

**Diebel and Dunham Reply:** Fiorentini and Lopez [1] have identified a lower energy structure for the  $F_4V$  complex than the higher symmetry structure which we considered in Ref. [2]. Our calculations using the methods described in Ref. [2] confirm the lower energy of this structure. By exploring a range of configurations, we also found lower energy structures for  $F_3V$ ,  $F_4V_2$ ,  $F_5V_2$ , and  $F_6V_2$ . The energy differences are most significant for higher F to V ratios, and these  $F_nV_m$  structures have rotated Si-F bonds similar to  $F_4V$ , which allow larger F-F spacing as noted in the Comment [1]. In this Reply, we have updated Table I and Fig. 3 from Ref. [2] to include these values. While some of the numbers have changed, the overall conclusions of our work on F in Si [2,3] remain valid (and are, in fact, confirmed in a recent paper by the authors of the Comment [4]): The strong binding of F to vacancies leads to immobilization and segregation of F in V-rich regions during ion implant annealing, giving rise to apparent uphill F diffusion and reduction of B transient enhanced diffusion.

In Table I, the formation and binding energies for different  $F_nV_m$  configurations are listed. For two or more F atoms,  $F_nV_m$  structures are favored over the interstitial configurations. For the  $F_nV$  structures, the binding energy gained by adding additional fluorine atoms is approximately constant ( $\approx -2$  eV). For  $F_nV_2$ , the binding energies of F to  $V_2$  are similar to that for  $F_nV$ , with slightly larger binding energies for the first two F atoms. The lower energy asymmetric structures show greater bond angle distortion but much smaller changes in bond length compared to the structures analyzed in Ref. [2]. With the updated values, the saturated  $F_4V$  structure (rather than the  $F_6V_2$ ) is stable in the presence of interstitials (apparent once Table II of Ref. [2] is updated with values of Table I).

TABLE I. Binding energies of  $F_nV_m$  for  $E_F = E_V + 0.45$  eV (intrinsic Fermi level at 650 °C [2]). For midgap Fermi level, clusters are predominantly neutral. The total binding energies ( $E_b^{\text{tot}}$ ) are calculated with respect to lowest energy interstitial fluorine configuration ( $F_{\text{int}}^-$ ) and neutral vacancies. The formation energies ( $E_f$ ) include energy to form required vacancies.

Structure	$E_b$ per F [eV]	$E_b$ last F [eV]	$E_b^{\text{tot}}$ [eV]	$E_f$ [eV]
V				+3.38
FV	-1.95	-1.95	-1.95	+1.43
$F_2V$	-1.88	-1.80	-3.75	-0.37
$F_3V$	-1.93	-1.96	-5.71	-2.33
$F_4V$	-1.91	-2.00	-7.71	-4.33
$V_2$			-1.45	+5.31
$FV_2$	-2.31	-2.31	-3.77	+3.00
$F_2V_2$	-2.37	-2.43	-6.20	+0.57
$F_3V_2$	-2.17	-1.78	-7.97	-1.21
$F_4V_2$	-2.13	-2.01	-9.98	-3.22
$F_5V_2$	-2.09	-1.90	-11.88	-5.12
$F_6V_2$	-2.09	-2.09	-13.98	-7.22

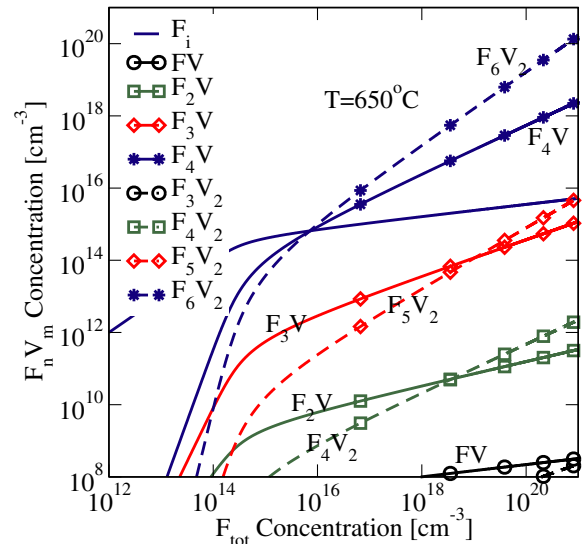


FIG. 1 (color online). Equilibrium concentration of various  $F_nV_m$  structures vs. total F concentration at 650 °C.

In Fig. 1, estimated equilibrium concentrations of F structures versus total F concentration are shown. The fully saturated clusters  $F_6V_2$  and  $F_4V$  are the most important in equilibrium. Out of equilibrium, a cascade of reactions involving point defects and  $F_nV_m$  clusters determine the dynamic behavior [3]. In the presence of nonequilibrium point-defect concentrations, the local equilibrium  $F_nV_m$  concentrations need to be multiplied by  $(C_V/C_V^*)^m$ . Thus, in the presence of excess vacancies during initial stages of implant annealing, almost all fluorine will reside in  $F_nV_m$  structures.

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