Atomistic simulations of metallic glass nanoparticles upon high velocity impact

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Abstract: New manufacture techniques of parts from metallic glasses have been developed in recent years. In particular, with the technique of cold gas dynamic spray (CGDS), metallic glasses can be produced in appreciable amounts. At present it is not yet well understood the deformation process that allows high degrees of compaction obtained with this technique. In this work we study through molecular dynamics (MD) simulations the deformation processes that occur when a metallic Cu-based glass nanoparticle impacts a metallic glass substrate at high velocities.

Introduction

Metallic glasses have attracted much attention due to their unique properties such as high hardness, elasticity and corrosion resistance [1]. Recently R. Fernandez et al [2], used the technique of cold gas dynamic spraying (CDGS) glass making compact deposits copper-based metal and zirconium. Following the good results in compaction interesting questions arise.

Method

An amorphous model of a ternary $Cu_{45}Zr_{45}Al_{10}$ alloy was generated by the melting-quenching technique using an NPT ensemble based on a crystalline B2 model structure. In the simulations we use the embedded atom type potentials from Y.Q. Cheng[3]. We analyzed and characterized the heated and cooled model structures using radial distribution functions and Voronoi tessellation. These generated amorphous models were then used to form a substrate-nanoparticle system for the impact simulation. The simulation of the impact was performed using a NVE ensemble with periodic boundary conditions in the x and y directions for the substrate. The MD simulations were carried out using the LAMMPS[4] software, while the structural analysis were performed using, and Voro++[5] and OVITO[6].

Results

Figure 1 shows the pair distribution function for: a) amorphous CuZrAl alloy at 300 K, b) liquid state from heating at 2000 K of the c) crystal B2 type. Figure 2 shows the Voronoi polyhedra histograms performed on $Cu_{50}Zr_{50}$ and $Cu_{45}Zr_{45}Al_{10}$ using two cooling rates. We observe that the presence of aluminium increases the <0,0,12,0> polyhedra fraction, same effect produce the lowest cooling rate. We choose the lowest cooling rate and containing 10% aluminium for impact samples.
Figure 3 shows the initial configuration. In the impact simulation we study the deformation of the nanoparticle by varying the velocity of impact and the temperature of the nanoparticle (Figure 4). We also studied the deformation processes in the presence of Cu and CuZr nano-crystals. Figure 5 shows the shear strain calculations performed with the atomic strain tensor modifier from OVITO. Finally, we analyzed the temperature reached in the impact. Figure 6 shows the temperature during a impact at 2000 m/s for the nanoparticle, substrate and three temperature control zones (TCZ).

Conclusions

-Embedding. According to the initial velocity of the particle, there are two schemes: for velocities less than 2000 m/s a fraction of the particle is outside the target, whereas at velocities greater than 2000 m/s a full inlay is verified.
-Variation of the particle temperature between 100 K and 300 K produces similar results for each initial velocity.
-We observe the formation of shear bands. For the inclusion of Cu nanoparticle the simulation shows dislocations in the nearest particles.

