

Materials Science and Engineering B97 (2003) 176-181



www.elsevier.com/locate/mseb

A comparative study of thermomechanical characteristics of Si_{34} and Si_{46}

W. Sekkal^a, A. Zaoui^{a,*}, S. Ait Abderrahmane^b

^a Condensed Matter Group, International Centre for Theoretical Physics, Trieste, Italy ^b Physics Department, University of Sidi Bel-Abbes, 22000 Sidi Bel-Abbes, Algeria

Received 30 July 2002

Abstract

A spherically averaged intermolecular potential type Lennard-Jones is used within molecular dynamics simulation in order to investigate the thermomechanical properties of silicon in the clathrates structures. This two-body potential describes well the intermolecular interaction between Si_{34} - Si_{34} and Si_{46} - Si_{46} . Results show that the diamond structure of silicon remains stable than the clathrates ones, although the difference in energy is quite small. We have also found that the volume of Si_{34} and Si_{46} increases by about 17% compared to silicon in the diamond structure. Several thermodynamics quantities are given for both materials. \bigcirc 2002 Elsevier Science B.V. All rights reserved.

Keywords: Chlatrates; Thermomechanical properties; Molecular dynamic

1. Introduction

The search for a direct energy gap materials based on a group IV semiconductors has been stimulated in the past few years by novel crystal growth techniques such as MBE and laser crystallization. Theoretical efforts for predicting group IV materials that are likely to have direct gaps have been concentrated in four areas. The first one is the investigation of materials where the cubic symmetry is broken and the zone-edge states are folded back to the center of the zone as in the models of porous silicon [1,2], and Si-Ge superlattices [3]. The second area focuses on predicting the properties of IV-IV alloys with a diamond structure [4]. This in fact alters the chemical and structural environment of the bulk material in a uniform way. The third area is the modifications of the electronic band structures of tetrahedral semiconductors by closed-shell atoms at the interstitial sites [5,6]. The fourth area is by lattice expansion effects, rather by universal substitutional

insertion. Applying negative pressure could produce more open structures [7,8]. However, it has not been studied thoroughly. The other results to band gap engineering has been the incorporation of large numbers of impurity atoms, around which the elemental semiconductors atoms nucleate.

One particular class of structures that grow according to this mechanism are the clathrate hydrate structure [9,10]: Si₃₄ and Si₄₆. Both structures are cubic. Si₃₄ is derived from a packing of dodecahedra and hexakaidecahedra (16-hedra) in the ratio 2:1 and the average ring size is 5.064. There are $4 \times 34 = 136$ Si atoms per facecentered cubic unit cell, which has the same symmetry as diamond (Fig. 1(a)). Si₄₆ lattice is a simple cubic (sc) lattice with a lattice constant near 10 Å and is shown in Fig. 1(b). At each sc lattice point, a Si_{20} icosahedral molecule is placed with another Si_{20} rotated 90° with respect to the first, placed at the body center of the cube. Each Si atom in the pentagonal dodecahedron is bonded to three other atoms within the same dodecahedron. The fourth bond is one of two types. The first type of bond connect one Si₂₀ unit with another. To make the solid fully fourfold coordinated, a second type of bond is formed by adding 12 atoms surrounding the Si_{20} ball.

The study of structural and thermodynamic properties of silicon in the clathrates structures are at present

^{*} Corresponding author. Address: Max Planck Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart, Germany. Fax: +49-711-689-3522

E-mail address: zaoui@marvin.mpi-stuttgart.mpg.de (A. Zaoui).