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Designing nanoindentation simulation studies by appropriate indenter choices: Case study on single crystal tungsten

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ABSTRACT

Atomic simulations are widely used to study the mechanics of small contacts for many contact loading processes such as nanometric cutting, nanoindentation, polishing, grinding and nanoimpact. A common assumption in most such studies is the idealisation of the impacting material (indenter or tool) as a perfectly rigid body. In this study, we explore this idealisation and show that active chemical interactions between two contacting asperities lead to significant deviations of atomic scale contact mechanics from predictions by classical continuum mechanics. We performed a testbed study by simulating velocity-controlled, fixed displacement nanoindentation on single crystal tungsten using five types of indenter (i) a rigid diamond indenter (DI) with full interactions, (ii) a rigid indenter comprising of the atoms of the same material as that of the substrate i.e. tungsten atoms (TI), (iii) a rigid diamond indenter with pairwise attraction turned off, (iv) a deformable diamond indenter and (v) an imaginary, ideally smooth, spherical, rigid and purely repulsive indenter (RI). Corroborating the published experimental data, the simulation results provide a useful guideline for selecting the right kind of indenter for atomic scale simulations.

1. Introduction

The majority of nanoindentation studies have focused on investigating the deformation of the substrate and the indenter is often considered as a smooth, rigid and otherwise inert body impenetrable by other bodies. This inert body assumption stems from the theory of continuum mechanics and usually the atomic description of the indenter is not taken into account. While this assumption is widespread in the atomistic simulation studies of nanoindentation [1,2], nanometric cutting or nanoscratching [3,4], there are some notable exceptions. These include MD simulations of nanoindentation of a gold substrate using a nickel tip [5,6], of a tungsten substrate using a deformable tungsten indenter [7], of aluminum using infinitely hard nickel [8] and of other engineering materials such as CaF_2, NiTi and gold using a hypothetical, purely repulsive type of spherical force field [9–11].

Recently, the fundamental mechanism between dislocations and a single nanotwin was elucidated by in situ transmission electron microscopy (TEM) nanoindentation [12]. High speed scratching or grinding using a single diamond tip are proposed [13], to address the fundamental mechanisms for abrasive machining, such as grinding, polishing and lapping. In these processes, as the chemical interaction changes with each type of indenter, the resulting magnitude and direction of the force being transferred by the indenter to the substrate for a given displacement differs. The implication of this change is not quantified in extant research. Our purpose in this study is to examine the specific role of tip-sample interaction perturbations on continuum contact mechanics concepts using state-of-the-art, fully atomistic molecular dynamics modelling. We focus on how modelling indenters with

Abbreviations: ABOP, Analytical bond order potential; BCC, Body centred cubic; CAT, Crystal analysis tool (software program); DXA, Dislocation extraction algorithm; MD, Molecular dynamics; NVE, Microcanonical ensemble; OVITO, Open Visualization tool (software program); PBC, Periodic boundary condition; TEM, Transmission electron microscope

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Nomenclature

a	contact radius of the spherical indenter
A	projected area
b	direction of Burgers vector
B	bulk modulus
DI	simulation using a rigid diamond indenter
TI	simulation using a rigid tungsten indenter
RI	simulation with a repulsive indenter (force potential)
C_{ij}	elastic constants of the material
DI-NA	diamond indenter with no pairwise attraction with the substrate
E	elastic modulus of the material
E_r	reduced elastic modulus of the material system
F or P	normal force or load on the indenter
F(r)	repulsive force potential
G	shear modulus (GPa)
h	instantaneous displacement of the indenter
h_f	residual depth of indentation
h_{max}	maximum depth of indentation
H	hardness of the material
K	force constant
L	total length of dislocations in Å
P-h	load-displacement curve
p_m	contact pressure
R	radius of the indenter
R_{pl}	radius of the plastic zone
r	distance between two dimers
r_0	cutoff radius between indenter and the substrate material
S	slope of the unloading curve
W	tungsten
$\sigma_{hydrostatic}$	hydrostatic stress
σ_1, σ_2 and σ_3	principal stresses
ε	strain
τ	shear stress

different material systems affects the extracted force data. Our exploration is important for understanding how the differences in adhesion (clinging between two different atomic species) and cohesion (clinging between the same atomic species) governs the initial contact and what subsequent effects it has on the contact mechanics at the meso and macro scales.

