dependency of strain rate, temperature and size on yield strength of hexagonal close packed (HCP) nanowires based on large-scale molecular dynamics (MD) simulation. A variance-based analysis has been proposed to quantify relative sensitivity of the three controlling factors on the yield strength of the material. One of the major drawbacks of conventional MD simulation based studies is that the simulations are computationally very intensive and economically expensive. Large scale molecular dynamics simulation needs supercomputing access and the larger the number of atoms, the longer it takes time and computational resources. For this reason it becomes practically impossible to perform a robust and comprehensive analysis that requires multiple simulations such as sensitivity analysis, uncertainty quantification and optimization. We propose a novel surrogate based molecular dynamics (SBMD) simulation approach that enables us to carry out thousands of virtual simulations for different combinations of the controlling factors in a computationally efficient way by performing only few MD simulations. Following the SBMD simulation approach an efficient optimum design scheme has been developed to predict optimized size of the nanowire to maximize the yield strength. Subsequently the effect of inevitable uncertainty associated with the controlling factors has been quantified using Monte Carlo simulation. Though we have confined our analyses in this article for Magnesium nanowires only, the proposed approach can be extended to other materials for computationally intensive nano-scale investigation involving multiple factors of influence.

Key words: hcp-nanowire; Yield strength; Surrogate; Monte Carlo simulation; Uncertainty; Sensitivity; Optimum design

1. Introduction

Nanoscale analysis has become immensely popular across all fields of research in the last few decades. The fundamental properties of any material such as strength, ductility, creep, fracture behavior, durability etc. can be controlled widely at nanoscale compared to its bulk specimen. Rapid advancements in electron microscopy and other devices that can manipulate materials at nano-scale along with the advancement in computing power are accelerating the progress of nanomaterials research. Numerous nanoscale simulations have been reported over the last two decades [1-7]. These studies reveal that there are several external and internal factors in a material, which affect the mechanical strength. Dislocation plasticity, dislocation movement, grain size, grain geometry and alloying elements control for the strength of a material, can be considered as internal factor while strain rate (*SR*), temperature (*T*) and size (or diameter of nanowire *d*) can be attributed as external factors. We focus on the effect of three external factors that affect mechanical strength in a nanowire. HCP-Magnesium nanowires have been considered in this study for the purpose of analysis. A novel methodology is proposed in the realm of nano-scale research for quantifying relative sensitivity of these three factors by analyzing their relative variances. Subsequently probabilistic analysis has been carried out using Monte Carlo Simulation (MCS) to study the relative coefficient of variation considering randomness in the three factors. Large-scale multiple-simulation ($\sim 10^3$) based statistical approach has been reported in scientific literature for nano-scale analyses that requires carrying out very large number of expensive and time consuming molecular dynamics simulations [8]. We propose a surrogate based molecular dynamics (SBMD) simulation approach where the number of actual MD simulations can be drastically reduced and thereby thousands of virtual simulations can be performed to investigate the material behavior thoroughly in a computationally efficient paradigm. Virtual simulation refers to the surrogate model predictions in this article. Application of the proposed SBMD

simulation approach has enabled us to apply global optimization algorithms in the field of MD simulation based investigations of materials, wherein we have optimized the size of nanowire to maximize the yield strength for different temperatures and strain rates. By implementing the SBMD simulation approach we practically replaced the expensive MD simulations by an efficient mathematical model that facilitates us to conduct a detail and robust analysis on the strength of the nanowire.

In the context of MD simulations there is considerable amount of available literature, where mechanical properties have been studied against variables such as strain rate, temperature or size effect [9-17]. Both temperature and strain rate have also been taken into account together and attempts have been made to carry out quantitative study of all the factors in nanoscale specimens [18-22]. The temperature sensitivity analysis has been carried out by an Arhennius expression [23] which is directly related to the activation energy of a reaction that can be a mechanical, physical or a chemical reaction. Temperature dependence determines the thermal softening of a specimen. Other than temperature, there are factors like work hardening, the strain rate sensitivity that also contribute and determine ductility. Explicit expression has been reported to quantify sensitivity of a single factor (strain rate) on a specific material response [24], but relative sensitivity analyses of multiple factors are still very scarce to find in nano-scale research. Few studies have attempted to correlate certain mechanical properties to cross-sectional size of nanowires by performing a regression analysis to arrive at some empirical formulae [25, 26]. Most of the studies reported so far in scientific literature present the variation of a response quantity of interest with respect to one factor, keeping all other factors constant. In reality all the factors act simultaneously in a process. The relative sensitivity of each controlling factor cannot be truly assessed unless we vary multiple factors simultaneously in an experiment/ simulation. In the proposed analysis of variance approach for sensitivity quantification, we have varied

