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Some critical issues for a reliable molecular dynamics simulation of nano-machining

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ABSTRACT

This paper investigates some critical issues in carrying out a reliable molecular dynamics simulation of nano-machining. Using monocrystalline copper as the workpiece material, this work shows that the Morse potential with compensation scaling can describe the interaction between copper atoms at a much better computational efficiency than the EAM potential. Based on a comprehensive study using the bond distance dynamics and cumulative error theories, the present investigation concluded that to avoid erroneous results the integration time step should be between the intervals of 4–12 fs, and that the machining speed should be less than 2062 m/s. The molecular dynamics simulation of nano-milling was then implemented as an application example.

1. Introduction

With the ever increasing needs for miniaturized ultra-precision components in micro/nano-electro-mechanical systems (MEMS/NEMS), the fabrication of nano-scale surface features has brought about significant challenges in both the understanding of the process design mechanisms and the technical realization of production [1]. Of the novel and effective manufacturing methods available today, micro/nano-mechanical machining has attracted extensive attention due to their simplicity and efficiency [2–4]. However, the material removal mechanism associated with nano-mechanical machining is still unclear. To understand the deformation mechanisms of a material, molecular dynamics (MD) has been recognised as a powerful tool to provide physical insights that are impossible to obtain from experiments [5–9]. Nevertheless, as have been pointed out by Zhang and Tanaka [10], Mylvaganam and Zhang [11] and Cheong et al. [12], an MD simulation may not give reliable results if improper algorithms, parameters or potential functions are used in the computation. For instance, in the analysis of a carbon nanotube subjected to tension [11], the use of the Tersoff–Brenner potential can describe the whole deformation process of the nanotube reasonably well, whilst the Tersoff potential cannot.

First, in an MD analysis it is important to select an appropriate interaction potential that can correctly describe the deformation of a material. In the investigation on copper with the aid of MD, for example, both the Morse potential and the embedded atom method (EAM) potential have been widely used to describe the interatomic interactions. The Morse potential is simple and computationally efficient in applications, because it takes only two-body interactions into account. In metals, however, thermal energy is mainly conducted by electron movements and hence needs to be compensated, as pointed out by Shimada et al. [13]. On the other hand, the EAM potential, which evolved from the density functional theory, includes the electron density induced by all the atoms in a material. Thus for metals, the EAM potential is commonly considered to be more accurate in describing the metallic bonding. However, the application of the EAM potential is not so efficient, because it requires more computational time and a greater memory space compared with the Morse potential [14]. For example, excessive memory is required, when using the EAM potential, to store electron densities and derivatives on all atoms in addition to the storage of neighbouring atoms for calculating the pairwise forces. A natural question is therefore: Which potential function is a better choice for the nano-machining simulation when efficiency and accuracy are considered together?

The second issue of primary importance is a proper selection of time step. In MD simulations, the motion equations are integrated by the finite difference method in which truncation and round-off errors are inevitably incurred [15,16]. The truncation error denotes the difference between the evaluation of the complete expression and the truncated expression. The round-off error encompasses all errors generated by the implementation of the finite-difference algorithm, including the number of significant figures used in the computation, the order by which the computations are performed,

