Supplementary material for

Assessment of phenomenological models for viscosity of liquids based on non-equilibrium atomistic simulations of Copper

MD Simulations of Solid and Liquid Phases of Copper Using Q-SC Force Field

The quantum effects modified Sutton-Chen type of many-body potential (Q-SC) has been tested for accurate property values of crystal phases.[8] In addition, we studied the static liquid structure and solid-liquid phase transition using the same force field before we extended it for viscosity studies of liquid copper. The radial distribution function and static structure factor obtained from simulations agrees with experimental values (Fig. 1). The solid-liquid phase transition was studied by both constant-rate heating and cooling (Fig. 2) and two phase simulations (Fig. 3). The melting point obtained from 10ps/100K rate heating is about 1250K, while the two phase simulations suggest a melting point around 1100K. Since the simulation time was very short and the heating rate was high, superheating effects were expected in heating process. Both melting temperatures are lower than the experimental value 1358K, which might arise from the small model system used in our simulations.

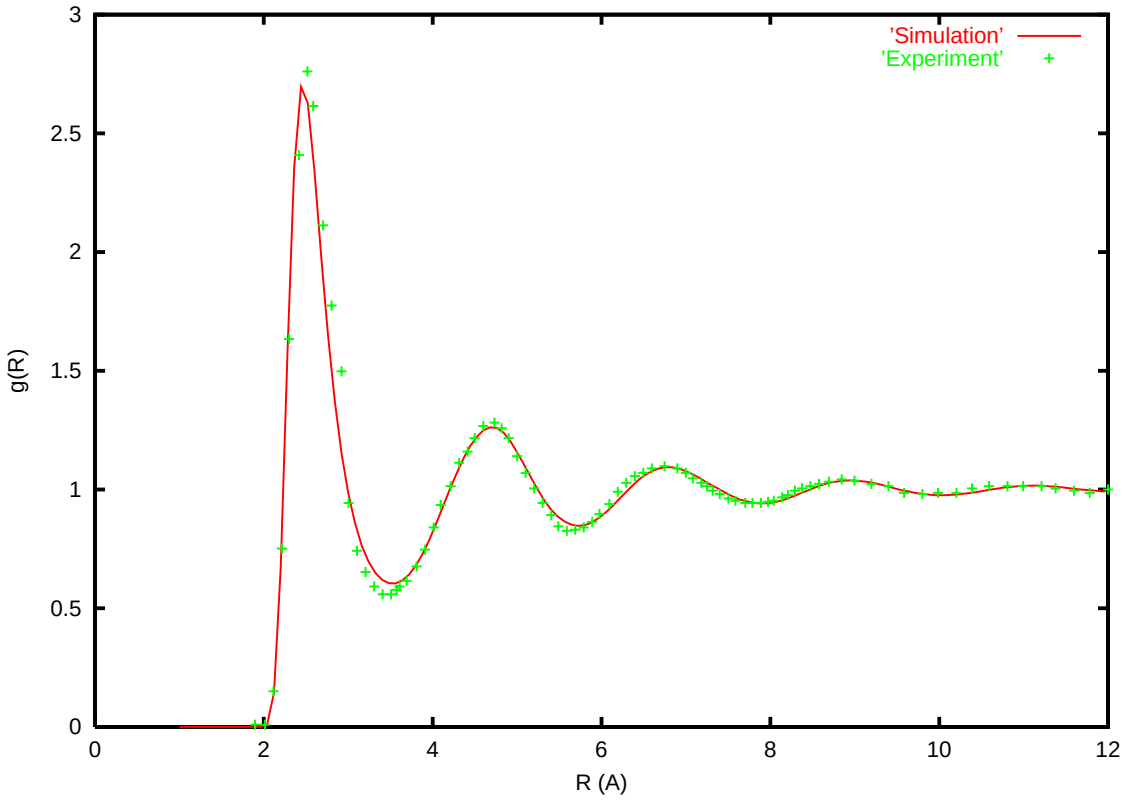
In summary, our results validate of the Q-SC potential for use in liquid copper study.