all the three considered factors simultaneously to quantify their relative sensitivity on the yield strength of the material. This article hereafter is organized as follows, section-2: description of the proposed SBMD simulation approach in details; section-3: Large-scale simulation based results and discussion on the yield strength of HCP nanowires; section-4: conclusion.

2. Surrogate Based Molecular Dynamics (SBMD) Simulation

In this section the proposed SBMD simulation approach is discussed along with the three analyses (sensitivity analysis, optimization and uncertainty quantification) performed for HCP nanowires to comprehensively study the behavior of this material (Fig. 1). Variance based sensitivity analysis has been carried out in conjunction with the SBMD simulation approach for quantifying relative sensitivity of the three considered factors. Variance based sensitivity analysis is a form of global sensitivity analysis that works in a probabilistic framework. It decomposes the variance of output of the system into fractions, which can be attributed to inputs, or sets of inputs [26]. The relative contribution of each of the three input parameters (including the contribution of the interaction terms) to the total model variance is obtained by dividing each individual sum of squares (SS) by the summation of all SS [27, 28]. Percentage relative contributions of variances are designated as sensitivity for different parameters. To achieve computational efficiency, a surrogate modeling approach based on D-optimal design coupled with polynomial regression [27, 28] has been developed in conjunction with MD simulations. On the basis of statistical and mathematical analysis, the surrogate modelling technique gives an approximate and efficient model which relates the input features ξ and output features y for a particular system.

$$y = f(\xi_1, \xi_2, \ldots, \xi_k) + \varepsilon \tag{1}$$

where f denotes the approximate response function and ε is the statistical error term having a normal distribution with mean zero and k is the number of input parameters. ξ is usually coded as

dimensionless variable having mean zero and a standard deviation of ξ. The surrogate model is fit approximately to a set of points in the design space (which may be chosen using design of experiment approach) following a multiple regression fitting scheme. Design of experiments is an efficient algorithm for planning experiments/samples so that the data obtained can be utilized to achieve any particular goal.

D-optimal design is one of the most efficient designs of experiment algorithms requiring fewer samples than standard design procedures and thus it needs much lesser number of molecular dynamics simulations/experiments to be carried out for forming the surrogate model [29]. In this design, position of design points is chosen algorithmically according to the number of factors and the desired model to meet the optimality criteria. Optimal designs can be used to create a good design for fitting a linear, quadratic, cubic or higher order models. There can be several types of optimality criteria such as D-optimality, A-optimality and E-optimality. Let X denotes the design matrix as a set of value combinations of coded parameters and X^t is the transpose of X, then D-optimality is achieved if the determinant of $(X^tX)^{-1}$ is minimal. A-optimality is achieved by minimizing the trace of $(X^tX)^{-1}$. E-optimality is achieved if the largest eigenvalue of $(X^tX)^{-1}$ is minimal. Among these, D-*optimal* design is the most commonly used owing to better accuracy of approximation than others. In D-optimal design, the total sample size (n) comprises of minimum design points (n_d), additional model points (n_a) and lack-of-fit points (n_l) i.e., $n = n_d + n_a + n_l$. The required model points (i.e., minimum design points) is the minimum number of samples to estimate the coefficients for model formation while additional model points are extra samples added by the user to improve precision estimates or coverage of the factor space and lack-of-fit points are the extra points to fill the factor space. The extra information provided by these points can test the fit of the model.