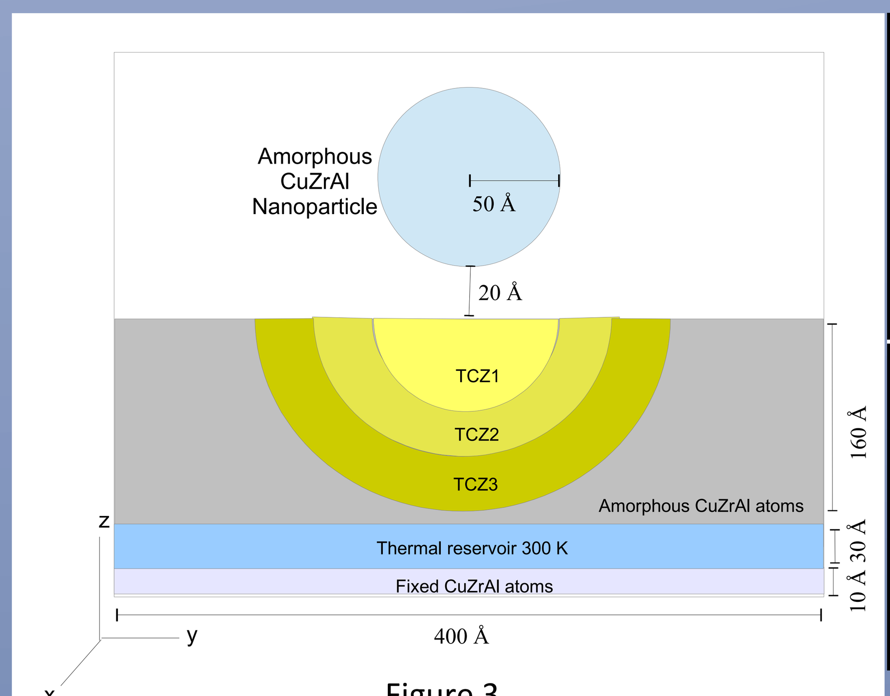
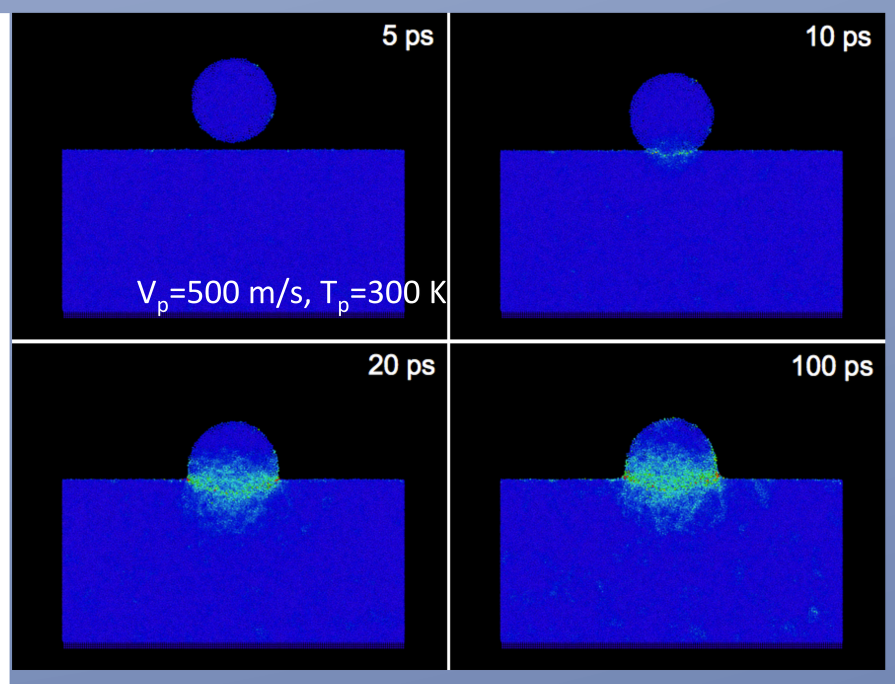
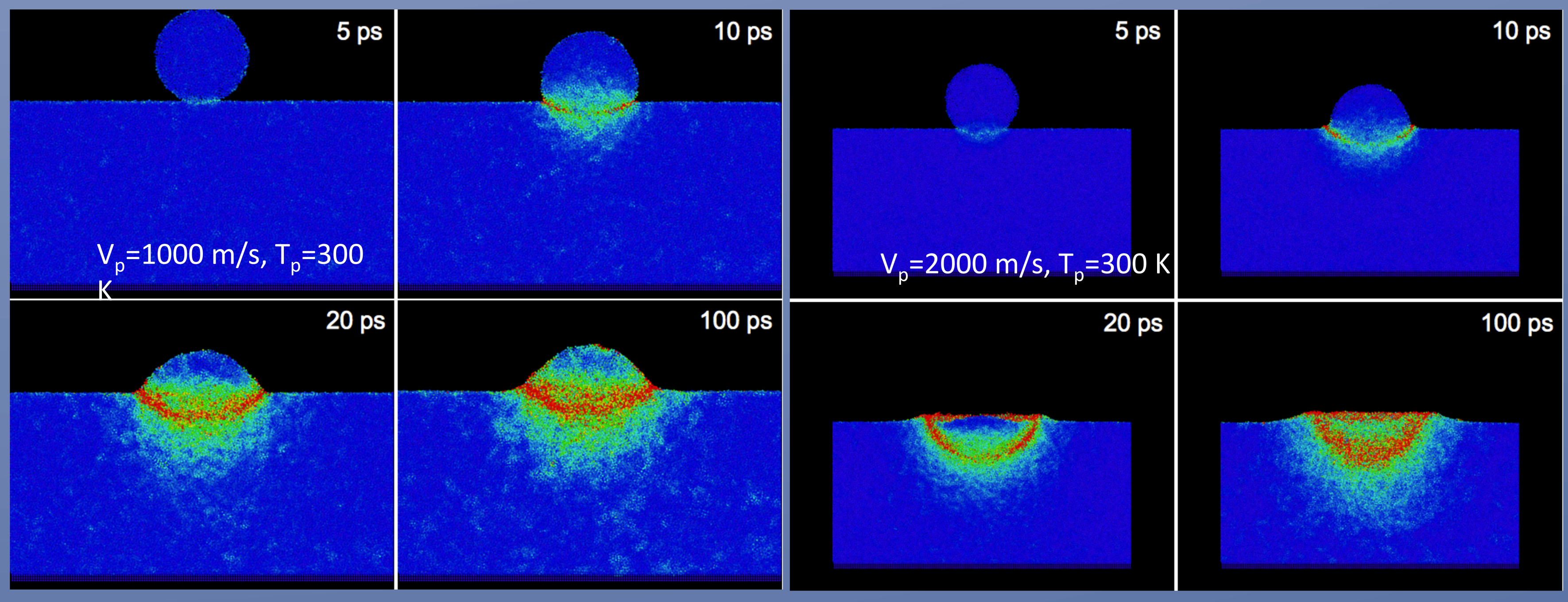


