Letter to Editor – Int J. of Machine Tools and Manufacture

The possibility of performing FEA analysis of a contact loading process fed by the MD simulation data

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Dear Editor,

In one of the previously published papers in Int. J. Mach. Tools Manuf. [1] an approach, namely the hybrid molecular dynamics-finite element analysis (MD-FEA) model was proposed. As a preliminary work in this area, the esteemed authors of the cited paper have attempted to gather the stress-strain data from the uniaxial tensile test simulation using a bottom up approach like molecular dynamics simulation and fed this data to an engineering toolbox like finite element analysis for performing micromachining simulation of silicon. However, we must account for the differences between uniaxial tension and deviatoric stress (that occurs during micromachining). In the latter case (machining or scratching), the diamond structure of silicon is sheared as well as having its volume and shape changed. Moreover, plastic deformation in MD simulation at its limiting length and time scales is typically observed due to dislocation glide or high-pressure phase transformation as opposed to larger experimental length scales where multiple events such as dislocation mediated plasticity, twinning, high pressure phase transformation and amorphisation can occur simultaneously. This tie in with the fact that the asymmetry in tension-compression behaviour [3] at nanoscale is more pronounced i.e. compression is dominated by dislocation glide while twinning is prominent during tensile pulling and therefore a tensile test data alone is not sufficient enough to inform a finite element model in the development of a hybrid MD-FEA model. It is therefore clear that the development of a hybrid MD-FEA is a more complicated situation and as a first step of a fundamental investigation, it would be more sensible to benchmark the hybrid-FEA model with respect to tensile, compression and shear data obtained from the MD simulation. In addition to this, there are other

considerations involved that must be accounted for in developing a robust hybrid MD-FEA model. In this letter, we communicate important technical insights on such considerations necessary to modify the existing hybrid MD-FEA method that will help the research community to further develop this idea.

It is worth noting that the plastic property data obtained from the MD is valid only for a specific strain rate and geometry of test sample. Any changes in the configuration of the tested system in MD (such as the aspect ratio or strain rate) leads to different plastic property data from the MD (even for the same material) which is not accounted for in the aforementioned model [1]. The variations in the strain rate and loading conditions are significant at the nanoscale [2, 3] (higher strain rate results in a higher fracture strain) and therefore a robust hybrid MD-FEA model must account for these dynamic effects. Taking example of a nanoscale tensile test problem, we show evidence in support of this argument and prove that such a hybrid MD-FEA model needs to be optimised further to account for the varying strain rates and geometric size effects.

Following our recent related work on this topic (a pure MD study [3]), we have brought FEA modelling into the comparison in this work. We begin by modelling a silicon nanowire of Ø20.68 nm (cross sectional area 336 nm^2) and length 48.98 nm (length/diameter ratio of 2.368) with the crystal orientation and direction of tensile pulling (parallel to the Y direction) as <010>. Due to circular symmetry of the wire, an axisymmetric model was considered in the FEA assuming 4-node bilinear axisymmetric quadrilateral elements (CAX4) with a mesh size of 2.5 nm. Initially, the wire was stretched at an applied engineering strain rate of 0.0005/ps = (5×10^8)/sec to compare it with the pure MD model. For FEA simulations, a commercial software Abaqus was used and following the procedure described by Aly et al. [1], the plastic data obtained from the MD simulation was fed to perform the FEA simulations at varying strain rates. The results were compared with the pure MD data as well as FEA simulation on silicon performed by using an established Johnson-Cook model (adopted from [4]) as follows:

$$\sigma = [A + B.\varepsilon^n] \times \left[1 + C.ln\left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right)\right] \times \left[1 - \left(\frac{T - T_{room}}{T_{melt} - T_{room}}\right)^m\right]$$

where σ is the material's flow stress, *A* is yield strength (**896.394 MPa**) of silicon, *B* is hardening modulus (**529.273 MPa**) for silicon, *n* is hardening coefficient (**0.3758**), *m* is thermal softening coefficient (**1**), *C* is

strain rate sensitivity coefficient (**0.4242**), ε is plastic strain, $\dot{\varepsilon}$ is the plastic strain rate and $\dot{\varepsilon}_0$ is the reference plastic strain rate (**1/s**), T is the workpiece temperature, T_{room} is the room temperature (**293 K**) and T_{melt} is the melting temperature (**1688 K**), elastic modulus of silicon was considered as 98 GPa for a silicon wire of diameter 20 nm oriented on the (001) orientation as obtained from MD and from the nanoscale experiments [5, 6] with Poisson's ratio of 0.23 and density of 2330 Kg/m^3.

