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 (≈ -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^{tot}) are calculated with respect to lowest energy interstitial fluorine configuration (F_{tet}^-) 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^{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

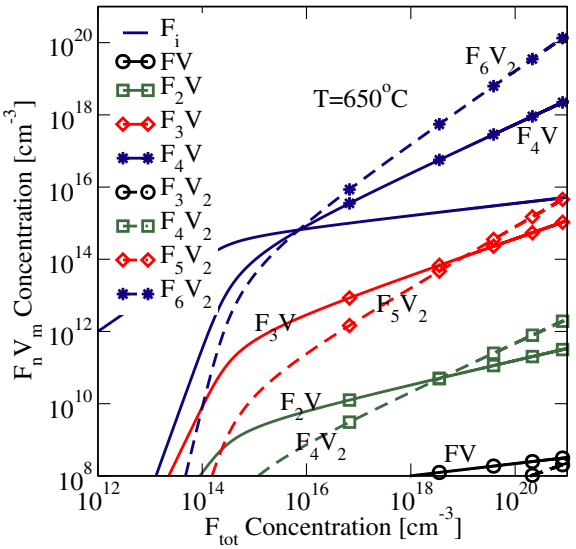

FIG. 1 (color online). Equilibrium concentration of various F_nV_m structures vs. total F concentration at 650 °C.

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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