After selection of the design points using D-optimal design algorithm as discussed above, a surrogate model, is constructed following a multiple regression technique, wherein it is assumed that random errors are identically distributed with a zero mean and a common unknown variance and they are independent of each other. The difference between the observed (y) and the fitted value ($\overline{y_i}$) for the i^{th} observation $\varepsilon_i = y_i - \overline{y_i}$ is called the residual. The criterion for choosing the β_i estimates of equation $y=X\beta+\varepsilon$ (Eq. (1)) is that they should minimize the sum of the squares of the residuals, which is often called the sum of squares of the errors (*SSE*) and expressed as,

$$SSE = \sum_{i=1}^{n} \varepsilon_i^2 = \sum (y_i - \overline{y_i})^2 \tag{2}$$

The residuals may be written as

$$\varepsilon = y - X\beta \tag{3}$$

The *SSE* thus becomes

$$SSE = \varepsilon^T \varepsilon = (y - X\beta)^T (y - X\beta) \tag{4}$$

Differentiating the *SSE* with respect to β using partial derivatives and equating it to zero, one can get $X\beta = y$. This over-determined system of equations can be solved directly to obtain the coefficients β as follows

$$\beta = (X^T X)^{-1} X^T y \tag{5}$$

After obtaining the coefficients β as described above, surrogate model can be easily constructed. The major drawback for this form of surrogate modelling is to fit the design points to a second order polynomial, as systems having high degree of nonlinearity cannot be replaced by a second order model. To overcome this lacuna, the data can be converted into another form using suitable

transformation scheme to capture the higher degree nonlinearity. For example, using logarithmic transformation or power transformation the surrogate model takes the following forms,

$$\ln y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \sum_{j>i}^{k} \beta_{ij} x_i x_j + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \varepsilon$$
$$y^n = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \sum_{j>i}^{k} \beta_{ij} x_i x_j + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \varepsilon \quad (6)$$

The quality of a model should be checked based on several criteria. An optimized model is formed by adding or deleting input factors through backward elimination, forward addition or stepwise elimination/addition. It involves the calculation of the *P*-value (probability value, gives the risk of falsely rejecting a given hypothesis) and *Prob. > F* value (gives the proportion of time one would expect to get the stated *F*-value if no factor effects are significant). The surrogate model constructed should be checked by some criteria such as R^2 (A measure of the amount of variation around the mean explained by the model), R_{adj}^2 (A measure of the amount of variation around the mean explained by the model, adjusted for the number of terms in the model. The adjusted R-squared decreases as the number of terms in the model increases if those additional terms don't add value to the model) and R_{pred}^2 (A measure of the prediction capability of the model) expressed as follows.

$$R_{pred}^2 = \frac{SS_R}{SS_T} = 1 - \frac{SS_E}{SS_T} \qquad (0 \le R^2 \le 1) \quad (7)$$

$$R_{adj}^2 = 1 - \frac{SS_E / (n-k-1)}{SS_T / (n-1)} = 1 - \frac{(n-1)}{(n-k-1)}(1-R^2) \qquad (0 \le R_{adj}^2 \le 1) \quad (8)$$

$$R_{pred}^2 = 1 - \frac{PRESS}{SS_T} \qquad (0 \le R_{pred}^2 \le 1) \quad (9)$$

where $SS_T = SS_E + SS_R$ is the total sum of square and *PRESS* is the predicted residual error sum of squares, which is a measure of how the model fits the samples in the design space. The values of R^2,

R^2_{adj} and R^2_{pred} should be close to 1. A difference between R^2_{adj} and R^2_{pred} within 0.2 indicates that the model can be used for further prediction. Another check is Adequate precision, which compares the range of the predicted values at the design points to the average prediction error. In general, a value greater than four indicates adequate model. Further, some plots should also be checked such as normal plot of residuals (indicates whether the residuals follow a normal distribution, in which case the points will follow a straight line), residuals vs. predicted plot (plot of the residuals versus the ascending predicted response values), actual vs. predicted plot (A graph of the actual response values versus the predicted response values for the design points used for meta-model formation. It helps to detect a value, or group of values, that are not easily predicted by the model) and Box-cox plot (helps to determine the most appropriate power transformation to be applied to response data).