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Nomenclature

a	copper cubic lattice constant
a'	contact area
a_0	contact area at load zero
a_c	contact area at P_c
A_{atomic}	atomic contact area
A_c	atomic contact area
B_e	bulk modulus at equilibrium
D_e	cohesive energy between two atoms
E_c	cohesive energy
E_{tot}	EAM energy
F_i	embedding energy of atom i
F_t	tangential cutting force
F_x	feeding force
F_y	traverse force
gre	global round off error
gte	global truncation error
h	feed per tooth
k	Boltzmann constant
K	material stiffness
K'	elastic constant in JKR model
K_m	material coefficient
m	mass of a copper atom
m_r	reduced mass of the system
M	number of steps
N	total number of atoms
N_c	number of contact pairs
P	load in JKR model
P_c	critical load in JKR model
r_a	theoretical radius of a copper atom
r_e	equilibrium distance between two atoms
r_{ij}	instantaneous distance between atoms i and j
R	indenter radius
T	absolute temperature
T_{melt}	melting temperature
T_v	period of vibration of an atom
U_i	scaled velocity of atom i
v	feed rate of machining tool
v_c	cutting speed of machining tool
v_i	indentation speed
v_{max}	threshold speed of nano-machining
V_i	velocity of atom i before scaling
V_m	mean square velocity
$V(r_{ij})$	pair-interaction energy between atoms i and j
α	material constant
γ	energy per unit contact area
ρ_ε	electron density at equilibrium
ω	angular velocity
Ω_ε	atomic volume at equilibrium
Δ_t	integration time step
Φ_ε	two-body central potential at equilibrium
$\rho_j(r_{ij})$	contribution to the electron density at i from atom j
$\bar{\rho}_i$	electron density at the site of atom i from all the other atoms

and the approximations used for calculating the square roots, exponentials, logarithms and so on. As illustrated in Fig. 1, both errors are determined by the integration step size (Δt), but affected in different ways. The global truncation error (*gte*) rises with increasing the integration step size; but the global round-off error (*gre*) drops due to the decline of the number of iterations. Usually, a big integration time step leads to an unstable motion of atoms or molecules due to the correspondingly big errors occurring in the integration. On the other hand, a small integration time step causes a high computational cost [11,16–18]. Consequently, the magnitude of Δt must be determined in such a way that acceptable small global errors are produced at as a lower computational cost as possible. In the current MD simulation exercises, the time step used in the nano-machining simulations varies in a wide range. For example, Zhang et al. used a time step of 0.5 fs [19] to investigate the deformation in the subsurface and 1 fs [20] to study the effect of cutting velocity, respectively, in the MD simulation of AFM-based nanometric cutting of copper. On the other hand, time steps of 10 fs and 15 fs were used in the studies on the effect of the negative rake tool in grinding and the exit failure in the cutting process, respectively [21,22]. These indicate that it is essential to clarify the selection of the integration time step that can guarantee a reliable nano-machining simulation.

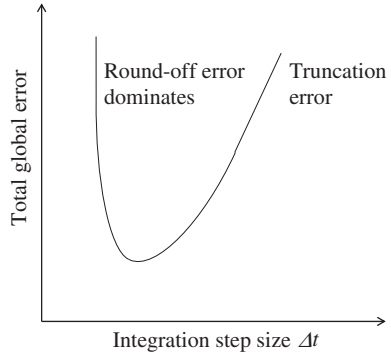

Fig. 1. Variation of global error with the size of integration time step.

The third issue that is vital to a reliable MD simulation is the selection of a rational range of machining speeds, which, on one hand, should be physically meaningful, but on the other hand, should be broad enough to allow to understand deeply the strain rate effect of a material. In a nano-scratching/cutting process, Pei et al. [23] found that increasing the cutting speed could lead to more lattice defects in the cutting region with higher cutting forces. Ye et al. observed that under a higher cutting speed, a machined surface became rough but the workpiece appeared to be dislocation-free. In contrast, under a lower cutting speed dislocations remained in the substrate and the machined surface was smoother [24]. Zhang et al. [25] reported that a higher scratching velocity causes a larger chip volume and the atoms at the chip surface connect to each other closely with a more amorphous structure. In a nano-milling process, a tool trajectory is the resultant of linear and rotary motions of the tool. As such, the two motion velocities of the tool for an MD simulation should reflect the feasibility in the fabrication practice and at the same time ensure the reliability of the MD simulation. However, little has been done in this regard and one has to refer to the parameter selections on the macro- and micro-scales, in which surface roughness, tool life and cutting forces have usually been used as the criteria to judge the machinability. It has been observed that increasing the cutting speed or decreasing the feed rate results in a lower surface roughness for most materials [26]. Nevertheless, this will shorten the lifespan of a tool [27]. It appears that the selection of the rotational speed and feed rate is decisive to the machined surface features and to the cost of production. A particular concern is that the cutting speed