FIGURE CAPTIONS

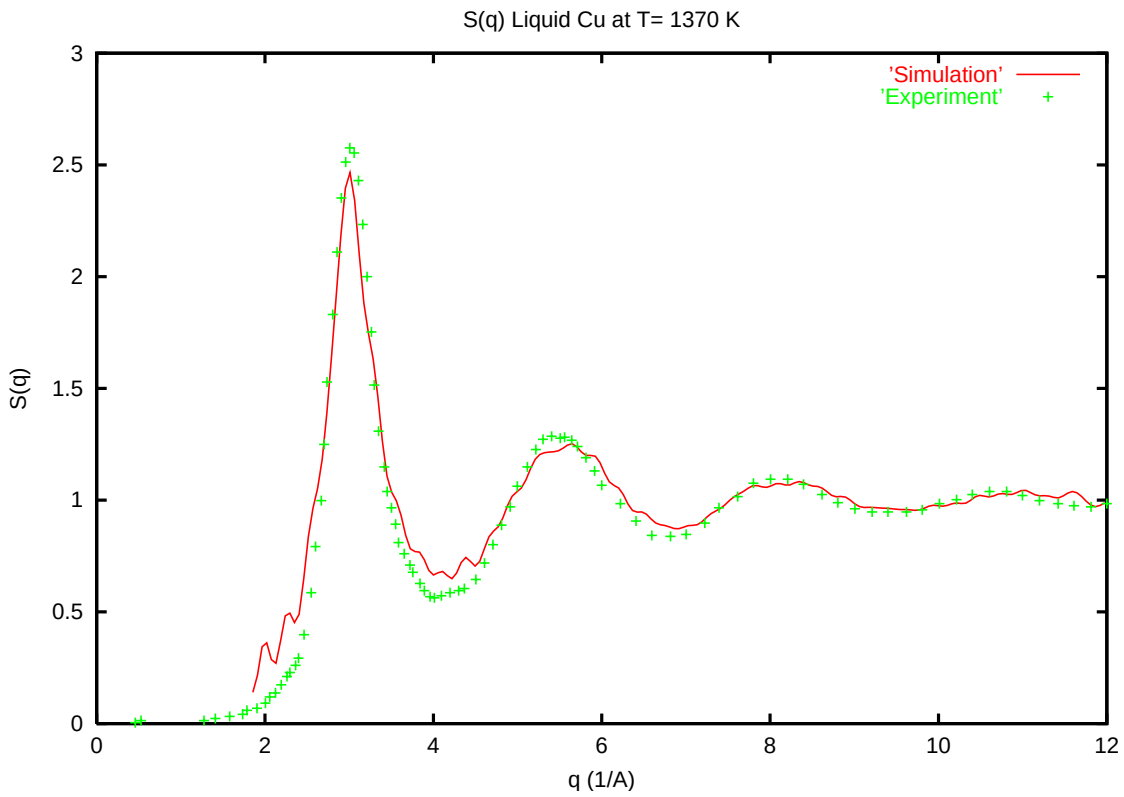
Figure 1: Radial distribution function (a) and static structure factor (b) from simulation at T=1370 K and experiment from *Y. Waseda, The structure of noncrystalline materials, McGraw Hill Publ. Co. NY, 1980*. The density of simulated liquid is 3% less than the experimental density.

Figure 2: Volume (a) and Total energy (b) variation during the heating and cooling process of Cu (1008 atoms). Characteristic temperatures Tm and Tg are obtained from the heating and cooling curves.

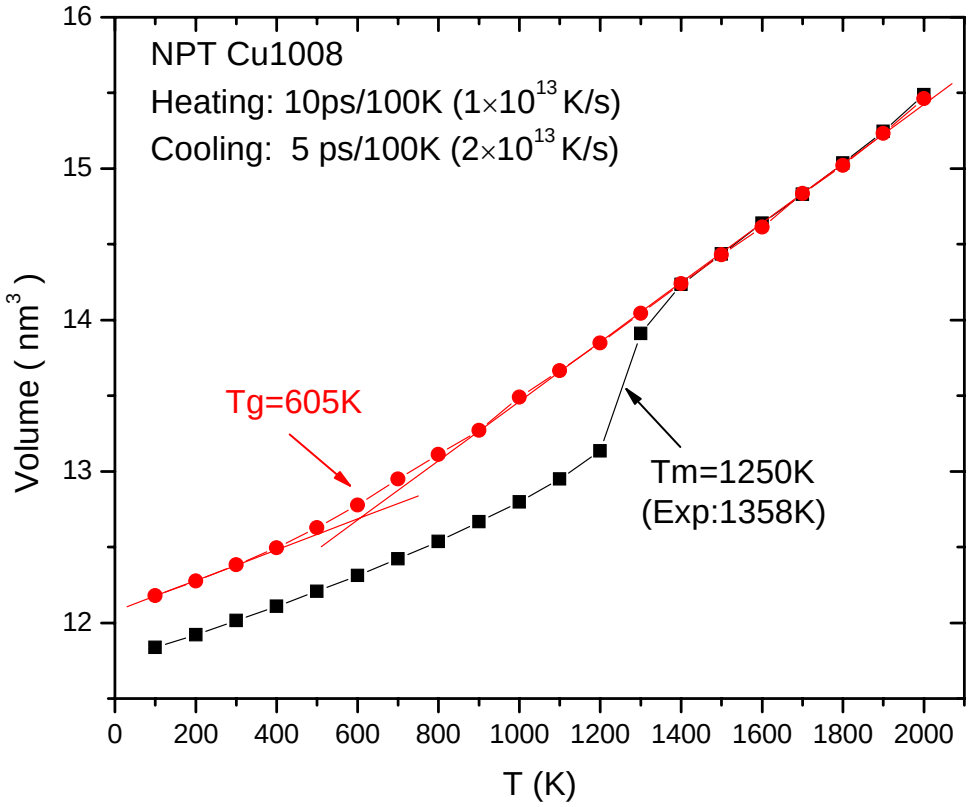
Figure 3: Total energy evolutions near melting point in two phase (crystal-liquid) NPT simulations of Cu. (a) FCC(111)-liquid interface, starting from 504 atoms in crystal phase and 504 atoms in liquid phase with interface period around 3.8nm. (b) FCC(100)-liquid interface, starting from 500 atoms in crystal phase and 500 atoms in liquid phase with interface period around 3.6nm.



