Studi teoritik mode vibrasi lokal silikon karbon amorf (a-Si1-xCx:H) dengan metode cluster kisi bethe

Efta Yudiarsah, author

Abstrak

Kerapatan keadaan vibrasi lokal dan fungsi korelasi pada beberapa struktur ikatan di dalam silikon karbon amorf (a-Si1-xCx:H) telah hitting dengan menggunakan model potensial Born dan metode "cluster" kisi Bethe. Mode-mode vibrasi lokal yang disebabkan oleh unit monohidrit (SiH dan CH), dihidrit (SiH2 dan CH2), dan trihidrit (SiH3 dan CH3) telah diidentifrkasi. Studi dilakukan pada dua jenis distribusi atom-atom penyusun bahan amorf yaitu "random sequence" dan "chemically ordered". Skema interpolasi digunakan untuk mendiskripsikan probabilitas ikatan dengan rasio percabangan pohon Cayley. Mode-mode vibrasi yang disebabkan keberadaan atom H di dalam pita fonon bulk silikon karbon sangat dipengaruhi oleh jenis atom tetangga terdekat kedua dari atom H. Mode-mode vibrasi yang disebabkan keberadaan atom H di luar pita fonon bulk silikon karbon hampir tidak dipengaruhi oleh jenis atom tetangga terdekat kedua dari atom H Hasil perhitungan yang diperoleh sesuai dengan data-data eksperimen.

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Vibration Local Modes of Amorphous Silicon Carbon (a-Si1-xCx:H): Theoretical Study by Using Cluster Bethe Lattice Methods. Local vibrational density of states and correlation function for various bonding structures in amorphous silicon carbon (a-Si1-xCx:H) have been calculated by employing Born potential models and cluster Bethe lattice method . The local modes induced by the monohydride (SiH and CH), dihydride (SiH2 and CH2), and trihydride (SiH3 and CH3) units are identified The study has been made for two types of distributions of constituent atoms of the alloy: a random sequence and a chemically ordered The interpolation scheme can relate the bonds probabilities to the branching ratios of a Cayley tree. The vibration modes induced by H atoms inside the bulk phonon region of an amorphous silicon carbon (a-Si1-xCx) are influenced very much by the presence of the kind of atoms lying on the next-nearest-neighboring sites of the H atom. On the other hand, the modes induced by H atoms lying outside the bulk phonon region of an amorphous silicon carbon (a-Si1-xCx) are nearly undisturbed by the presence of the kind of atoms lying on the next-nearest neighboring sites of the H atom. The calculated results are in a good agreement with the available experimental data.