# A Theoretical Study on Ratcheting Fatigue Behavior of Copper Nanowire Using Classical Molecular Dynamics Simulation

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## INTRODUCTION:

Fatigue behavior of nano-wires however, is one of the most essential aspects, as in all engineering applications fatigue of components is a crucial damage mechanism. In comparison with fatigue studies carried out for strain-controlled cyclic loading, asymmetric fatigue cycling or ratcheting is rather new domain of research. Ratcheting is defined as accumulation of progressive plastic strain at the time of application of asymmetrical cyclic loading to structural components. Moreover, study of fatigue behavior of materials at high temperature is important because it causes reduction in flow stress of materials and thus affects fatigue properties. But performing fatigue experiments at high temperature is highly difficult, expensive and time consuming. Therefore simulation based studies become very effective ways to predict the fatigue behavior of materials at varying temperatures [1].

The study of mechanical properties of nano-structured copper becomes important research topic worldwide due to fast advancement of electronic industries. Earlier investigators have studied the properties of copper nano-wire under static loading while very few studies have been conducted to test the effect of cyclic loading as it consumes a lot of time when the experiment is conducted in real life. In this work, asymmetric fatigue cycling or ratcheting simulations have been carried out up to a specified number of cycles to understand the nature of strain accumulation in copper nano-wire. Prior to conduct fatigue simulation, tensile behavior of copper nano-wire has been examined over a range of temperatures.

## COMPUTATIONAL DETAILS:

MD simulations of copper nano wires have been carried out using well tested and widely used LAMMPS (Large Scale Atomic/Molecular Massively Parallel Simulator) code using EAM FS (Embedded Atom Model Finnis-Sinclair) potential. In Finnis/Sinclair model total energy of an atom is represented by:

$$E_i = F_\alpha\left(\sum_{j\neq i}\rho_{\alpha,\beta}(r_{i,j})\right) + \frac{1}{2}\sum_{j\neq i}\varphi_{\alpha,\beta}(r_{i,j})$$

where *r*, the electron density is a functional specific to the atomic types of both atoms *i* and *j* so that different elements can contribute differently to the total electron density at an atomic site depending on the identity of the element at that atomic site and alpha and beta are the element types of atom *i* and *j*. The simulation box size was 40 Å × 100 Å × 40 Å in which total number of atoms were 14812 with 9349 movable atoms. Figure 1a illustrates a typical simulation box. The fixed (grip portion) and movable (region that undergoes deformation) regions are indicated in the figure.

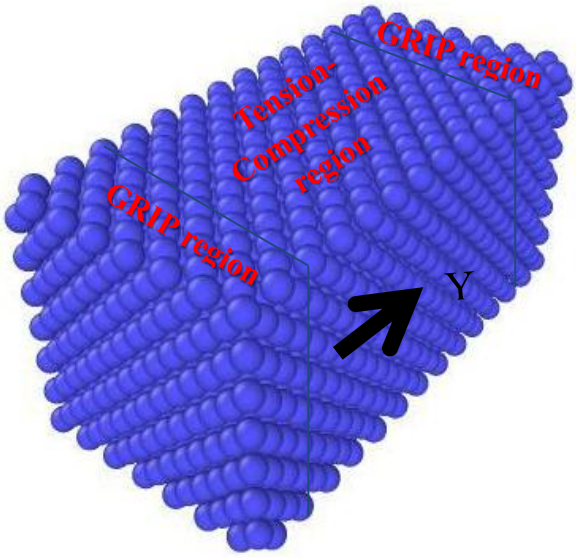


**Figure 1:** VMD snapshot of the sample undergoing simulation

**LOADING DETAILS:**

MD simulations of copper nano wires have been carried out to estimate the tensile properties at three different temperatures. Asymmetric stress controlled fatigue that is ratcheting simulations have been done for different stress ratios and with varying temperatures. Ratcheting strain is calculated using the formulae:

$$\%\ \text{Ratcheting strain} = \left[\frac{\left(Y_{hi} + |Y_{lo}|\right) - L}{2L}\right] \times 100$$

**RESULTS:**

Typical results of tensile simulation are shown in Figure 2. It can be seen that tensile strength reduces with increasing temperature, as expected. The tensile simulations have been done to select the specific maximum loads for the fatigue studies for the selected nanowires.

