Anomalous Structural Change Induced by Strong Electron Exchange-Correlation in an Expanded Liquid Alkali Metal

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One of the central issues in condensed matter physics is to understand the strong exchange-correlation (XC) effect between electrons which may cause some kinds of attraction related to a variety of phenomena such as superconductivity, ferromagnetism, and Wigner crystallization. Besides those kinds of attraction, the XC effect always acts as an attraction in the symmetric Landau's Fermi-liquid interaction for the entire region of the electron density n; this attraction increases monotonically with decreasing n, leading to a strong tendency toward electronic phase separation, which is, however, prohibited from developing macroscopically by the charge neutrality.

An expanded liquid alkali metal is an interesting system in which the latter attraction plays an essential role not only in transport properties but also structural ones. This attraction is, in fact, a driving force for the liquid-gas phase transition necessarily accompanied by the metal-insulator transition [1].

Here we report on our recent study of the local ionic structure of an expanded liquid alkali metal on the basis of a model ionic system derived from the first-principles Hamiltonian by treating the electron-ion pseudopotential as perturbation [2]. Near the liquid-gas phase transition, we have found that R_{NN} the distance between adjacent ions *decreases* despite the increase of the mean interionic distance (or r_s the Wigner-Seitz radius) as shown in Fig. 1. This anomalous structural change is in sharp contrast with the normal one in compressed liquid alkali metals near the liquid-solid phase transition, for which R_{NN} increases with increasing r_s.

In order to elucidate the physical origin of the local contraction of R_{NN}, we consider the interionic equilibration distance R_{eq}, which is determined by the minimum position in the effective interionic interaction potential, because R_{NN} coincides with R_{eq} for low n. From Fig. 2, it is found that R_{eq} *decreases* against the increase of r_s provided that the condition of $2r_c < r_s < 4r_c$ is satisfied with r_c being the radius of the ion core. By the careful analysis on the spatial dependence of the effective interionic interaction, we have revealed that this decrease of R_{eq} is attributed to an enhanced attraction working between valence electrons (or the strong tendency toward electronic phase separation caused by the XC effect), combined with the effect of excluding those electrons from the ion cores.

In Fig. 2, we have also indicated R_{eq} at n_{solid} (the solid densities at ambient pressure and temperature) and at $n_{critical}$ (the critical densities) for Na, K, Rb, and Cs. Since the density in the expanded liquid state is smaller than n_{solid} but larger than $n_{critical}$, we can conclude that the local contraction of R_{eq} and therefore R_{NN} is a universal phenomenon of an expanded liquid alkali metal.

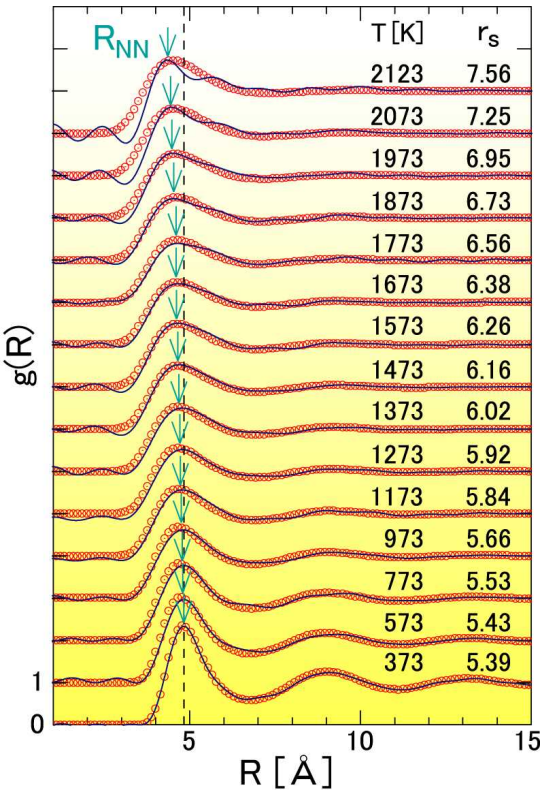

Fig. 1. Comparison between our theoretical results of the radial ion-ion distribution function $g(R)$ obtained by Monte-Carlo simulations on the model ionic system (the red open circle) and the experimental results by Matsuda *et al*. [Phys. Rev. Lett. **98**, 096401 (2007)] (the blue solid curves) for Rb. The distance between adjacent ions R_{NN}, which is determined by the first-peak position in $g(R)$, decreases with increasing r_s.

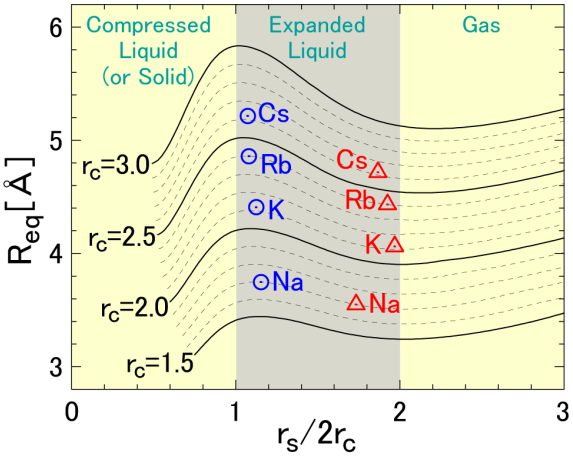

Fig. 2. Interionic equilibration distance R_{eq} with changing r_c from 1.5 to 3.0 by 0.1 versus the ratio of r_s to $2r_c$. For each species, R_{eq} at n_{solid} is marked by a blue circle, while R_{eq} at $n_{critical}$ by a red triangle. R_{eq} decreases against the increase of r_s in the region of $1 < r_s/2r_c < 2$, roughly corresponding to the expanded-liquid regime.

References

[1] H. Maebashi and Y. Takada, J. Phys.: Condens. Matter **21**, 064205 (2009).

[2] H. Maebashi and Y. Takada, J. Phys. Soc. Jpn. **78**, 053706 (2009).

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