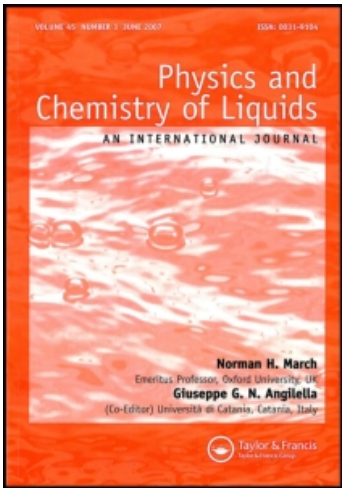

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Comment on Dual-Hard-Sphere Models for Liquid Semiconductors Si And Ge

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COMMENT ON DUAL-HARD-SPHERE MODELS FOR LIQUID SEMICONDUCTORS Si AND Ge

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Various generalized dual-hard-sphere (DHS) models are reviewed on calculating the liquid structure factor for semiconductor elements Si and Ge. It is found that the model generalized by Canessa, Mariani and Vignolo gives the best fitting of experimental structure factor $S_{exp}(k)$ in the range $k < 2k_F$, (k_F, the Fermi wave vector), and all previous models including a new generalized model by the author fail to reproduce the experimental structure factor $S_{exp}(k)$ of Si and Ge in the whole range of k vector.

KEY WORDS: Hard sphere model, structure factor, silicon, germanium, non-simple metals.

It is well known that anomalous behaviour on the first peak of the static structure factor $S(k)$ is found in some liquid metals, such as so-called non-simple metals, Hg, Ga, Sn, Bi, Sb, and semiconductors Si and Ge. Though both group elements show a subsidiary shoulder on the high-k side of the main peak of $S(k)$, there are also some differences between such two groups. For the non-simple liquid metals, the main-peak values of structure factor $S(k)$ are within 2.0–2.5 like the normal liquid metals; while for the liquid semiconductors Si and Ge, the main-peak values of structure factor are around 1.5, which is much lower than the normal liquid metals.

Many attempts have been devoted to explain such anomalies on the main peak for non-simple metals. Orton[1–4] presented originally a dual-hard-sphere (DHS) model to calculate the structure factor $S(k)$ of non-simple liquid metals and liquid semiconductor Si and Ge. Later this model was improved by Canessa, Mariani, and Vignolo (CMV)[5,6] to calculate $S(k)$ for liquid metals Hg, Bi, Ga, Sn[5], and Sb[6]. The CMV model includes six parameters, the packing densities (η_1 and η_2), the hard sphere diameters (σ_1 and σ_2), and the correlation amplitudes (δ_1 and δ_2). The calculated results by the CMV model are in better agreement with experimental $S_{exp}(k)$ than the original Orton DHS model, though the calculation is limited to within twice the Fermi wave-vector, $k \leqslant 2k_F$. Recently, Zou, Jin and Shang (ZJS)[7] have presented another generalized model based on the Orton DHS picture to calculate the structure factor $S(k)$ for non-simple liquid metals Bi, Ga, Sb, and Sn. They use five parameters, the packing densities (η_1 and η_2), the hard sphere diameters (σ_1 and σ_2) and the atomic concentration x of the second type of hard sphere. The advantage of the ZJS model over the CMV model is that ZJS model can fit the experimental $S_{exp}(k)$ in the whole range of k-space instead of the range within twice of the Fermi wave-vector.

Table 1 Parameters used in calculation of $S(k)$. ρ is the atomic density; T_m is the melting temperature.

