ANALYSES OF VIBRATIONS OF Ar_n AND Ar_nCO_2 CLUSTERS BY MOLECULAR DYNAMICS CALCULATION

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Previously, we analyzed intracluster vibrational motions of Ar_n, n=13–55, clusters by use of molecular dynamics method [a]. It was shown that a number of collective vibrations were excited. The vibrations were assigned to breathing, quadruple spheroidal and quadruple torsional vibrations corresponding to the modes of a dense sphere with the radius of Ar_n and the phonon velocities in solid Ar. Such vibrations were observed for Ar clusters by the energy loss of colliding He atoms [b]. The frequencies of these vibrations were found to decrease with the increasing cluster size, suggesting that these vibrational motions are new physical properties of clusters obeying a scaling law.

In this work, the motions of Ar atoms and CO_2 molecule in Ar_nCO_2 cluster produced by addition of CO_2 to the surface of Ar_n cluster, are simulated by use of the classical molecular dynamics method. The potential is calculated by overlapping two-body Lennard-Jones potentials, where an anisotropic potential is used for the Ar-CO_2 interaction. By extracting the breathing and quadruple spheroidal vibrations, the frequencies of these modes are calculated to be: e.g., 33 and 20 cm^{-1}, respectively, for $Ar_{13}CO_2$. These values are almost identical to those for Ar_{13}. This indicates that the addition of CO_2 causes little effect on the vibration of Ar_{13} when the CO_2 molecule is on the surface of Ar_{13}. Cluster-temperature and cluster-size dependence of the frequencies will be presented.

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[a] Y. Ozaki, M. Ichihashi and T. Kondow, Chem. Phys. Lett. 182, 57 (1991); ibid. 188, 555 (1992).

[b] U. Buck and R. Krohne, Phys. Rev. Lett. 73, 947 (1994).