Heterogeneous melting- New insight from atomic mechanism

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Introduction

Melting in reality is always influenced by the effects of free surface.

There is an evidence that melting initiates at the surface and propagates into the interior of crystals. The mobility of surface atoms plays a fundamental role [1]

Ref [1]: F. Delogu, Phys. Rev. B 73, 184108 (2006)

There is no work related to the monitoring spatio-temporal arrangements of liquid-like atoms during the heating process.

It motivates us to carry out this study

Calculations

Using classical Molecular Dynamics simulation with the Embedded Atoms Method Potential proposed in [2].

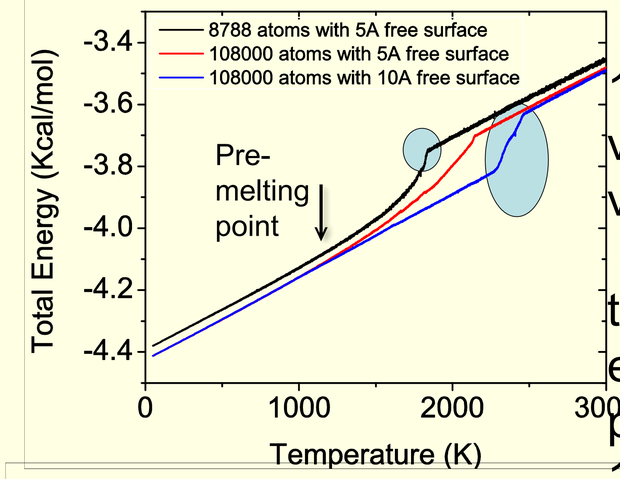
Ref [2]: SM Foiles et al, Phys. Rev. B 33, 7983 (1986)

Two free surfaces in the z direction and periodicity in x, y directions are used in this simulation.

Models include the perfect fcc Nickel lattice of the size 13x13x13 and 30x30x30.

Models are relaxed at 50K and heated up to 3000K with $3x10^6$ MD step. Time step is 1.0fs.

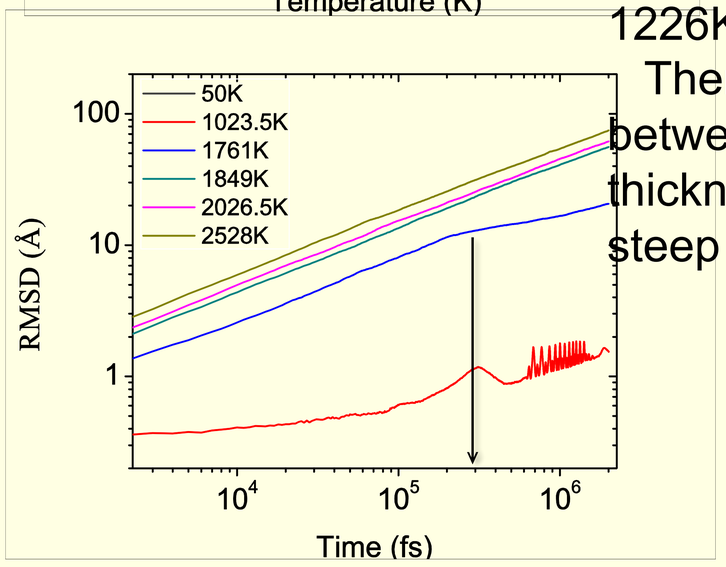
Thermodynamic properties



Melting point of model 13x13x13 is 1826K versus experimental value – 1728K.

Due to deviation from the linearity of total energy, the pre-melting point is defined to be 1226K.

There is a relation between the vacuum thickness size and the steep of caloric curves.



RMSDs show that although there is just below the melting point (1761K), displacement of atoms increases then approaches the limit value after a long relaxation. This indicates a stability of the crystalline matrix at T below a melting point.

Atomic mechanism

Using the Lindemann melting criterion to define the liquid-like atoms. [3,4]

Ref [3]: F. A. Lindemann, Z. Phys. 11, 609 (1910)
[4]: Z. Shi, P. G. Debenedetti, and F. H. Stillinger, J. Chem. Phys. 134, 114524 (2011).

Fig 3. shows the same behavior of the caloric curve: liquid-like atoms occur in the pre-melting region and rapidly increase toward the melting point.