Elements	$T_m(K)$	$\rho(\text{Å}^{-3})$	η_1	$\sigma_1(\text{Å})$	δ_1	η_2	$\sigma_2(\text{Å})$	δ_2
Si	1683	0.05553	0.157	2.284	4.320	0.285	1.816	1.397
Ge	1210	0.04612	0.103	2.384	7.579	0.542	2.214	0.3178

In this comment, some results are obtained on fitting experimental[8] $S_{exp}(k)$ for liquid Si and Ge by using these generalized DHS model. At first, both CMV and ZJS models are used to fit $S_{exp}(k)$ in the whole range of k-space. It turns out that neither of them can give a good fitting, expecially around the range of the subsidiary shoulder of $S_{exp}(k)$. This problem was also met by Orton[1,4] before. Next, the ideas of both CMV and ZJS, are tentatively extended by using seven parameters $\eta_1, \eta_2, \sigma_1, \sigma_2, \delta_1, \delta_2$, and

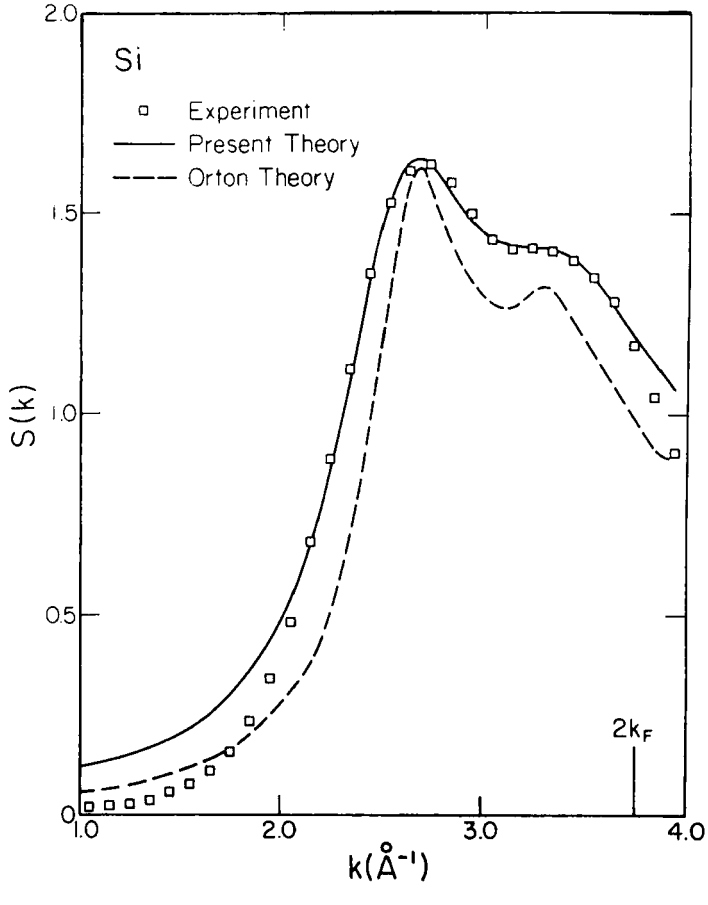

Figure 1 Calculated structure factor $S(k)$ of liquid Si in comparison with experimental data[8] $S_{exp}(k)$, the theoretical fitting curve by Orton[4] is also quoted.

x, to obtain a good fit of $S_{exp}(k)$ for liquid Si and Ge. The structure factor of this new generalized modes is expressed as

$$S(k) = (1 - x)S_1^{CMV}(k) + xS_2^{CMV}(k), \tag{1}$$

where $S_i^{CMV}(k) = 1/(1 - \delta_i n C_i(k))$ $(i = 1, 2)$ is the structure factor of each kind of hard sphere, and $C_i(k)$ is the direct correlation function. The results of fitting $S_{exp}(k)$ indicate that this generalized model still fails to reproduce $S_{exp}(k)$ for liquid Si and Ge in the whole range of k-space. Therefore, one can conclude that even though liquid Si and Ge behave like metals, they belong to a different class of non-simple metals.