Figure 3





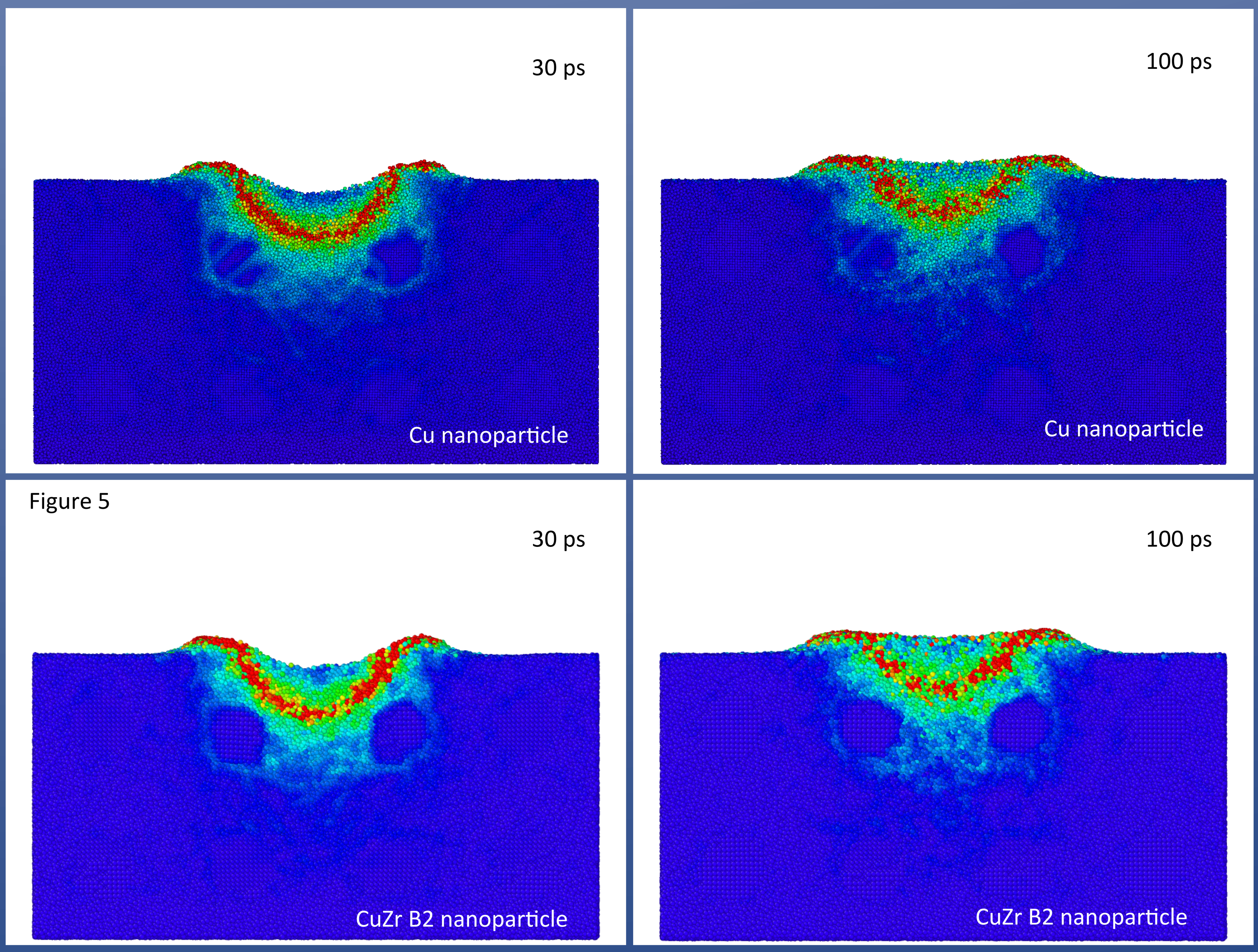


Figure 5

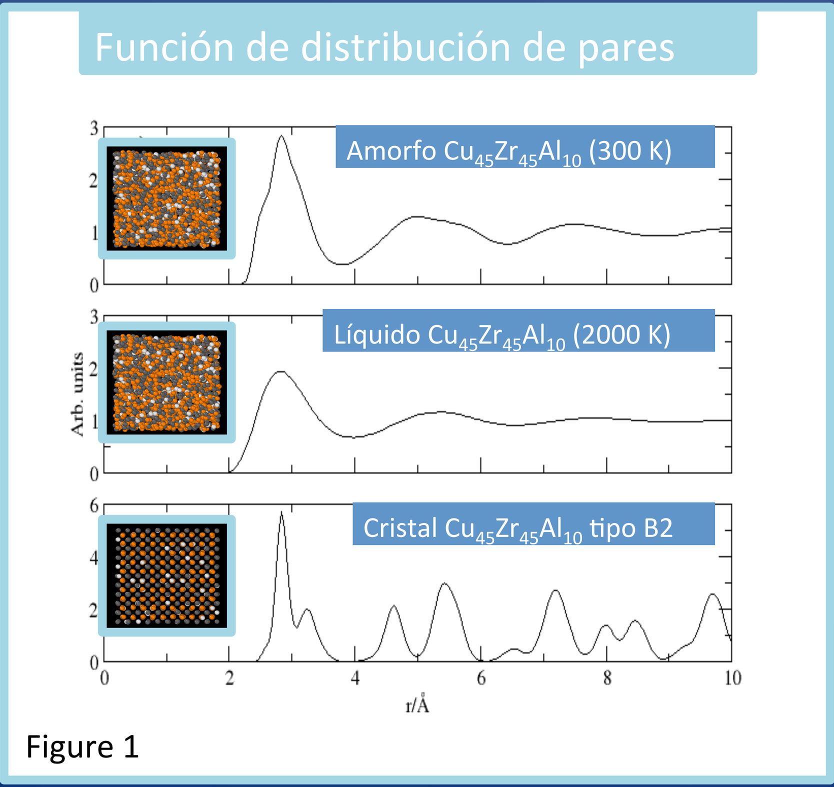


