The Embedded Ring Approach
Applied to Annealed Graphitic Amorphous Carbon
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QUESTION: HOW DOES THE MICROSCALE STRUCTURE OF GRAPHITIC AMORPHOUS CARBON CHANGE WITH ANNEALING TEMPERATURE?

ABSTRACT

Determination of the nanoscale structure and bonding of atoms in highly disordered materials is extremely difficult, but essential in understanding these ubiquitous materials. We perform complex calculations that allow the determination of the medium range order of constituent atoms in graphitic amorphous carbon (g-C) by modeling its Raman spectra, which correspond to the in-plane motion of atoms. Specifically, a dynamical model, the embedded ring approach (ERA), is applied to predict the evolution of vibrations and structure of annealed g-C. We find that the graphitic nature of g-C increases with annealing temperature as evidenced by a greater fraction of 6-membered rings and by sharper peaks in the Raman spectra.

RESULTS AND CONCLUSIONS

The quantitative effects of annealing on the structure of graphitic amorphous carbon can readily be seen in the development of two peaks in the Raman spectra. Raman spectroscopy is a probe of the in-plane motion of the carbon atoms.

REFERENCES


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