# Stair-rod dislocation cores acting as one-dimensional charge channels in GaAs nanowires

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Aberration-corrected scanning transmission electron microscopy and density-functional theory calculations have been used to investigate the atomic and electronic structure of stair-rod dislocations connected via stacking faults in GaAs nanowires. At the apexes, two distinct dislocation cores consisting of single-column pairs of either gallium or arsenic were identified. *Ab initio* calculations reveal an overall reduction in the energy gap with the development of two bands of filled and empty localized states at the edges of valence and conduction bands in the Ga core and in the As core, respectively. Our results suggest the behavior of stair-rod dislocations along the nanowire as one-dimensional charge channels, which could host free carriers upon appropriate doping.

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### I. INTRODUCTION

III-V semiconductor nanowires (NWs) are low-dimensional structures receiving increasing interest from the research community due to their superior physical properties. Compared to silicon, a higher electron mobility combined with the possibility of band-gap engineering makes these materials particularly suited for electronic and optoelectronic devices [1–6]. Furthermore, due to their high aspect ratio, nanowires are attractive building blocks to be integrated on Si for a broad range of applications, such as photovoltaic devices, field-effect transistors, and lasers [7-11]. However, besides the novel device architecture possibilities [12-15], what makes nanowires superior to their thin-film counterparts is that below a certain critical nanowire diameter the density of misfit dislocations can be significantly reduced, allowing improved growth efficiencies and better device performances [16–19]. In this context, the presence of bulk crystallographic defects (i.e. partial dislocations, stacking faults, etc.) might play a decisive role on the device properties.

In order to implement III-V nanowires in state-of-the-art devices, it is crucial to analyze and control the presence of all lattice imperfections as their occurrence can lead to the formation of electrically active states within the band gap with the consequent reduction of carrier mobility [20–28]. For example, a particular class of steps in twin boundaries has been demonstrated, via density-functional theory (DFT), to be nonradiative recombination centers inducing deleterious effects in GaAsP nanowires [29]. On the other hand, it has been proven that crystallographic defects can also have a beneficial effect on the device properties. DFT calculations performed on II-VI CdTe thin films for solar cells reported the presence of electrically inactive states in defective regions. In particular, a charge transfer between two nearby 90° partial dislocation

cores was observed, increasing the separation of the carriers by band bending. This phenomenon should theoretically improve the cell efficiency [30,31].

A first step in evaluating the impact of a particular defect on the device performance is to investigate its exact atomic configuration. For this purpose, transmission electron microscopy (TEM) provides the lateral spatial resolution to study the structure of nanodevices at the atomic level and has been successfully used over decades in the study of semiconducting materials [32–36]. A correlation with the electronic properties of the defect is achieved by the aid of theoretical modeling and *ab initio* methods.

In this work, we used aberration-corrected scanning transmission electron microscopy (STEM) and energy-dispersive xray (EDX) spectroscopy to characterize two stair-rod dislocation cores formed at the intersection of three intrinsic stacking faults in a gallium arsenide (GaAs) nanowire. Based on the experimental observations, a 3D atomic model was developed and used to perform DFT calculations. Our simulations reveal the presence of quasi- $s p^2$  hybrid orbitals at the two defect cores and the presence of highly localized projected density of states (PDOS) shifting along the stacking fault from the valence band in the gallium core to the conduction band in the arsenic core. This confirms the antithetical nature of these two types of defects, suggesting for this particular case the creation of parallel localized potential paths along the nanowire.

## **II. METHODS**

GaAs horizontal NWs were grown via template-assisted selective epitaxy (TASE) in a metal-organic chemical-vapordeposition tool as reported previously [37]. The TEM lamella was prepared by means of an FEI Helios Nanolab 450S focused ion-beam instrument. After protecting the nanowire with a platinum layer and performing the cut in the region of interest, the lamella was transferred to a TEM grid and thinned down to electron transparency. We employed a double-spherical

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FIG. 1. HAADF-STEM micrographs, recorded along the [110] zone axis, showing (a) the front section of the nanowire and (b) an enlarged view of the square indicated in panel (a). The intrinsic stacking faults intersecting at  $70.5^{\circ}$  are visible as v-shaped planar defects. The stair-rod dislocations at the vertexes are highlighted with red circles. The two cores are  $\sim 15$  nm apart.

aberration-corrected JEOL JEM-ARM200F microscope operated at 200 kV and equipped with a JEOL Dry SD100GV silicon drift detector with 100-mm<sup>2</sup> detection area for EDX analysis. In STEM mode, a convergence semiangle of 25 mrad was used in combination with a high-angle annular dark-field (HAADF) detector with inner and outer collection semiangles of 90 and 370 mrad, respectively.