3. Results and Discussion

In this section we have discussed details about surrogate model formation including validation of the model with respect to original data and thereby results on the surrogate based analysis of HCP nano-wire. For surrogate model formation, we have chosen ranges of the controlling factors on the basis of available literature as: *SR* [10^7 s^{-1}, 10^{10} s^{-1}], *T* [200 K, 600 K] and *d* [4 nm, 12 nm]. From this analysis domain, we have algorithmically selected 21 efficient combinations of the three controlling factors using D-optimality criteria and thereby the yield strength of the nanowire have been evaluated corresponding to each of the combinations using MD simulations (Table 1). On the basis of these 21 design points (thus 21 MD simulations) a surrogate model has been formed which effectively eliminates the need of any further MD simulation to obtain the yield strength of the nanowire corresponding to any arbitrary combination of the three controlling factors within the design space. Description about the molecular dynamics simulations is furnished next. The atomistic simulations

have been performed in LAMMPS [30], visualized in OVITO [31] and Atom Eye [32]. The embedded atom potential used for the simulation was developed by Sun *et al.* [33]. Initially we ran equilibration run for checking the stability of the nanowires are various temperature keeping all three direction periodic and under NPT ensemble. After this we change the boundary condition to be periodic in *Y* & *Z* directions and applied different constant strain rate in *X* direction where free boundary condition is applied. For all the MD simulations that have been performed, the stress-strain relationships are found to be similar to each other in nature. HCP metals usually need twinning to accommodate plastic deformation in addition to dislocation slip due to their lack of sufficient slip systems (Only 3 in {0 0 0 1} Mg). A typical stress-strain curve indicating different stages (I, II, III, IV) in the deformation process along with formation of slip planes is shown in Fig. 2(a, b). Fig. 3 shows the prediction capability of the surrogate model with respect to actual MD simulation considering multiple points; wherein less deviation of the tested points from the diagonal line indicates high accuracy of the model. The R^2, R^2_{adj} and R^2_{pred} values of the constructed surrogate model have been found to be close to 1, indication validity of the model further.

The sensitivity analysis results for individual and interaction effects on the basis of the aforementioned approach are presented in Fig. 4(a). The figure reveals that the strain rate is the most sensitive factor for the yield strength of the nano-wire, followed by temperature and size. Among the interaction effects, the terms containing both strain rate and temperature are most sensitive, while sensitivity of the size effect is relatively lesser. In an earlier study on polycrystalline graphene, strain rate has also been identified as one of the most influential factors for fracture strength [34, 35]. Thus, along with the findings of the present study, strain rate can be regarded as one of the most influencing factors for mechanical behavior of nano-scale materials.

It is always necessary to understand a material's behavior under certain conditions so that we get necessary information for using the material as a component in nano-mechanical application [36-38]. The materialistic information can be extracted from multiple set of repetitive experimentation/ computation or we can adopt a statistical method. We have carried out MCS using the surrogate model to analyze effect of the three controlling factors (with 10,000 samples for each case) on the yield strength in a probabilistic framework. The probability density function (pdf) for random variation of the controlling factors following a uniform distribution is presented in Fig. 5 considering both individual and combined effects. We have performed 40,000 virtual experiments for MCS using the SBMD simulation based approach by actually carrying out only 21 expensive MD simulations. It is interesting to notice that the probabilistic characteristics of yield strengths follow a normal distribution (Fig. 5), even though distribution of the controlling factors has been considered as uniform. Relative coefficient of variation (RCV) [39] obtained from the MCS results for the three factors are shown in Fig. 4(b). RCV provides a quantitative idea about relative importance of the controlling factors on the response of interest. The relative sparsity in the pdf plots and RCV for different factors are in good agreement with the sensitivity analysis results of Fig. 4(a).

Fig. 6(a, b) presents a deterministic analysis on the variation of the yield strength with size for different temperatures and strain rates respectively. From the figures, it is possible to clearly identify maximum and minimum yield strength for different combinations of size temperature and strain rate. This plot will provide a comprehensive understanding about the material behavior for subsequent analysis and design. It has been possible to present such a rigorous analysis on the yield strength only because of adopting the SBMD simulation based approach that facilitates us to carry out numerous virtual experiments for different combinations of the input parameters instead of performing actual MD simulations thousands of times.

The primary aim of any experiment or computational study related to strength of material is to search an optimum configuration of controlling factors for maximizing the strength. However, direct implementation of any standard global optimization algorithm in the realm of nano-scale simulation/experiment is very scarce because of the fact that these algorithms generally follow an iterative search procedure requiring large number of function evaluations. The expensive nature of the MD simulations makes it difficult to carry out such a huge number of simulations. We have proposed a surrogate based approach to mitigate this lacuna in the context of this problem, wherein practically huge number of function evaluations can be carried out utilizing only 21 MD simulations. We have applied Genetic algorithm [40-42] to optimize the size of the nano-wire (a controllable factor) for maximizing the strength considering different strain rates and temperatures. Optimized yield strength is plotted with respect to strain rate for different temperatures in Fig. 7. There exists a critical strain rate ($5.15 \times 10^9\ s^{-1}$), below which the optimized diameter of the nanowire is 4 nm (i.e. the lower range of size in the design domain) and above which the optimized diameter ranges within 10.09 nm to 10.60 nm for all temperatures. This finding is in good agreement with the plots of Fig. 6(a, b), where two peaks of the yield strength can be spotted for the same values of the diameter.

