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First Principles Calculations on Σ 3 Grain Boundary Impurities in Polycrystalline Silicon

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1. Introduction:

Currently, over half of all solar cells produced worldwide are made from polycrystalline silicon (pc-Si). While these devices have comparatively lower efficiencies mainly due to transition metal impurities (10^{14}–10^{16} cm^{-3}) in most of the pc-Si materials[1]. Metal silicide precipitate is observed to increase with decreasing atomic coincidence within the grain boundary (i.e. increasing Σ values) [2]. The effect of impurity in the grain boundary (GB) of pc-silicon was studied using Σ 9 tilt boundaries by Fujita *et al*[3]. In the present study we used DFT method to understand relationship between sigma value and impurity precipitation. First we study the dopant position and the nature of interaction between the GB and transition metal. Finally we have studied the electronic changes that occurred up on doping the transition metal impurities in the GB region.

2. Results and discussion

Σ 3 (112) grain boundary of pc-silicon was constructed using GB studio[4]. We used VASP code for geometrical optimization. The calculations were performed with monkhorst-pack of 4x4x4, using projector augmented wave (PAW) pseudopotentials with a wave cutoff of 240 eV. The Perdew – Wang (PW91) functional is used for the generalized gradient approximation (GGA) [5]. Periodic boundary condition was applied along x and y axis of the super cell containing 96 atoms. To validate our studies we used one Copper, Iron, Nickel and Chromium atom as dopants and compared our findings with the experimental results[2]. The optimized structures of Σ 3 GB along with the interstitial and substitution site doped Cr is shown in Figure 1. To know the suitable position of dopant we optimized structures by placing dopants both at the interstitial and at the substitution sites. Up on complete relaxation atomic migration of atoms were found to be minimal along the grain boundary plane, which is inline to the experimental results.

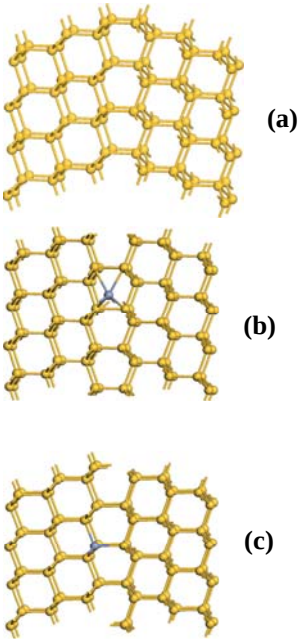

Figure 1: Full optimized structure of (a) of Σ 3 grain boundary (b) chromium doped at the

Interstitial site and (c) chromium doped at the substitution sites

Table 1 shows the segregation energy, Barder charge both at the interstitial and substitution sites for the dopants. It is evident for the table substitution sites are favorable for doping compare to interstitial site. Among the metal impurity copper has highiest segregation energy which is consistent with the experimental observation[6]. The Fermi energy for the system decreases upon doping. Bader analysis shows that charge transfer occurs from the metal to silicon for the Cr but in the other cases silicon to metal charge transfer was observed.

Table1. Bader charge, segregation energy and Fermi energy for metal doped in Σ 3 GB of pc-Si

System		Bader charge on metal (*e*)	Segregation Energy SE# (eV)	Fermi Energy E_f (eV)
M	Site			
Cr	I*	0.8997	7.32	4.14
	S*	0.8507	1.59	3.94
Fe	I	-0.2358	6.75	4.06
	S	-0.3385	1.28	4.05
Ni	I	-0.3022	5.36	4.03
	S	-0.3219	0.57	3.87
Cu	I	-0.1489	2.79	4.07
	S	-0.4052	2.82	3.89

* - I – interstitial & S- substitution ; $\#SE = (1/2)[E_{MGB} - E_{SiGB}] - (1/2)[E_{Mbulk} - E_{Sibulk}]$

3. Conclusions

In conclusion we have carried out DFT studies on the Σ 3 (112) GB of pc- silicon and its doped transition metal structures. Doping process reduces the Fermi level of the system. Energy calculation shows substitution site is the preferred for the transition metals in the GB region of Σ 3 (112) pc-silicon. Due to replacement of silicon with metal atoms a minimal dislocation of atom along the GB plane was observed.

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References:

1. D. Macdonald, A. Cuevas, A. Kinomura, Y. Nakano, and L. J. Geerligs, J.Appl. Phys. **97** (2005) 033523.

2. T. Buonassisia , A. A. Istratov, M. Heuer, M. A. Marcus, J. Isenberg, Barry Lai, Z. Cai, S. Heald W. Warta, R. Schindler, G. Willeke and E. R. Weber J. Appl. Phys. **97**(2005) 074901.

3. K Masuda – Jindo and Y. Fujita **Polycrystalline Semiconductor II** J.H Werner (eds) Springer Proceeding in Physics Vol. 54. 139 - 144.

4. H. Ogawa, Mater. Trans. **47** (2006), 2706-2710.

5. G. Kresse, D. Joubert, Phys. Rev. B 59, 1758 (1999).

6. Scott A. McHugo Appl. Phys. Lett. **71** (1997), 1984-1986