Finally, these generalized DHS models are applied again to fit $S_{exp}(k)$ only in the range $k \leqslant 2k_F$. The CMV model has been found to show the best agreement in this k-range than any other models, especially, it gives good fitting around the range of the subsidiary shoulder. The results of six parameters in the CMV model are listed in

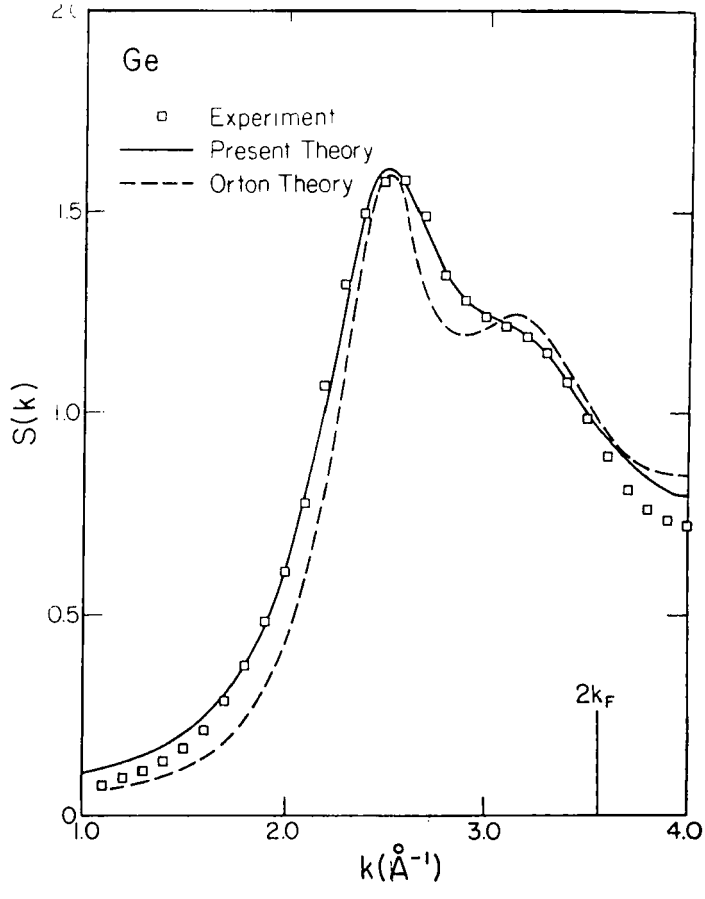

Figure 2 Calculated structure factor $S(k)$ of liquid Ge in comparison with experimental data[8] $S_{exp}(k)$, the theoretical fitting curve by Orton[4] is also quoted.

Table 1 for liquid Si and Ge, the experimental and the calculated structure factors of liquid Si and Ge are shown in Figure 1 and Figure 2.

In summary, the generalized dual-hard-sphere models are tested to reproduce the experimental structure factor $S_{exp}(k)$ of liquid Si and Ge. The model generalized by Canessa, Mariani, and Vignolo gives the best fitting of $S_{exp}(k)$ in the range of $k \leq 2k_F$, however, all versions of DHS models fail to fit $S_{exp}(k)$ in the whole range of k-space. Unlike the non-simple metals Hg, Ga, Sn, Bi, and Sb, further ansatz beyond the simple dual structure picture demands to be taken into account for reproducing $S_{exp}(k)$ of liquid Si and Ge in the whole range of the k-space.

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References

1. B. R. Orton, *Z. Naturf.*, **30a**, 1500 (1975).
2. B. R. Orton, *Z. Naturf.*, **31a**, 397 (1976).
3. B. R. Orton, *Z. Naturf.*, **32a**, 332 (1977).
4. B. R. Orton, *J. Physique, Suppl.*, **41**, C8-280 (1980).
5. E. Canessa, D. F. Mariani, and J. Vignolo, *Phys. Stat. Sol.* (b) **124**, 465 (1984).
6. E. Canessa, D. F. Mariani, and J. Vignolo, *Phys. Stat. Sol.* (b) **126**, K1 (1984).
7. Xian-Wu Zou, Zhun-Ahi Jin, and Ya-Jun Shang, *Phys. Stat. Sol.* (b) **139**, 365 (1987).
8. Y. Waseda, *The Structure of non-crystallic materials, liquids, and amorphous solids* (McGraw-Hill Publ. Co., New York, 1980).