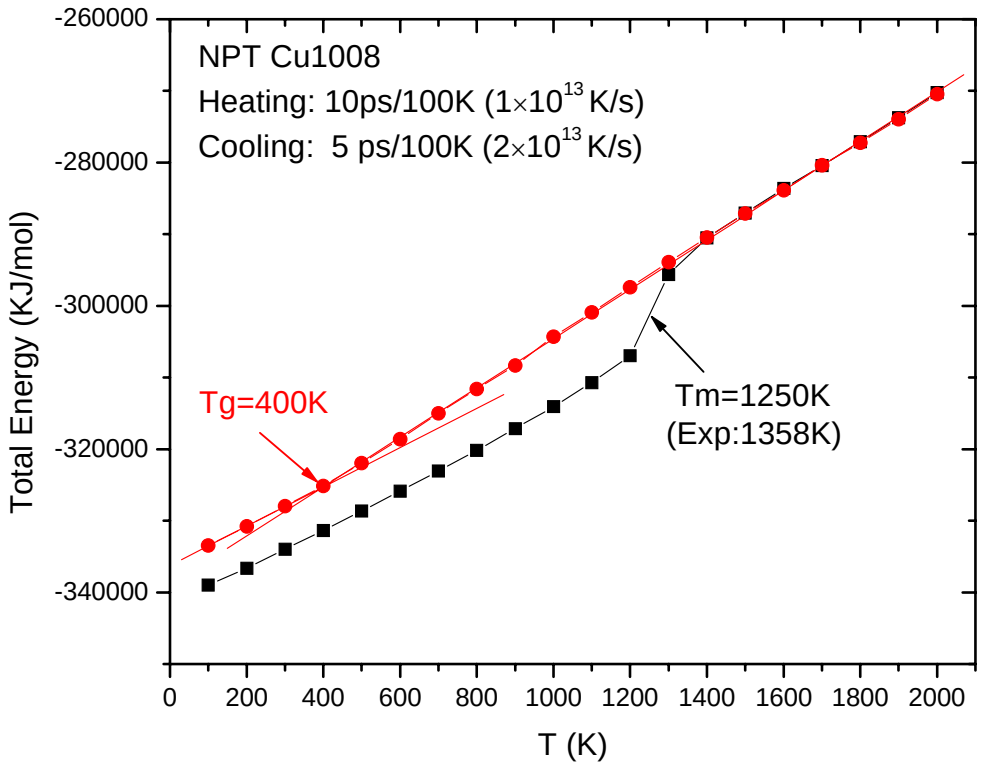
Peng Xu et al., Fig. 1a



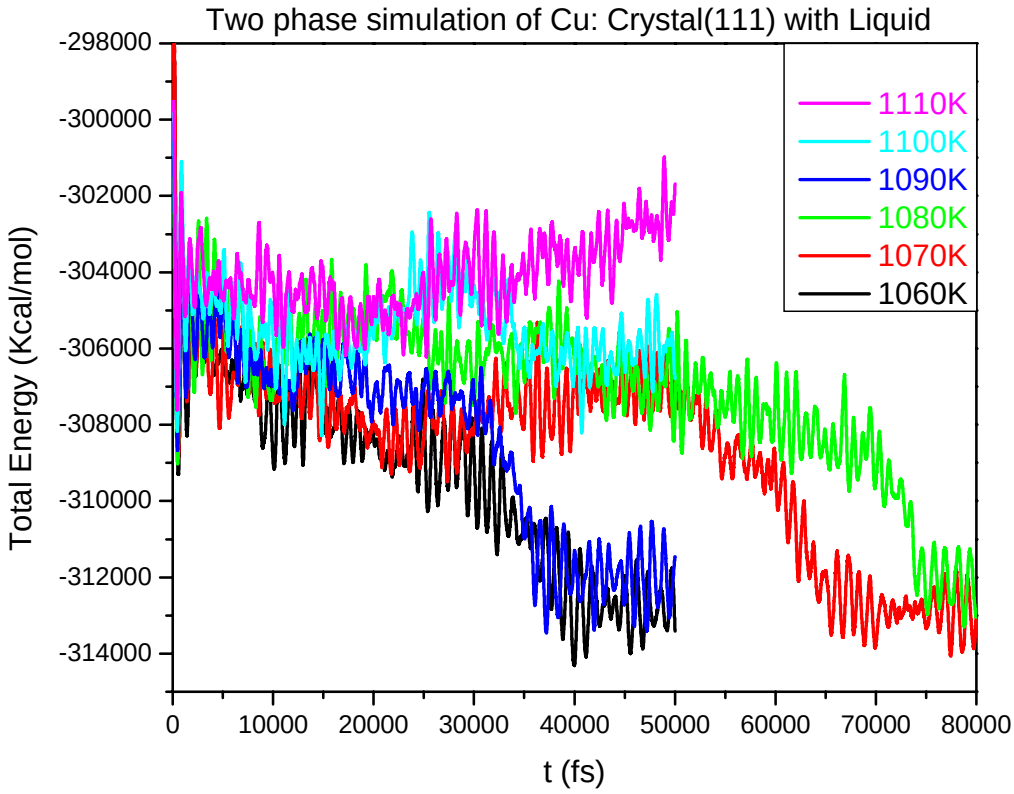
Peng Xu et al., Fig. 1b