2. Literature review

The word Tungsten is derived from the Swedish words 'tung sten' meaning 'heavy stone' while its chemical symbol W comes from the German name Wolfram. Scheelite and Wolframite are the two naturally occurring tungsten ores important for industrial use. For an ideal cubic crystal, the reciprocal elastic modulus can be expressed as $\frac{1}{E} = S_{11} - 2\left[(S_{11} - S_{12}) - \frac{1}{2}S_{44}\right](l^2m^2 + m^2n^2 + l^2n^2)$ where l, m and n are the direction cosines of the specimen axis with respect to the crystallographic axis [14]. This is an identical expression to that expressed by Zhang et al. [15] by introducing the (h,k,l) vector $\frac{1}{E(hkl)} = S_{11} - 2S_A\frac{h^2k^2 + h^2l^2 + k^2l^2}{(h^2 + k^2 + l^2)}$ with $S_A = S_{11} - S_{12} - \frac{1}{2}S_{44}$. Interestingly, for tungsten, the value of S_A is close to zero, i.e. the material response of W is close to that of an isotropic material.

Due to its inert nature, W has been proposed as a candidate material to be used for plasma facing, as part of structural components required for applications like limiters, first wall armour and divertor components in nuclear fusion reactors [16] and in military applications such as reinforcing materials in alloyed composites for making bullet shot and radiation shields [17]. Furthermore, due to the importance of tungsten in the carbide tooling industry, British Geological Surveys, US Department of Defense and European Commission (EC) have identified tungsten as a 'critical' raw material due to its supply risk.

Tungsten is a BCC transition metal, and such metals commonly shear in ⟨1 1 1⟩ directions on the (1 1 0), (1 1 2) and (1 2 3) planes [18] and/or sometimes these deformations resemble "pencil glide" on arbitrary planes along the ⟨1 1 1⟩ direction whereas ⟨1 0 0⟩ (1 0 0) was recognized as easy cleavage crystallographic directions. Bahr et al. [19] also observed that when the shear stress prior to yield is slightly higher than the flow stress, a phenomenon referred to as "staircase yielding" prevails.

Noticeably, identical values of shear strength for tungsten (18 GPa = 0.11 G) with failure strains of about 17–18% in the ⟨1 1 1⟩ direction were obtained regardless of the slip plane whereas the ideal tensile strength of the (0 1 0) surface obtained was 29 GPa. The ideal shear stress (18 GPa) found by Roundy et al. [18] was calculated using a Hertzian solution for the stress field of an elastic indenter, and is considerably lower than the value obtained by Bahr et al. [19], who reported a maximum shear stress for tungsten (oxidized for 32 h) of 28.6 GPa, and gave an estimation for the shear stress required for dislocation nucleation in pure W of 26 GPa. This difference was attributed to the linear elastic assumption which is used to calculate the values from the experimental data. Consequently, a correction factor in the form of sinusoidal stress-strain relations (to the experimental data by a factor of $2/\pi$) was proposed to eliminate this difference [18]. A summary of these results is shown in Table 1.

In another study, Lassner et al. [20] asserted that slip is the basic mechanism in the plastic deformation of single crystal tungsten, and it occurs in the most densely packed ⟨1 1 1⟩ direction on (1 1 0) or (1 2 2) planes, and additionally on the (1 1 1) plane at elevated temperatures. They also noted that twinning is a less dominant deformation mechanism and occurs mainly on the (1 1 2) plane in the ⟨1 1 1⟩ direction. Argon et al. [21] examined low temperature deformation of single crystal tungsten (in the range of 77–450 K) and concluded that it exhibits an anisotropy on the (1 1 2) plane producing slip on unexpected slip systems.

Simulations on BCC metals is an emerging area of research, since little is known about their deformation behaviour at the nanoscale [22,23]. This was the major motivation for choosing tungsten as the reference material for this work while comparing different choices of indenters.

3. Molecular dynamics (MD) simulation of nanoindentation

3.1. Simulation setup

In this work, the "Large-scale Atomic/Molecular Massively Parallel Simulator" (LAMMPS 17th November 2016 version) [24] was used to perform a series of MD simulations. OVITO [25] was used to visualize and analyse the atomistic simulation data while an automated "dislocation extraction algorithm" (DXA) [26] and crystal analysis tool (CAT) [27] were used for automated identification of crystal defects, dislocation lines and their Burgers Vector from the output of the MD data. The algorithm and the necessary considerations required and used in this work are quite similar to that of simulating nanometric cutting

Table 1
Experimental data on nanoindentation of tungsten [18].

Maximum normal stress (σ_{max})	Maximum shear stress (τ_{max})	Normalized shear stress (τ_{max}/G)
69.6 GPa	21.6 GPa	13.5 (%)