Document category	:	ISI Web of Science
Title	:	The Raman Spectra of Nanocomposite Clusters of Atoms in Phosphorous-Selenium Glassy State
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Abstract	:	We make clusters of atoms of the size of less than 1 nanometer by using the density functional theory and from that we obtain the bond lengths corresponding to the minimum energy configuration. We are able to optimize large clusters of atoms and find the vibrational frequencies for each cluster. This calculation provides us with a method to identify the clusters present in an unknown sample of a glass by comparing the experimental Raman frequency with the calculated value. We start with the experimental values of the Raman frequencies of PSe (Phosphorous-Selenium) glass. We calculate the structural parameters of PSe, P4Se, P2Se2, P4Se5, PSe4, P4Se3 clusters of atoms and tabulate the vibrational frequencies. We compare the calculated values with those measured. In this way we find the clusters of atoms present in the glass. Some times, the same number of atoms can be rearranged in a different symmetry. Hence we learn the symmetries of molecules. We find that certain symmetries are broken due to self-organization in the glassy state.
Subject	:	Density-functional theory; Raman spectra; glass; cluster; vibrational frequency
Type	:	Proceedings Paper
Conference	:	Nanosynthesis And Nanodevice
ISSN	:	1022-6680
ISBN	:	978-3-03785-630-7
Publisher	:	Trans Tech Publications Ltd
Year issue	:	2013
Language	:	English