First principles calculations of liquid Mo under pressure

Byeongchan Lee[1]* and Geun Woo Lee[2]

[1]*Kyung Hee University, 1732 Deogyeong-daero, Yogin, Gyeonggi, Republic of Korea*
[2]*Korea Research Institute of Standards and Science, 267 Gajeong-ro, Yuseong, Daejeon, Republic of Korea*

Keywords: local order, Mo, first principles calculations

*e-mail: airbc@khu.ac.kr

Many properties of a transition metal liquid can be predicted from first principles molecular dynamics, but the structural properties are of great importance because the detailed information on the liquid structures are not available from experiment yet. The local order calculations can be used to predict the various transitions including the liquid-liquid transition under pressure [1].

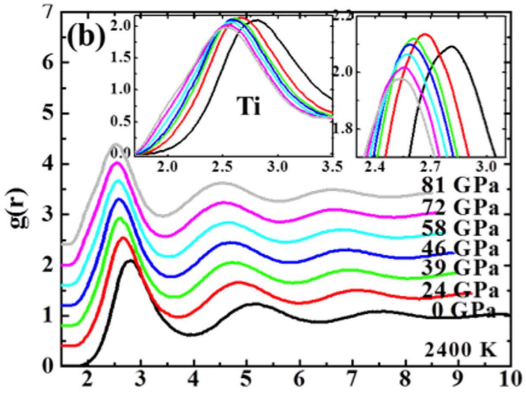

Figure 1. Pair correlation function of liquid Ti at 2400K as a function of pressure [1]. The liquid-liquid transition is observed from the first peak as shown in insets.

Here we present first principles calcullations in liquid Mo. First, the change in local order of liquid Mo is discussed as a function of pressure. The temperature and pressure are kept above the melting curve such that Mo maintains the stable liquid state. Local structures are analyzed with standard techniques such as pair correlation function, and the results are compared and contrasted with those from other liquid transition metals such as Ti and Ni. Ti, Mo, and Ni stand in distinct places in the periodic table, and the difference in the structural properties is related to the effects of valence electrons as we move from the early to the late transition metal zone. The pressure effect is compared with the temperature effect [2].

Second, thermophysical properties such as viscosity are discussed via related functions such as velocity autocorrelation function. The atomic vibration is deteremined from the balance between the viscous effect and the caging effect, and we see a few clear differences between Mo and Ti in the velocity autocorrelation function. The origin of the difference is discussed.

Last, we try to connect the material properties and the melting curve, and discuss the driving force of the liquid-liquid transitions found in some elelmental metals.

Acknowledgments: This work was supported by the Korea Research Institute of Standards and Science and by the Basic Science Program of the National Research Foun- dation of Korea (NRF).

[1] B. Lee, G. W. Lee, *Scientific Reports* 2016, **6,** 35564.
[2] B. Lee, G. W. Lee, *The Journal of Chemical Physics* 2008, **129,** 024711.