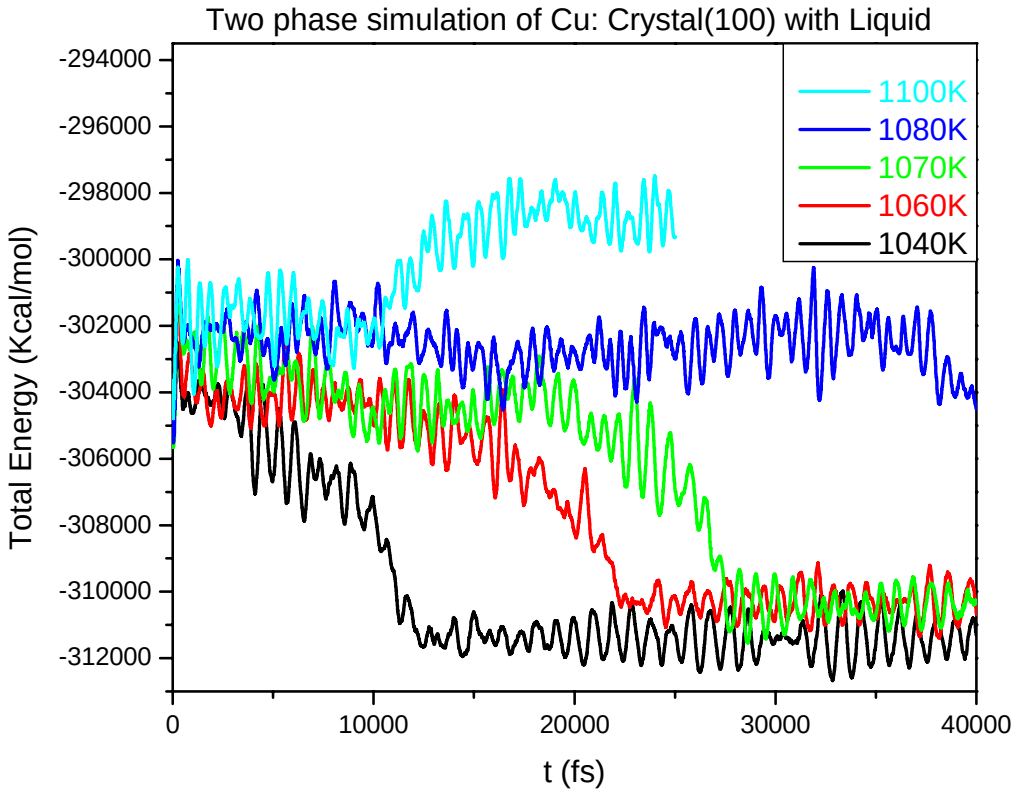
Peng Xu et al., Fig. 2a



Peng Xu et al., Fig. 2b



Peng Xu et al., Fig. 3a



Peng Xu et al., Fig. 3b