There is always some degree of uncertainty associated with the controlling parameters in actual implementation/experimentation. This in turn affects the response quantity of interest (yield strength in the present study). Literature concerning the quantification of uncertainty in nano-scale investigations based on molecular dynamics simulation is very scarce. The main reason behind this is the fact that uncertainty quantification following a non-intrusive Monte Carlo simulation approach is computationally very expensive and time consuming. The present SBMD approach is capable of mitigating this lacuna effectively. To explore the effect of uncertainty, we have performed MCS (using 10,000 simulations in each case) with different degree of randomness (Δ) in the controlling factors

with respect to optimized configuration of the nanowire. Representative results of the uncertainty analysis are furnished in Fig. 8, which shows the response bounds and distribution of yield strength with increasing degree of randomness in the controlling factors. The mean value of yield strength is found to decrease with the increase in temperature. For a particular temperature, response bounds and standard deviations are found to increase with increasing degree of stochasticity, while the variation in the mean values is marginal. From the significant variability in yield strength due to stochastic input parameters, it is quite evident that the effect of uncertainty should be accounted in the investigation of HCP nano-wires for precise analysis and design of the system. Following the proposed SBMD simulation based approach, optimization can be performed in an efficient manner considering the uncertainties associated with the system parameters.

4. Conclusion

A critical analysis on yield strength of HCP magnesium nano-wires following an efficient SBMD simulation approach is presented in this article. The proposed SBMD simulation approach in nano-scale has enabled us to carry out large-scale simulation based analyses in a computationally efficient way and subsequently furnish new results for deterministic as well as stochastic analyses concerning yield strength of the material. Sensitivity of the three controlling factors (strain rate, temperature and size) on the yield strength has been quantified considering simultaneous variations of all the three factors, wherein strain rate has been identified as the most sensitive factor followed by temperature and size. Deterministic studies have been performed on the basis of numerous virtual simulations to characterize strength of the nano-wire in its full inherent complexity. Subsequently a probabilistic analysis has been carried out to explore the effect of inevitable uncertainty associated with the controlling design parameters using Monte Carlo simulation. Probabilistic description of yield strength has been presented considering individual as well as combined variation of stochastic input

parameters. Thousands of different combinations of the controlling factors have been considered throughout the study to obtain corresponding yield strengths for different analyses using only 21 actual MD simulations by following the SBMD simulation approach. Application of the proposed methodology enables us to predict the strength of the nanowire within a continuous domain of the controlling factors by obtaining a complete map/bridge between the design parameters and the response to find an optimized configuration for maximizing the yield strength. The number of input factors to explore their effect on the responses of HCP nano-wires can be increased in future investigations. This will however increase the required number of actual molecular dynamics simulations marginally. The efficient SBMD simulation approach is general in nature and therefore, it can be extended to other problems in the realm of nano-scale analysis.