Figure 1

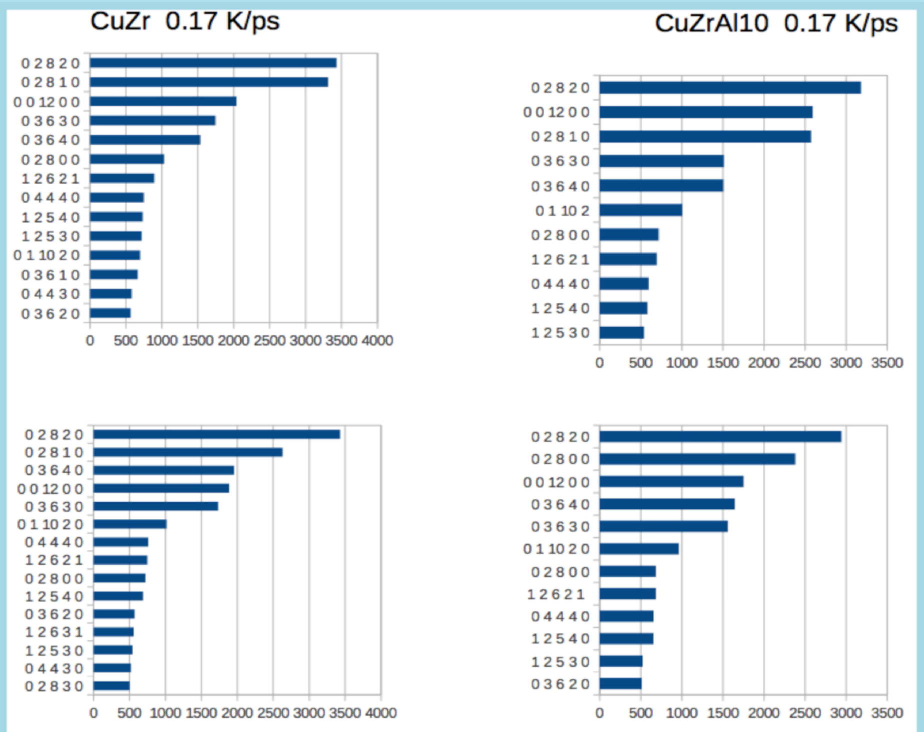


Figure 2

