# Studying Atomic Vibrations by Transmission Electron Microscopy.



Studying Atomic Vibrations by Transmission Electron Microscopy

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**Abstract [en]**

We employ the empirical potential function Airebo to computationally model free-standing Carbon-12 graphene in a classical setting. Our objective is to measure the mean square displacement (MSD) of atoms in the system for different average temperatures and Carbon-13 isotope concentrations. From results of the MSD we aim to develop a technique that employs Transmission Electron Microscopy (TEM), using high-angle annular dark filed (HAADF) detection, to obtain atomic-resolution images. From the thermally diffusive images, produced by the vibrations of atoms, we intent to resolve isotopes types in graphene. For this, we establish a relationship between the full width half maximum (FWHM) of real-space intensity images and MSD for temperature and isotope concentration changes. For the case of changes in the temperature of the system, simulation results show a linear relationship between the MSD as a function of increased temperature in the system, with a slope of 7.858Ã—$10^{-6}$ Ã…$^2$/K. We also note a power dependency for the MSD in units of [Ã…$^2$] with respect to the FWHM in units of [Ã…] given by FWHM(MSD)=0.20MSD$^{0.53}$+0.67. For the case of increasing isotope concentration, no statistically significant changes to the MSD of $^{12}$C and $^{13}$C are noted for graphene systems with 2,000 atoms or more. We note that for the experimental replication of results, noticeable differences in the MSD for systems with approximately 320,000 atoms must be observable. For this, we conclude that isotopes in free-standing graphene cannot

be distinguished using TEM.

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