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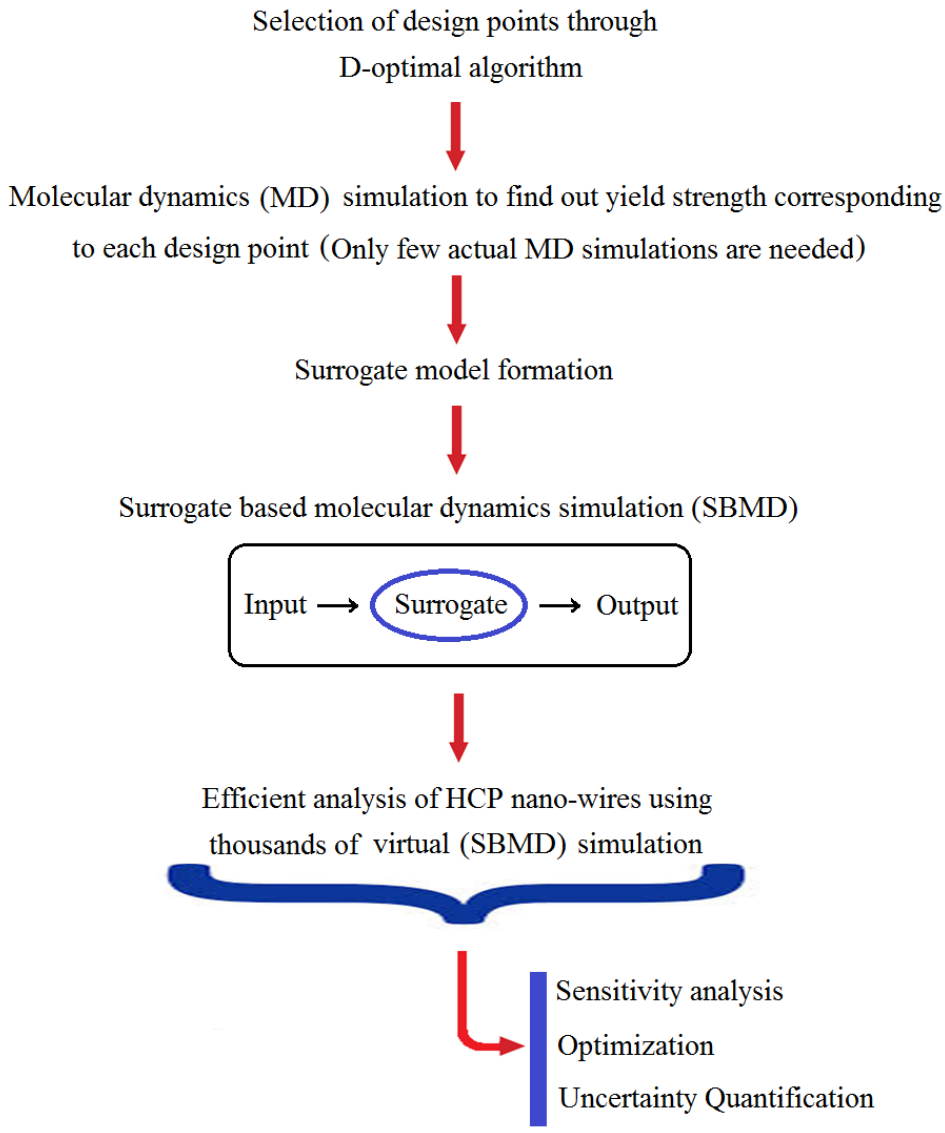

Fig. 1: Surrogate based molecular dynamics (SBMD) simulation approach for efficient but comprehensive analysis of HCP nanowires.

