Vegard's Law in the $Si_{1-y}C_y$ alloys

RAHMANI MOHAMED
Laboratoire d'Étude des Matériaux & Instrumentations Optiques ,Physics Department
University Djillali Liabes of Sidi Bel Abbes,Algeria
eddrre@yahoo.fr-rahmani_m77@yahoo.fr

YAKOUBI ABDELKADER
Laboratoire d'Étude des Matériaux & Instrumentations Optiques ,Physics Department
University Djillali Liabes of Sidi Bel Abbes,Algeria
Yakoubi_aek@yahoo.fr

***Abstract*—In this work, we presented a calculated of structural properties of the $Si_{1-y}C_y$ binary alloys, the atomic structure of this alloys is important for understanding its properties. We used theories of bond-length of Vegard's approach based of the method of linear augmented plane wave (FP-LAPW) based on the theory of density functional (DFT). We also studied the structural properties of this alloys with the LDA approximation for the potential for exchange and correlation. Our study affirms that the lattice constant is approximately equal to the composition-weighted average of the lattice constants of the pure materials.**

Keywords:Alloys;Vegar'slaw;Structural properties;SiC

I. INTRODUCTION

In this paper we report the calculation of structural properties of Si,C and $Si_{1-y}C_y$ binary alloy in their use of a supercell 08 and 16 atmos to understand and detailed the effect of the cell size as well that the concentration of C in the Si. The physical properties of binary alloys are usually investigated with the Vegard's law, assuming that the lattice constant of a binary alloy can be expressed as a linear combination of the lattice constants of the two forming silicon and carbon materials. In this work, we first investigate the equilibrium lattice constant deviation from the Vegard's law in the diamond structure for Si, C and their binary. which are carried out of first principles calculations by means of a supercell with plane wave pseudo potential based density functional theory (DFT) in the local density approximation (LDA).

II. METHOD CALCULATES

The calculations were made using the FP-LAPW approach used in the WIEN2k code [1] that operates under the DFT [2, 3]. This approximation is set by Perdew and Wang[4]. This last calculates the self consists of Kohn and Sham solution [5] who decry the valence electron in a potential created by a periodic array. Basic functions, electron densities and potential are extended in combination of spherical harmonics around atomic sites, that is to say the atomic spheres with a cutoff Imax = 10 and Fourier series in the interstitial region. to obtain the convergence of the Eigen values, the plane wave functions with a cutoff Rmt * Kmax = 7 in these calculations we treated the statements Si ($1S^2 2S^2 2P6$) and C ($1S^2$) as valence. for the elements Si and C we used the muffin-tin radii, RMT of 1.9 and 1.8 Bohr respectively.

III. RESULTS AND DISCUSSION

to study the structural and electronic properties of $Si_{1-y}C_y$ it is essential to study first those parent elements Si and C, the calculated values of the equilibrium lattice parameters, compressibility modules and their derivatives for Si and C and their binary alloy of the supercell 08 atoms and 16 supercell atoms are given in Table1 and Tabel2 respectively, results compared with other calculations and experimental data available.

Good agreement is observed with the experimental and theoretical data with an underestimation of network parameters for the two elements Si and C, and an overestimation of the modulus versus the experimental because the use of LDA, compared to C we notice that the bulk modulus of Si is much lower, so we can expect that Si is less hard than C.

the variation in lattice parameter depending on the concentration for the binary alloy $Si_{1-y}C_y$ lighters shows a deviation from that of the linear interpolation of binaires. this deviation is due to the relaxation lengths Si-C.

The Variation of the concentration depending on the network parameter y (solid line), compared with that obtained by the Vegard law (red line).given in Table1 and Table2 respectively

TABLE I. **THE VALUES RESULTED FROM VEGARD'S LAW AND THEIR DEVIATIONS FROM THIS CALCULATIONS OF 08 SUPERCELL**

Y	*a*(Å)	*a*(Å) VCA	Other cal.	dev. values	Exp.
0	5.463	5.463	5.314[a]	0	5.429[b],5 .431[c]
0.125	5.213	5.222	5.218[a]	-0.009	
0.25	4.979	4.981	4.979[a]	-0.002	
0.375	4.690	4.740	4.694[a]	-0.05	
0.5	4.332	4.499	4.329[a]	-0.167	
0.625	4.201	4.258	4.202[a]	-0.057	
0.75	4.033	4.017	4.038[a]	0.016	
0.875	3.816	3.776	3.821[a]	0.04	
1	3.535	3.535	3.540[a]	0	3.567[b]

[a], [b] **Ref. [6], [7]**

[c] **Ref.[7]**

TABLE II. **The values resulted from vegard's law and their deviations from this calculations of 16 supercell**

Y	*a*(Å)	*a*(Å)Vegard's law	dev. values	Other cal.	Exp.
0	5.463	5.463	0		5.429[b]
0.0625	5.375	5.3425	0.032		
0.125	5.238	5.222	*0.016*	*5.238*[a]	
0.1875	5.154	5.1015	0.052		
0.25	5.062	4.981	0.081	*5.062*[a]	
0.3125	4.954	4.8605	0.093		
0.375	4.663	4.740	-0.077	*4.663*[a]	
0.4375	4.775	4.6195	0.155		
0.5	4.668	4.499	0.169	*4.668*[a]	
0.5625	4.544	4.3785	0.165		
0.625	4.41	4.258	0.152	*4.410*[a]	
0.6875	4.257	4.1375	0.119		
0.75	4.138	4.017	0.121	*4.138*[a]	
0.8125	4.005	3.8965	0.108		
0.875	3.853	3.776	0.077	*3.853*[a]	
0.9375	3.681	3.6555	0.025		
1	3.535	3.535	0		3.567[b]

[a], [b] Ref. [6], [7] [c] Ref.[7]

IV. CONCLUSION

In the results presented here, both positive and negative deviations from Vegard's law were obtained and the deviation values are listed in table(1) and (2). Such deviations, as mentioned in introduction were also reported by previous results.

The properties structural of the binary alloy $Si_{1-y}C_y$ were calculated using the empirical pseudopotential method. By adjusting the form factors of the pseudopotential, agree well with reported experimental data.

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