Supplemental material for: Assessing the potential of perfect screw dislocations in SiC for solid-state quantum technologies

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(Dated: April 24, 2023)

I. SUPERCELL CONFIGURATION

To study perfect stoichiometric and decorated screw dislocations in 3C-SiC, we used supercells containing a dislocation dipole in a quadrupolar arrangement, which minimizes the interaction between dislocations [1–3]. Such structural model is created in a 576-atom SiC supercell using anisotropic elasticity via the software package BABEL [4]. This configuration can be seen in Fig. 1(a), and it guarantees a minimum distance between dislocation cores of ∼16Å. In Fig. 1(a), the position of dislocations and their line directions (in- and out-of-plane) are depicted using red marks that follow the usual vector notation. In Fig. 1(b), we use the dislocation analysis tool available within OVITO [5, 6] to detect and inspect the created screw dislocations within the supercell. Also in Fig. 1(b), dislocation lines as extracted by OVITO are shown as red lines, green atoms refer to bulk-like atomic sites and gray atoms signal atomic sites that cannot be clasify as diamond-like, i.e., the sites composing the core of the dislocation.

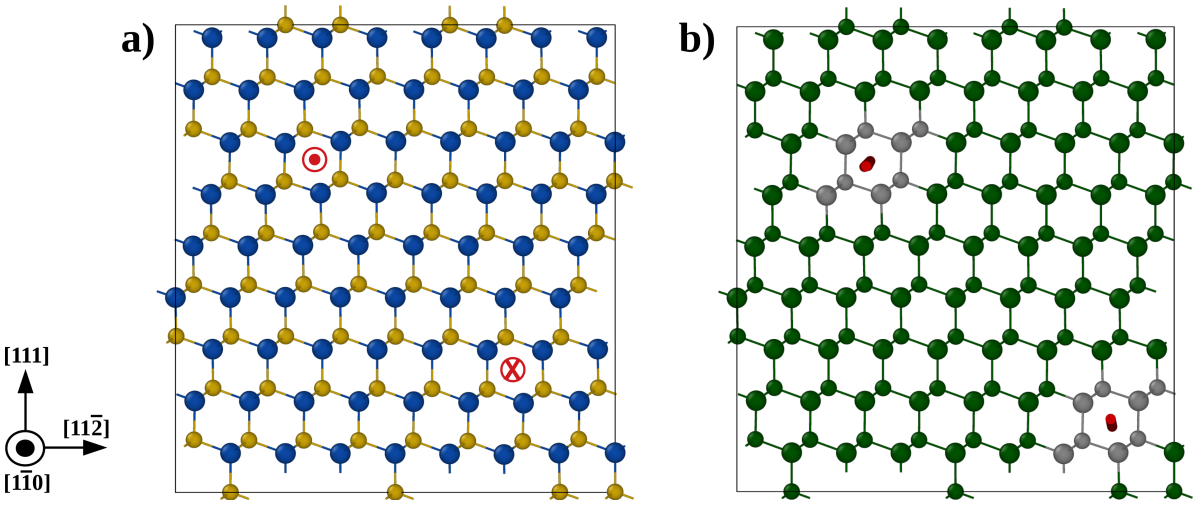

FIG. 1. (a) Screw dislocation dipole in a 576-atom supercell of 3C-SiC, with the position of dislocations and their line directions (in- and out-of-plane) depicted using vector notation (carbon and silicon atoms are shown in yellow and blue, respectively). (b) Dislocation analysis of the created supercells with dislocations shown as red lines, green atoms refer to bulk-like atomic sites and gray atoms signal atomic sites that cannot be clasify as diamond-like, i.e., the sites composing the core of the dislocation. Figures and analysis were obtained using OVITO [5].

II. CHARGE LOCALIZATION

In Figs. 2(a) and 2(b) we show two different perspectives of the charge density difference between a DV0 and a negatively charged DV when located directly at the core of the dislocation. As can be seen there, the additional charge is localized near the DV and it is not associated to any of the cores composing the dislocation dipole. This localization is a key requirement for the validity of our formation energy calculations and it confirms the electrical inactivity of the screw dislocations in 3C-SiC, which is one of the conditions that need to be satisfied for dislocations to be useful for quantum applications.