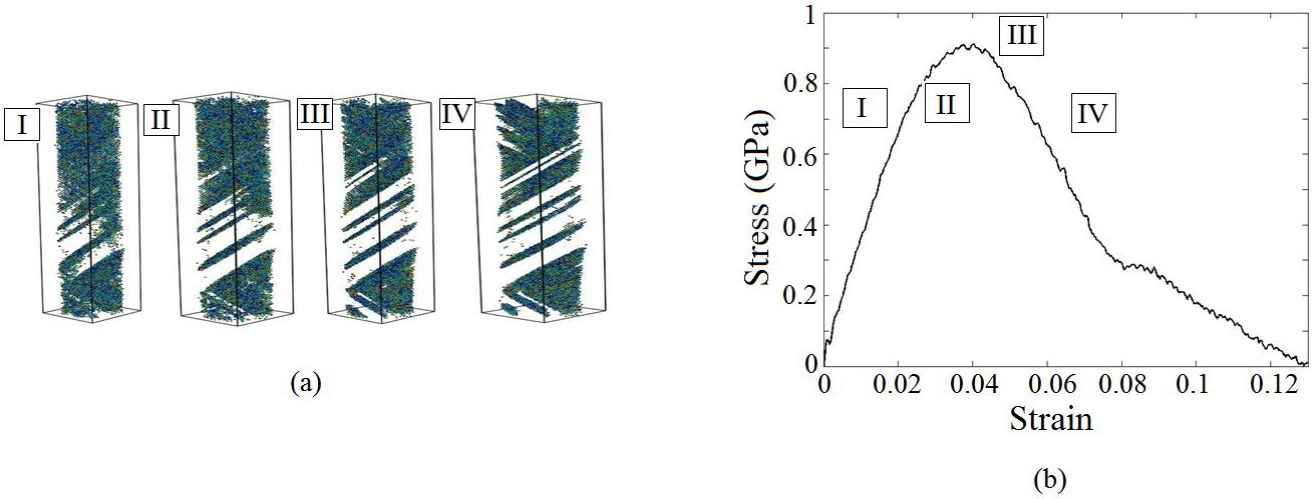

Fig. 2: (a) Slip planes corresponding to the stress-strain curve shown in Fig. 2(b). The green color of atoms denotes the Mg-atoms and the empty planes signify the slip planes in cylindrical nanowires. (b) A typical stress-strain plot showing different stages (I, II, III, IV) during the formation of slip planes in Magnesium Nanowire under uniaxial tension.

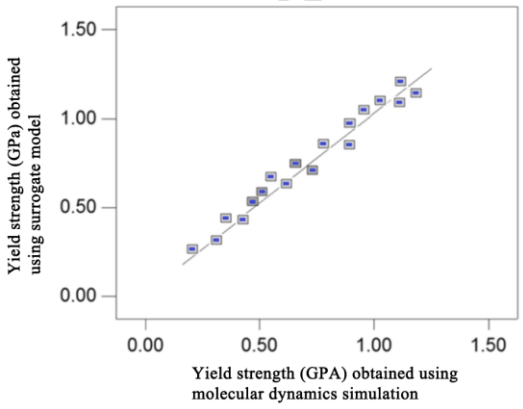

Fig. 3: Surrogate model validation plot showing actual MD simulation results vs surrogate model results considering multiple points for yield strength.

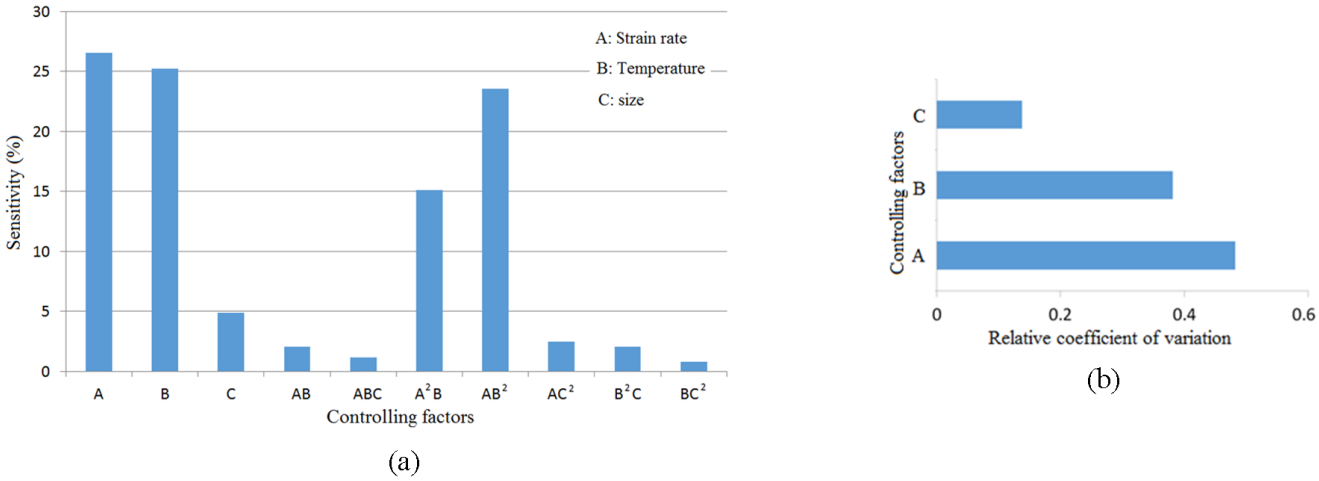

Fig. 4: (a) Sensitivity analysis results for yield strength of HCP nanowire including interaction effects, (b) relative coefficient of variation for different controlling factors.