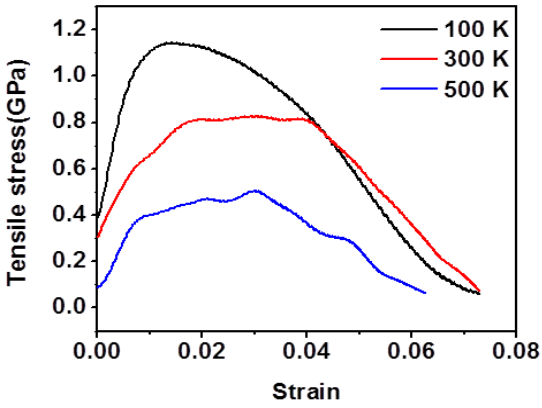


**Figure 2:** Effect of temperature on tensile properties of the selected copper nano-wire.

Figure 3 indicates the VMD snapshots of the selected specimen box under tension and compression during ratcheting fatigue. It can be noticed the variation in the specimen length in the Y direction during fatigue.

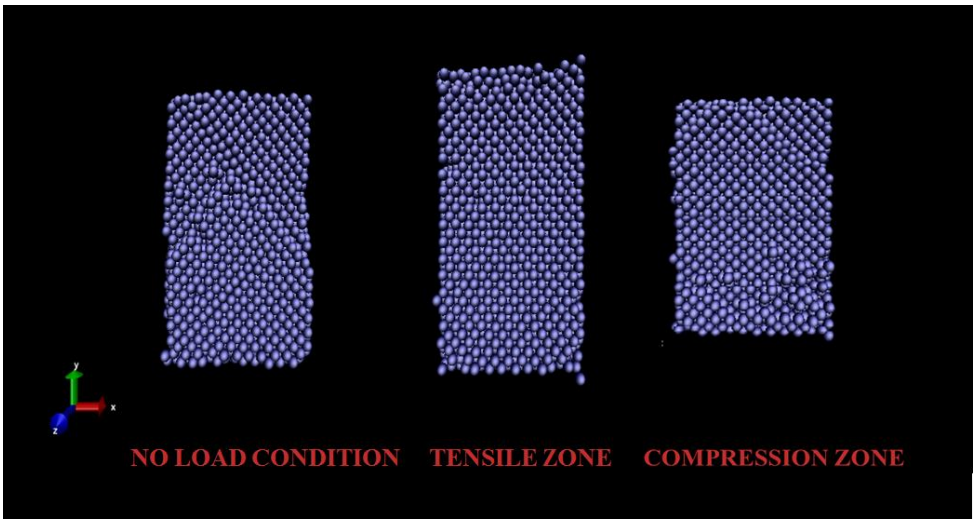


**Figure 3:** VMD snapshot of the sample taken during simulation.

As mentioned above, the ratcheting simulations have been done for different stress ratios and temperatures; the results generated from these simulation studies are shown in Figure 4. One can note that for different stress ratios like R = -0.2, -0.4 and -0.6, strain accumulation increases with increasing the R value. Similarly, with increasing temperature, strain accumulation increases. Further, the strain accumulation attains a saturation plateau after the second cycle. To see the effect of number of cycles on strain accumulation, a few simulation studies have been conducted for 50 cycles, although that produced similar trend of results at different temperatures (Figure 5).

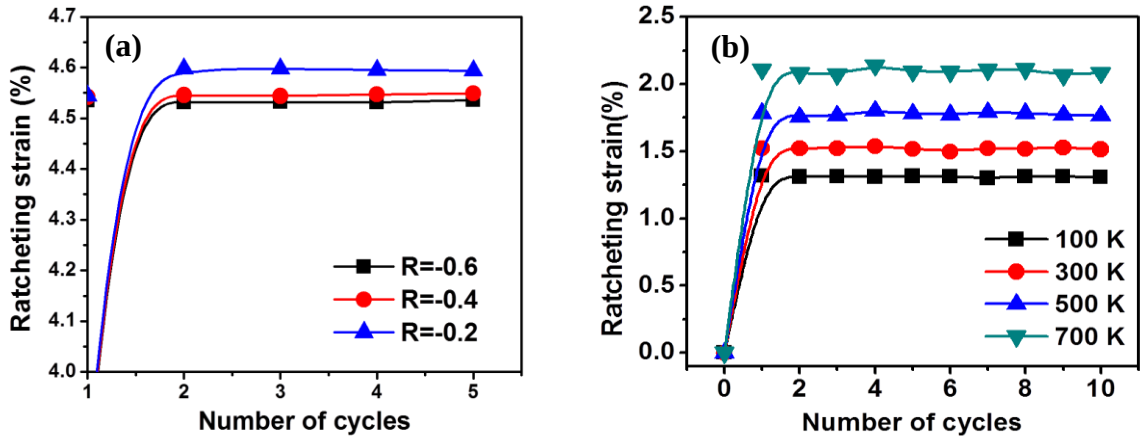


**Figure 4:** Effect of simulation parameters on accumulation of ratcheting strain for (a) varying stress ratios and (b) for varying temperatures.