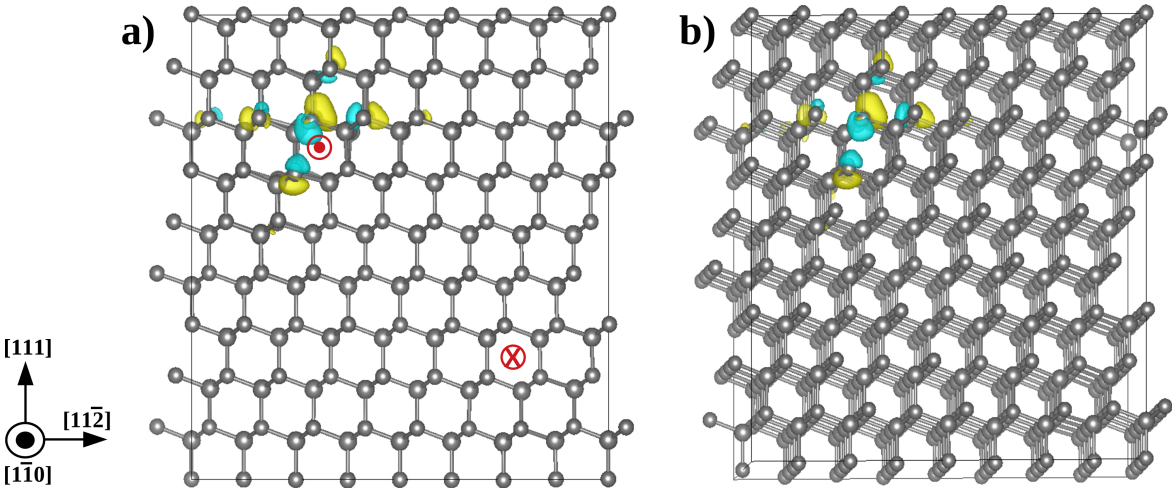

FIG. 2. (a) and (b) Two different perspectives of the charge density difference between a DV0 and a negatively charged DV when located directly at the core of one of the screw dislocations composing the dipole. Figures were obtained using VESTA [7]. The isosurfaces are shown at 5% of the maximum.

III. SECOND- AND THIRD-PREFERRED CONFIGURATIONS

In Figs. 3(a) and 3(b) we show examples of the second- and third-preferred configurations for DV near the cores of perfect screw dislocations in 3C-SiC. The second-preferred configuration, Fig. 3(a), has the silicon vacancy directly at the core and the carbon vacancy siting outside the core. The third-preferred configuration, Fig. 3(b), has both vacancies directly outside the core and in the second ring from the center.

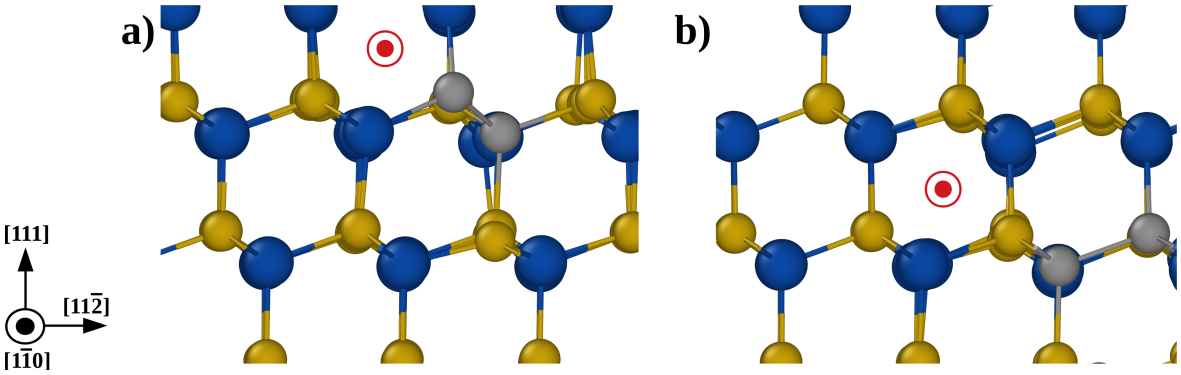

FIG. 3. (a) Second- and (b) third-preferred configurations for DV near the cores of perfect screw dislocations in 3C-SiC. Carbon and silicon atoms are shown in yellow and blue, respectively. Vacancies are shown as gray spheres. Figures were obtained using OVITO [5].

IV. COORDINATION ANALYSIS

In Fig. 4 we show the radial pair distribution function, $g(r)$, of both the pristine 3C-SiC supercell and that of its dislocated counterpart. As can be seen, the bulk case is characterized by a single nearest neighbour distance. However, once the dislocation dipole is created, the bonding distribution of the supercell exhibits a disorder that explain both the band tail states and the symmetry breaking that lifts the degeneracy of the e states associated to the neutral DV.

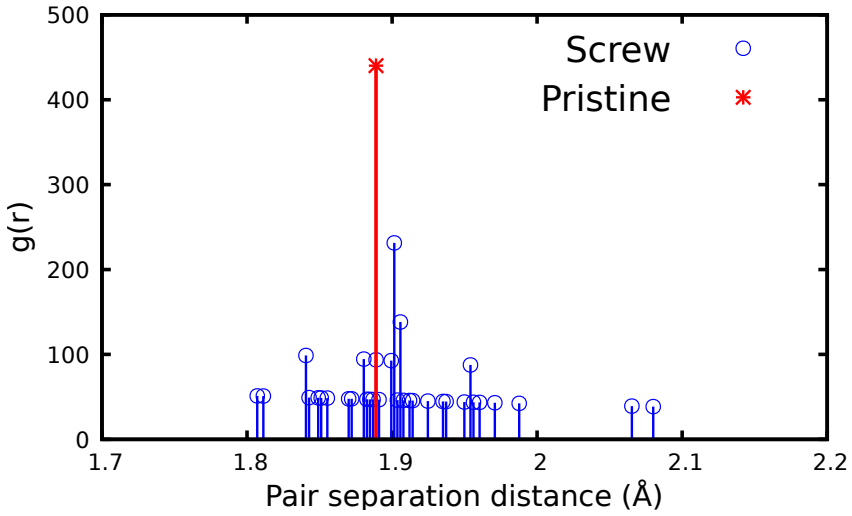

FIG. 4. coordination analysis of both the pristine 3C-SiC supercell and that of its dislocated counterpart.. The analysis was carried out using OVITO [5].

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