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Carbon plasmas in the infrared: The first steps of a new method

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Mid infrared time-resolved emission (IrLIBS) spectra were recorded from laser-induced carbon plasma at Hampton University, Virginia, USA. These spectra constitute the first report of carbon materials LIB spectroscopy in the mid infrared range. The plasma was induced using a Q-switched Nd:YAG laser. The laser beam was focused to high purity graphite pellets mounted on a translation stage. Mid infrared emission from the plasma in atmospheric pressure background gases was detected by a cooled MCT detector in the range 4.5-11.6 micrometer, using long-pass filters. The spectra were taken in argon, helium and also in nitrogen and were background corrected and noise filtered. A 0.15 m spectrometer with gratings blazed at 8 micrometer was used. Spectral resolution was around 80 nm. Several spectral runs were averaged using a boxcar averager. Even though a gate delay of 10 to 20 microseconds was used, there were strong backgrounds in the spectra. Superimposed on this background broad and noisy emission bands were observed, the form and position of which depended somewhat on the ambient gas. In argon, for instance strong bands were observed around 4.8, 6.0 and 7.5 micrometer. Using atomic spectral data by NIST it could be concluded that carbon and argon lines from neutral and ionized atoms are very weak in this spectral region. The width of the infrared bands also supports molecular origin. The infrared emission bands were thus compared to vibrational features of carbon molecules and clusters of various sizes on the basis of previous carbon cluster infrared absorption and emission spectroscopic analyses in the literature and quantum chemical calculations. Application of these results is expected in materials science, environmental chemistry and also in astrophysics.

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Packing structures and electronic properties of Si-Ge alloy clusters from DFTB calculations

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Over the past few decades, much attention has been paid to the understanding of the structures and properties of SiGe alloy materials owing to their potential applications in a variety of microelectronic and optical-electronic devices. Ge crystallizes in the same diamond structure as Si does, and Ge and Si can be mixed in any ratio to form SiGe alloy materials. These systems may have properties markedly different from those of their macroscopic counterparts and that depend in a highly non-trivial way on the composition and size of the clusters. Accordingly, a detailed understanding about the composition and size effects of SiGe clusters can provide information that is relevant not only for basic science but also for applications. The structural, energetic and electronic properties of small-sized SixGey (x+y=2-9) alloy clusters are studied by using the density functional tight binding (DFTB) method combined with unbiased structure optimization using a genetic algorithms (GAs) method. The results demonstrate a strong dependence of all properties not only on cluster size but also on cluster composition. In general, the Si atoms prefer to be closer to the center of the cluster (defined as the arithmetic average of all nuclear positions), whereas the Ge atoms are further away from the center. Although, in general it is difficult to identify particularly stable clusters containing more than one element; some SixGey clusters are found to be more stable. According to the Mulliken gross populations, an electron transfer from the Ge atoms to the Si atoms is observed, especially for the atoms most far from the center.

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