INTISARI

Efek Vibrasi Atomik pada *Konsentrasi Vacancy* α-Sn (*Grey Tin*): Komputasi Berbasis *Density Functional Theory*

Oleh

ZOHAN SYAH FATOMI
14/362761/PA/15810

Kajian efek vibrasi terhadap *konsentrasi vacancy* dan kalkulasi energi formasi sistem kristal Gray Tin (α-Sn) dengan menggunakan *Density Functional Theory* telah berhasil dilakukan. Sistem vacancy dimodelkan dengan menggunakan *supercell* 64 atom dengan absensi 1 atom pada daerah sentral *supercell*. Efek vibrasi dilakukan dengan melakukan *komputasi phonon density of states* (phonon-DoS) untuk sistem kristal murni dan vacancy melalui pendekatan fungsi Gaussian. Kemudian frekuensi vibrasi phonon yang telah dihasilkan digunakan untuk menghitung konsentrasi vacancy sistem. Didapatkan nilai energi formasi untuk sistem monovacancy kristal Gray Tin (α-Sn) adalah sebesar 1.89 eV dan nilai konsentrasi vacancy Gray Tin (α-Sn) di titik lebur adalah sebesar 3.68 x 10^3 cm^{-3} namun ketika efek vibrasi atomik dipertimbangkan nilai konsentrasi vacancy bertambah 10^6 x menjadi 6.48 x 10^9 cm^{-3}. Peningkatan nilai konsentrasi tersebut dipengaruhi oleh *softening* yang terjadi pada kristal akibat *defect monovacancy*.

Kata-kata kunci: α-Sn, energi formasi, *konsentrasi vacancy*, *softening*.

ABSTRACT

Atomic Vibrational Effect On Vacancy Concentration α-Sn (*Grey Tin*): Computation Based On *Density Functional Theory*

By

ZOHAN SYAH FATOMI
14/362761/PA/15810

The study of vibrational effect on vacancy concentration and energy formation of Gray Tin (α-SN) using Density Functional Theory (DFT) has been successfully carried out. The vacancy system is modeled by using supercell 64 atoms with an absence of one atom at the central area of the supercell.In this research, The vibrational effect is calculated by computing the phonon density of states (Phonon-DoS) of pure and vacancy systems through Gaussian function approach. Then, The vibrational frequency of the phonon which has been produced is used to calculate vacancy concentration of the system. From our calculation, We obtained that formation energy value of the monovancy crystal system is 1.89 eV, and the vacancy concentration of Gray Tin at the melting point is 3.68 x 10^3 cm^{-3}. However, when the atomic vibration effect is considered to the system the value of the vacancy concentration is increased to be 6.48 x 10^9 cm^{-3}. The results of the calculation showed that the increasing value of the vacancy concentration is influenced by the softening that occurs in crystal systems due to monovacancy defect.

Kata-kata kunci: α-Sn, formation energy, concentration vacancy, softening