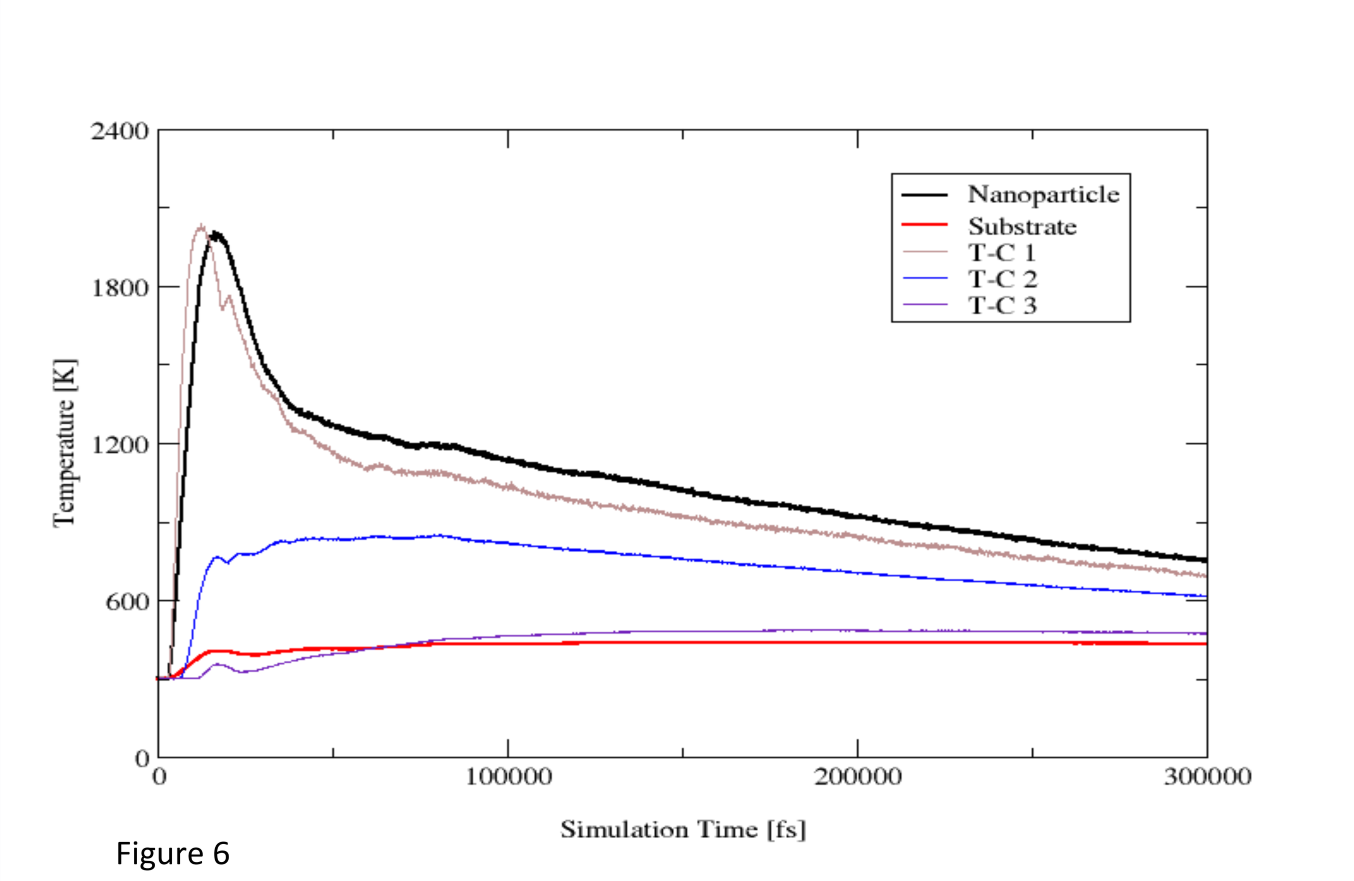


Figure 6

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