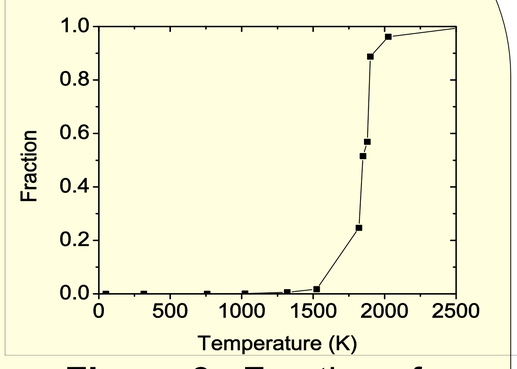


Figure 3: Fraction of Liquid-like atoms upon heating

Liquid-like atoms firstly occur in the surface shell but do not form a purely liquid skin.

The liquid-like atoms propagate into the interior (Fig. 4) and then homogeneous melting of the interior occurs

Figs. 4 and 5: close to the melting point, liquid-like clusters (playing the role of melting nucleation sites) also occur in the interior. This means the homogeneous melting is started.

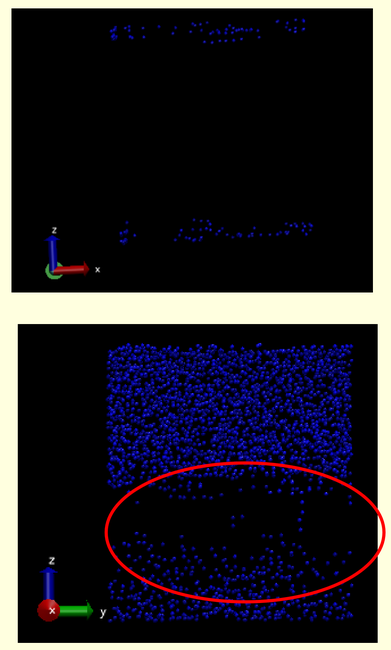


Figure 4: Snapshots of liquid-like atoms at 1525K and 1820K, respectively

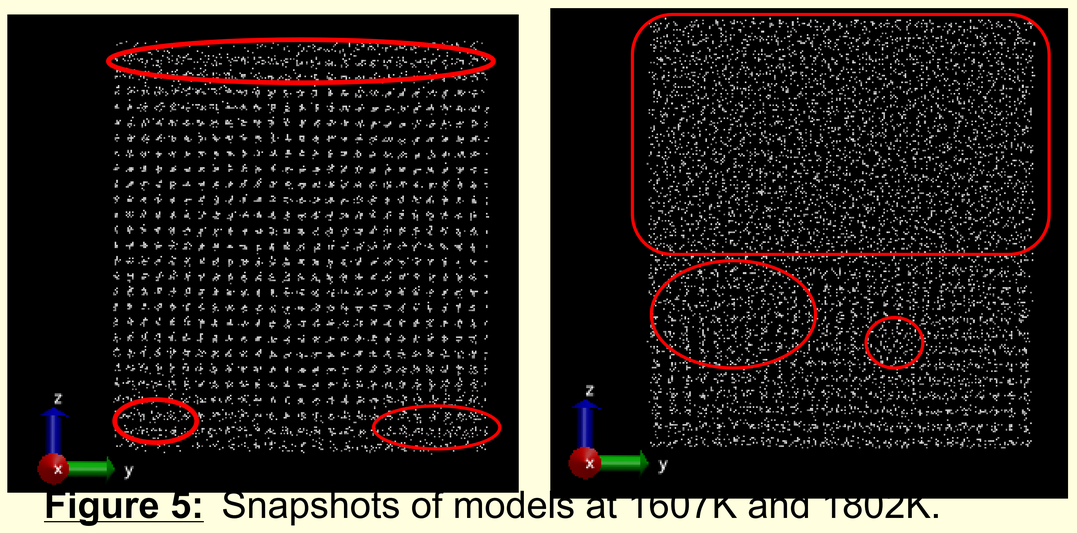


Figure 5: Snapshots of models at 1607K and 1802K. Red circles and squares is used for marking disorder regions

Conclusions

Heterogeneous melting should be undergone as follows: pre-melting of the surface occurs first until the interior reaches the limit of superheating leading to the homogeneous melting of the latter.

This study is helpful to predict the stability of materials surface upon heating up to high temperatures.