Transverse wave and cage effect in monoatomic liquids from molecular dynamics

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Transverse wave (TW) does not propagate in fluids because there is no shear elasticity. In atomic scale, however, this is not true. The existence of atomic-scale TW in some liquids has been well known since the pioneering study of molecular-dynamics (MD) simulation for collective dynamics of liquid argon [1]. Due to recent developments of inelastic x-ray scattering technique, Hosokawa et al (e.g. [2]) finally succeeded to observe the TW's in some liquid metals. Recent ab initio MD studies (e.g. [3]) show that the cage effect is always observed when TW's occur in liquids. Therefore it is possible that the existence of TW is attributed to the cage effect in liquids. So far, however, no detailed investigation has been reported about quantitative relation between the frequency of the TW and that of the atomic oscillation in a cage.

The purpose of this study is to clarify the relation between TW and cage effect in monoatomic liquids quantitatively from MD simulations. To obtain a high statistical accuracy of dynamic structure, we performed a classical MD simulation for liquid copper. The reasons why we chose the liquid copper are the experimental dynamical structure factor [2] and a reliable interatomic potential [4] are available. The calculated dynamic structure factor and dispersion relation are in excellent agreement with the experimental data [2]. We have found that the frequency of the TW coincides with that of the atomic oscillation in a cage by the time-correlation function of the relative velocity between arbitrary two atoms in a cage.