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A molecular simulation based computational intelligence study of a nano-machining process with implications on its environmental performance

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ABSTRACT

Determining the optimum input parameter settings (temperature, rotational velocity and feed rate) in optimizing the properties (strength and time) of the nano-drilling process can result in an improvement in its environmental performance. This is because the rotational velocity is an essential component of power consumption during drilling and therefore by determining its appropriate value required in optimization of properties, the trial-and-error approach that normally results in loss of power and waste of resources can be avoided. However, an effective optimization of properties requires the formulation of the generalized and an explicit mathematical model. In the present work, the nano-drilling process of Boron Nitride Nanosheet (BNN) panels is studied using an explicit model formulated by a molecular dynamics (MD) based computational intelligence (CI) approach. The approach consists of nano scale modeling using MD simulation which is further fed into the paradigm of a CI cluster comprising genetic programming, which was specifically designed to formulate the explicit relationship of nano-machining properties of BNN panel with respect to process temperature, feed and rotational velocity of drill bit. Performance of the proposed model is evaluated against the actual results. We find that our proposed integrated CI model is able to model the nano-drilling process of BNN panel very well, which can be used to complement the analytical solution developed by MD simulation. Additionally, we also conducted sensitivity and parametric analysis and found that the temperature has the least influence, whereas the velocity has the highest influence on the properties of nano-drilling process of BNN panel.

1. Introduction

In today's world, the growth of manufacturing industries has resulted in an increase in the demand for energy. In industry, several manufacturing operations such as machining (turning, drilling, grinding and milling), and 3-D printing processes (fused deposition modeling, selective laser sintering, selective laser melting, etc.) are carried out which draw the (electrical) energy from the power grid [1]. Among these operations, machining is widely used in the manufacturing industries. Since energy is an essential and expensive component for driving the machining operations, the saving of energy would result in higher environmental performance and productivity. For example, if the energy is drawn from the thermal power station, lowering the energy consumption would result in the lower emission of harmful gas, and would result in saving of water resources, if the route chosen is drawn from hydraulic plants [2,3]. Survey studies conducted by peer researchers [4–7] reveal that an extensive focus has been paid in optimizing the machining operations of materials such as steel and composites based on the two components: cost and productivity. Recently, few studies are conducted that address the implications of conducting machining operations on its environmental performance [8–10]. However, to the best of authors' knowledge, any study that discusses the implications of machining of nanomaterials such as carbon nanotube, graphene and boron nitride nanosheets (BNN) on the environmental aspect is hardly noticed.

Among these nanomaterials, the research in BNN has attracted significant interest in material science due to its attractive physical and mechanical properties [11,12]. The exceptional qualities of BNN have been widely studied and investigated to explore its diverse possible applications in real world. These include applications in electric circuits such as BNNT-based integrated circuits (ICs), structural composite materials and hydrogen storage applications [13–15]. These

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applications of BNN require it to be machined at nanoscale, leading to production of BNN based nano-components of complex geometry and functionality. In addition, the increasing demand to manufacture BNN based nano-sensors for NEMS industry is one of the major incentives to study the mechanical characteristics of BNN subjected to nano-drilling.

Numerous studies have been undertaken to predict the mechanical properties of BNN under various nano-machining operations. Tang et al. [16] determined the strength of BNN under axial stretching using *in situ* Transmission Electron Microscopy (TEM) and MD simulation approach. It was found that the mechanical properties and deformation behaviors are correlated with the interfacial structure under atomic resolution, which clearly demonstrates a geometry strengthening effect. Chiu et al. [17] studied the radial rigidity of BNN subjected to radial nano-drilling process. It was found that the radial thickness has a greater influence on the structural stability of BNN under nano-drilling. Zheng et al. [18] studied the nano-mechanical properties of BNN subjected to cutting operation using atomic force microscopy (AFM) technique. It was predicted from the experiments that the tested BNNs exhibit fracture strengths ranging from 9.1 to 15.5 GPa. Boldrin et al. [19] studied the mechanical strength of BNN subjected to manufacturing process using an analytical model based on energy equivalence principles. They found that the results obtained from the analytical model compared well with data obtained using MD simulations. In addition, the model also helped to understand various deformation mechanisms in BNN under nano-machining conditions. The above mentioned literature studies clearly indicate that the mechanical properties of BNN depend on various nano-machining process parameters such as system temperature, feed and rotational velocity of drill bit. Hence, understanding the influence of each factor on the nano-drilling process is important for optimizing the mechanical properties of BNN. One way of optimizing system properties of nanoscale materials is to form an explicit model formulation which can then be used to extract system input variables for desirable material performance.

