DEPARTAMENTO DE FÍSICA
UNIVERSIDAD DE SANTIAGO DE CHILE

Examen de Grado

Para optar al grado de Magíster en Ciencia con Mención Física

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"Langevin Dynamics for Gas Transport in Carbon Nanotubes"

In this thesis, a one-dimensional Langevin stochastic dynamics algorithm implemented in MATLAB is studied to calculate the self-diffusion of diatomic nitrogen molecules within a single-walled carbon nanotube, of radius 4.3Å, in a temperature range between 10K and 300K. The Langevin dynamics algorithm introduces a damping parameter γ that can be conveniently chosen to adequately capture thermal and interatomic interactions in the system. The nitrogen molecule is considered as a solid sphere with the mass of diatomic nitrogen. Effective potentials were obtained between molecular carbon-nitrogen interactions and intermolecular nitrogen interactions. It was found that the azimuthal potential is not relevant for axial diffusion. Furthermore, the radial potential has two minima, which are the privileged positions where the nitrogen molecules are able to diffuse along the nanotube. The axial potential has a depth of approximately 17K and has the periodicity of the unit cell of the nanotube.

To compare the precision of the results obtained with a stochastic propagation, the 3D molecular dynamics program LAMMPS was used to obtain the diffusion of a molecule of molecular nitrogen at different temperatures within the carbon nanotube. A parameter γ was searched in such a way that the data matched. The parameter γ that is consistent with the data obtained with LAMMPS corresponds to the value of 0.1 THz, where differences were observed below 10K and above 300K. Diffusions at different nitrogen concentrations were calculated with LAMMPS and 1D Lagenvin, where after comparing them it was found that at low concentrations the diffusions are in the same order of magnitude, but at high concentrations close to the saturation point of the nanotube, the 1D Langevin algorithm underestimates the diffusion coefficient, which can be explained by the greater availability of axial diffusion paths in 3D, compared to 1D modeling.

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