While revisiting the literature, we noticed that the full scale MD models [2] reveals that the fracture strain is strongly dependent on the applied strain rate. In conjunction with this, we expected the tabularly fed FEA model shown and compared in figure 1 to predict these strain rate dependent effects. The pure FEA model does not show such variations obviously because it is fed by the MD specific data valid for a particular strain rate test which is the major bottleneck that we are alluding to in this work. For a given strain rate and geometry though, the FEA model predicts close alignment with the MD results, both showing incipient inelastic behaviour. It may be seen from figure 1 that the rupture strength and strain largely depended on the strain applied in the MD for an instance at an applied strain rate of 0.0005/ps, our simulations revealed a value of ultimate rupture strength and separation strain of (001) oriented silicon to be up to <13 GPa and 0.14 respectively in contrast to a high values of 24 GPa and 0.22 obtained earlier for a smaller aspect ratio wire [1]. These results are also compared with the J-C model that showed lower magnitudes of stress for a given strain in the plastic regime. Based on these observations we conclude that a newer kind of material model would be necessary if MD data is to be fed into the FEA, particularly accounting for the strain rate and geometry of the sample because size effects at the nanoscale cannot be discarded. Also, it might be more sensible to develop and test such a hybrid MD-FEA model in a uniaxial stress situation prior to testing in a deviatoric stress condition.

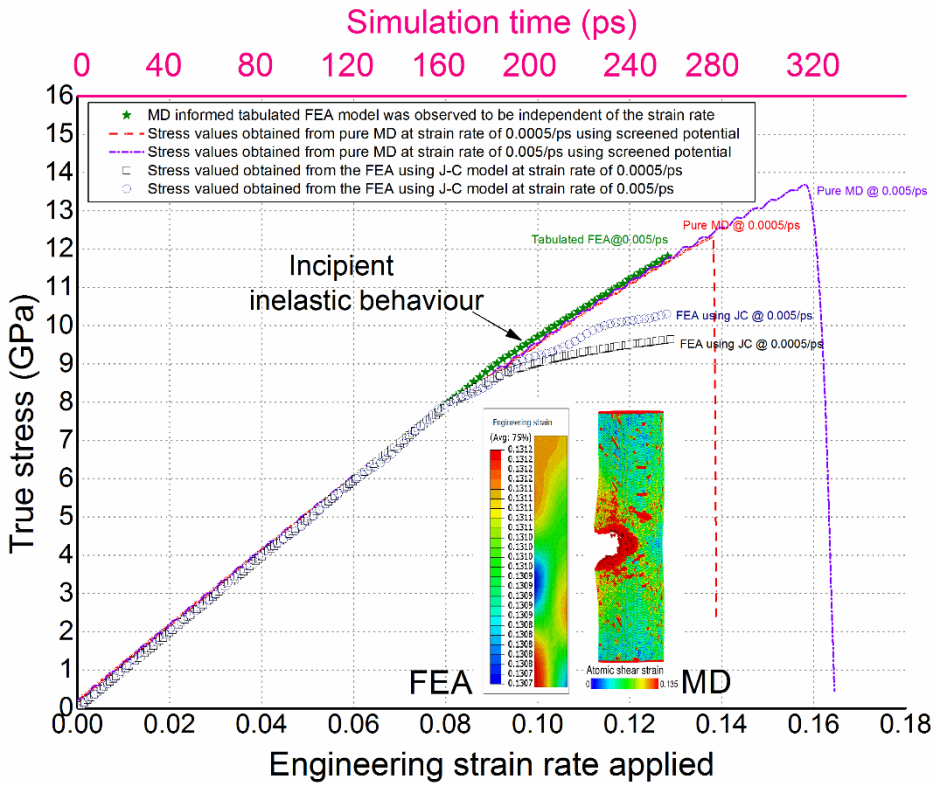

Figure 1: Comparison of the pure MD results with the FEA results using (i) J-C model and (ii) tabulated MD fed FEA model

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