

Studi teoritik mode vibrasi lokal silikon karbon amorf ($a\text{-Si}_{1-x}\text{C}_x\text{:H}$) dengan metode cluster kisi bethe

Efta Yudiarsah, author

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Abstrak

Kerapatan keadaan vibrasi lokal dan fungsi korelasi pada beberapa struktur ikatan di dalam silikon karbon amorf ($a\text{-Si}_{1-x}\text{C}_x\text{:H}$) telah diteliti dengan menggunakan model potensial Born dan metode "cluster" kisi Bethe. Mode-mode vibrasi lokal yang disebabkan oleh unit monohidrit (SiH dan CH), dihidrit (SiH_2 dan CH_2), dan trihidrit (SiH_3 dan CH_3) telah diidentifikasi. 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 ($a\text{-Si}_{1-x}\text{C}_x\text{:H}$): Theoretical Study by Using Cluster Bethe Lattice Methods. Local vibrational density of states and correlation function for various bonding structures in amorphous silicon carbon ($a\text{-Si}_{1-x}\text{C}_x\text{:H}$) have been calculated by employing Born potential models and cluster Bethe lattice method. The local modes induced by the monohydride (SiH and CH), dihydride (SiH_2 and CH_2), and trihydride (SiH_3 and CH_3) 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 ($a\text{-Si}_{1-x}\text{C}_x$) 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 ($a\text{-Si}_{1-x}\text{C}_x$) 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.