**DISCUSSION:**

Asymmetric cyclic loading causes deposition of remnant dislocations during each load reversals on the substructure of a material [2]. This fact in turn accumulates plastic strain to a material in each cycle. The material fails in significantly lower number of cycles as that compared to the low cycle fatigue life under symmetric loading. The strain accumulation depends on cyclic loading parameters as well as on working temperature. Temperature induced softening is responsible for higher strain at high temperature. It is known that fatigue crack initiates on the free surface [3]. To check this, a few simulation studies have been done with higher load and that results in crack initiation on the surface. Typical VMD snapshot is illustrated in Figure 6.

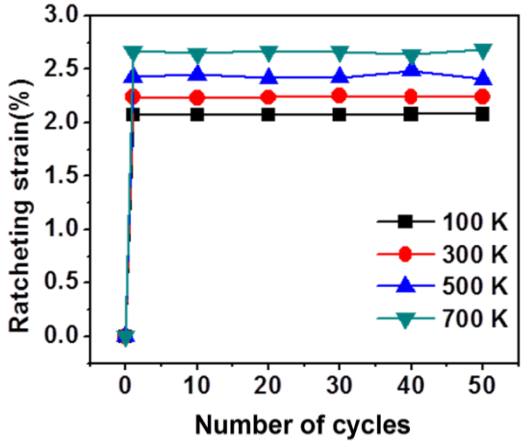


**Figure 5:** Effect of number of cycles on accumulation of ratcheting strain at varying temperatures.

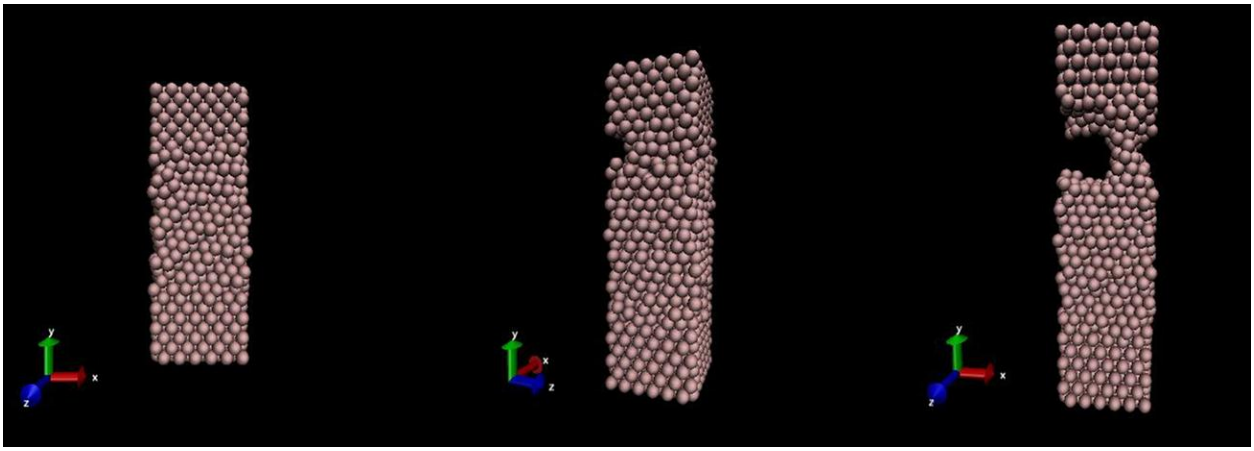

**Figure 6:** VMD snapshot of ratcheting induced crack initiation from the surface of the nano-wires.

## CONCLUDING REMARKS:

☞ MD simulation is used for the first time to assess ratcheting strain.

☞ Accumulation of ratcheting strain increases with increasing stress ratio (due to increased remnant dislocations) and temperature.

☞ Strain accumulation attains a saturation level after the initial two cycles and it does not vary up to the investigated number of cycles. It occurs due to attainment of stable dislocation configuration in the substructure of the material.

## REFERENCES


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