Theoretical studies based on MD simulation have become more popular to study the mechanical properties of BNN when compared to that of laboratory based experiments. This is due to the reason that MD simulation allows rapid restructuring nano-machining parameters [20,24,25]. This is useful to understand the influence of system parameters on the nano-machining properties of BNN. Hence, MD simulation models can be used as a viable alternative compared to time consuming and expensive experiments for monitoring nano-machining process. In addition, MD simulation is capable of generating accurate solutions in predicting engineering properties of nanoscale system with minimal cost and high rapidity [21–23,26,27]. However, the MD simulation does not provide information on relationship between the input parameters and the generated output. Computational intelligence (CI) methods (artificial neural network, support vector regression, genetic programming (GP), etc.) can prove to be a useful tool for predicting the relationship between generated output properties and the input parameters [28–32]. However, they cannot be used to predict system properties in nanoscale materials.

Therefore, there is a need to develop a MD based CI simulation approach for modeling the material properties of nanoscale materials such as BNN. The proposed approach combines powerful advantages of accuracy and low cost of MD simulation with the explicit model formulation ability of the CI methods. These methods require input training data which can be obtained from the MD simulations which are based on a specific geometry, cutting conditions and temperature. Among the various available CI methods, the GP offers the advantage of a fast and cost-effective formulation of a functional expression based on the multiple input variables without any incorporation and need of the existing analytical models [33–35]. It is to the best of author's knowledge that limited or no work exists on the application of MD based CI simulation model on evaluating the output properties such as mechanical strength and completion time of the nano-drilling of the nanoscale system. Additionally, the potential future applications of BNN in electronics industry require a thorough understanding and investigation of various input parameters on the output properties of BNN.

In present work, the proposed MD based CI approach is employed to investigate the effect of input parameters: rotation velocity, temperature and feed rate on the two output properties: nano-machining force and completion time of nano-drilling of BNN. The functional expression (model) of nano-machining force and nano-machining time with respect to rotation velocity, temperature and feed rate is obtained. The performance of the proposed model is evaluated against the actual data obtained from the literature. Further the parametric and sensitivity analyses conducted are used to validate the robustness of the proposed model by unveiling dominant hidden input parameters and non-linear relationships. The potential implication arises from the present study includes the improvement in its environmental performance. This is because by the formulation of generalized MD based CI model, the optimum input parameters settings (temperature, rotational velocity and feed rate) can be determined which optimizes the properties (strength and time) of the nano-drilling process. This also results in improvement in environmental performance because the rotational velocity is an essential component of power consumption during drilling and therefore by determining its appropriate value required in optimization of properties, the trial-and-error approach resulting in the loss of power and waste of resources can be avoided.

2. A MD based CI approach

The output properties of nano-drilling phenomenon of BNN (hereafter referred to as BNN panel) described in this work are modeled entirely using an MD based CI simulation approach as shown in Fig. 1. In this approach, the MD is integrated in the paradigm of popular CI method, GP. For understanding the notion of the approach, each of MD and GP method is discussed as follows.

The empirical Tersoff potential [36] is used to model the nano-machining characteristics of BNN panel based on potential parameters for describing the covalent bonding of boron and nitride atoms developed by Albe et al. [37,38]. These potential parameters are determined from experimental studies involving impact of nitrogen on hexagonal boron nitride target [39] and ion-beam deposition on boron nitride thin films [40]. The Tersoff potential is described mathematically as,

$$E_{Tersoff} = \frac{1}{2}\sum_{i}\sum_{i \neq j} f_{cut}(r_{ij})\left[A_{ij} f_R(r_{ij}) - B_{ij} f_A(r_{ij})\right] \quad (1)$$

where r_{ij} represents scalar distance between the atoms i and j, $f_{cut}(r_{ij})$ represents the cutoff function, f_R and f_A denotes the repulsive and attractive pair terms respectively. The A_{ij} and B_{ij} terms are used to include the Tersoff empirical bond order between the atoms.

The data obtained from the MD simulation is further fed into GP cluster. GP based on Darwin's theory of 'survival of the fittest' finds the optimal solution by mimicking the process of evolution in nature. Due to which, GP has been extensively applied for solving symbolic regression problems of various systems.

The initial population of models is obtained by randomly combining the elements from the function and terminal sets. The elements in the function set can be arithmetic operators (+, −, /, and ×), non-linear functions (sin, cos, tan, exp, tanh, and log) or Boolean operators. The elements of the terminal set are input process variables and random constants. The present study has three input process variables chosen as elements of terminal set. The constants are chosen randomly in the range as specified by the user since these accounts for the human or the experimental error. The performance of the