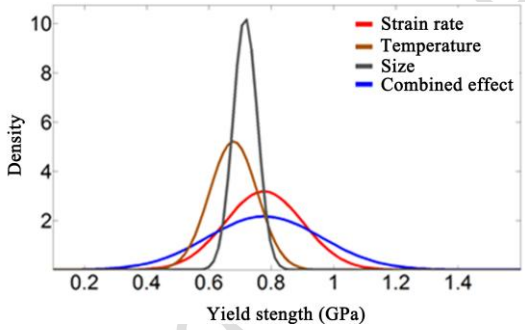

Fig 5: Probability density function plots for random variation due to individual and combined effect of the controlling factors

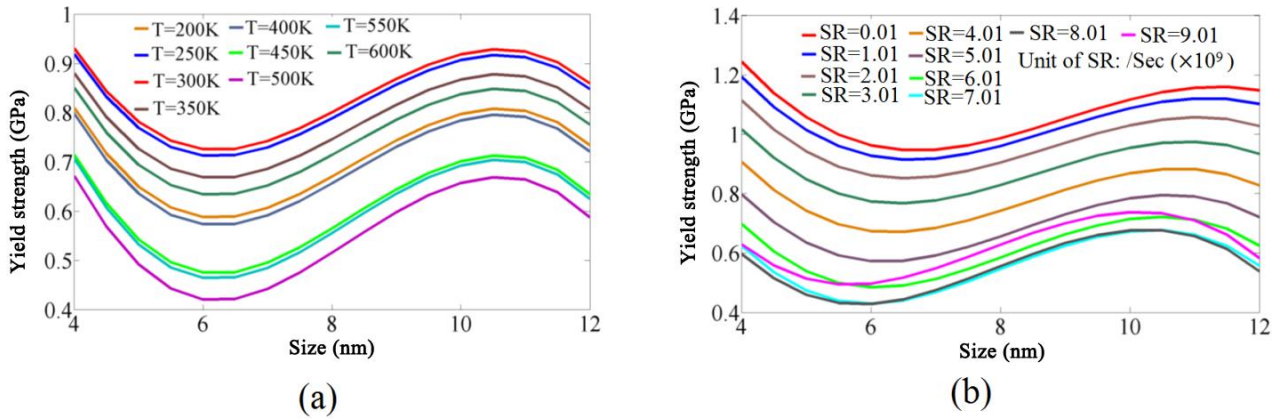

Fig. 6: (a) Variation of yield strength with size at different temperatures (b) variation of yield strength with size at different strain rates (SR)

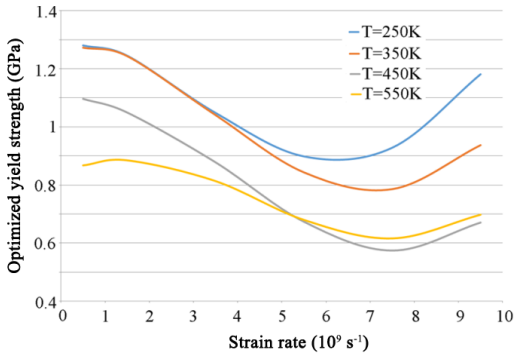

Fig. 7: Optimized yield strength for different strain rates at various temperatures

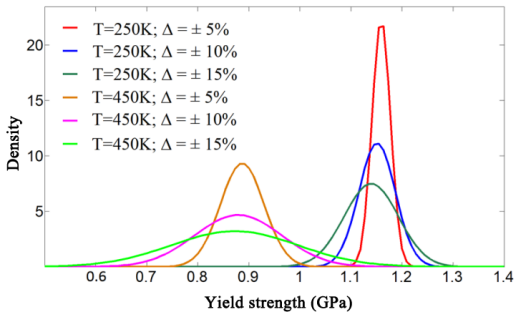

Fig. 8: Representative results on effect of uncertainty in the controlling factors considering optimized sizes for a strain rate of 3.5×10^9 s^{-1}.

Table 1 Set of molecular dynamics simulations on hcp-Mg nanowire presenting the chosen design points through D-optimal algorithm along with corresponding yield strengths and yield strains.

Serial No.	Strain rate (s^{-1})	Temperature (K)	Diameter (nm)	Yield stress (GPa)	Yield strain
1	8.32×10^{9}	208	8	0.9101	0.03727
2	5.005×10^{9}	400	8	0.6879	0.03705
3	1×10^{10}	400	11	0.807	0.0438
		⋮			
21	5.005×10^{9}	246	11.2	0.9214	0.044