## **III. RESULTS AND DISCUSSION**

Figure 1(a) shows a low-magnification HAADF-STEM micrograph of a GaAs nanowire front section projected along the [110] zone axis. This front section exhibits an average width and height of 100 and 38 nm, respectively. Unless otherwise specified, the same orientation and zone axis of the nanowire is maintained for all subsequent micrographs and models. An atomically resolved image of the inset marked with a white square in Fig. 1(a) is displayed in Fig. 1(b). Three intrinsic stacking faults on different {111} glide planes intersect at an acute angle of  $70.5^{\circ}$  and create the dislocation cores highlighted with two red circles labeled 1 and 2. These two cores, connected via an intrinsic stacking fault, are about 15 nm apart and are expected to propagate along the whole length of the nanowire. The dumbbell atomic columns in the intrinsic stacking faults exhibit the typical change in orientation



FIG. 2. HAADF-STEM atomically resolved images of the (a) first and (b) second dislocations cores. (c), (d) Atomic-scale EDX chemical maps corresponding to the red dashed area in panels (a) and (b), respectively. The nature of the unpaired single-atomic columns, i.e., gallium (blue) for core 1 and arsenic (green) for core 2, is distinctly revealed.

due to the removal of one close-packed plane from the perfect zinc-blende crystal structure [38].

The Burgers circuits performed on both cores were used to determine the Burgers vectors of the dislocations. The identification of the Burgers vectors of a stair-rod dislocation is obtained by subtracting the vectors of two circuits; the first circuit runs around one stacking fault and the second one around both the second stacking fault and the stair-rod dislocation, considering the crystal unfaulted at the position of the first stacking fault. A detailed analysis of the Burgers vectors is given in the Supplemental Material in Fig. S1 [39]. In this case, the cores are formed by the interaction of  $30^{\circ}$ Schockley partial dislocations annihilating each other in two different stair-rod dislocations. Their interaction results in an energy reduction. This particular type of stair-rod dislocation was previously reported in nanostructured metals and semiconductors [33,40,41] and is commonly present in the GaAs nanowires grown in planar SiO<sub>2</sub> templates investigated here. Stair-rod dislocations are characterized by the presence of single unpaired atomic columns [33], clearly visible in Figs. 2(a) and 2(b), where the two dislocation cores, previously marked as 1 and 2, are illustrated at higher magnification. The mirrored symmetry between the two structures with the unpaired atomic columns (marked with white circles) located on different lattice sites is distinctly visible.

Due to the small atomic number difference between Ga (Z = 31) and As (Z = 33), the  $Z^2$  contrast intensity difference, usually used to recognize atomic species in HAADF micrographs, was not significant enough to safely determine the nature of the single elements. For this reason, atomic-scale

EDX chemical maps were recorded in the red dashed area of the two cores. As illustrated in Fig. 2(c), the core in panel (a) exhibits Ga single-atomic columns, while in Fig. 2(d) the core corresponding to panel (b) consists of As single-atomic columns, where gallium and arsenic atoms are colored in blue and green, respectively.

Subsequently, 3D atomic models of the dislocation cores were created with RHODIUS software [42,43] and used as input for the DFT calculations in order to study the effect they might induce on the band gap and on its electronic structure. DFT calculations were performed within the Gaussian plane-wave method as implemented in the CP2K package [44] with double-zeta valence polarized (DZVP) basis sets for the representation of Kohn-Sham orbitals, with plane-wave cutoff for the charge density of 600 Ry. An initial geometry optimization was performed using the Perdew-Burke-Ernzerhof (PBE) [45] generalized gradient approximation (GGA) exchangecorrelation functional. This, as it is well known, fails, however, to determine the band gap accurately; therefore, single-point calculations were performed using the hybrid functional developed by Heyd-Scuseria-Ernzerhof (HSE06), with the exchange screening parameter  $\omega$  set to 0.11 as recommended in Ref. [46].

To speed up the calculations, the auxiliary density matrix method [47] with FIT6 auxiliary basis sets was employed. Maximally localized Wannier functions [48] were extracted using CP2K. In order to investigate the effect of the stair-rod defects on the electronic properties of GaAs, DFT calculations were performed on two different models. A  $6 \times 6 \times 6$ supercell (corresponding to 16.96 Å in each direction) with 1728 atoms was adopted for the bulk structure, while the defective area was incorporated in a supercell with 924 atoms consisting of  $12 \times 12 \times 2$  unit cells. After properly relaxing the structure, the models were imported in STEM\_CELL and used to simulate HAADF images [49,50]. Strain mapping was performed by the use of geometric phase analysis (GPA) [51] within the FRWR plugin in order to verify the validity of the model. Subsequently, GPA maps of the modeled structure were compared with the experimental ones. Concordantly, both experimental and simulated data show quantitatively comparable strain and rotational maps at the intrinsic stacking faults with no long-range strain fields contributions stemming from the dislocation cores (Supplemental Material Figs. S2 and S3 [39]). This confirms the structural validity of the adopted DFT model.

Figures 3(a) and 3(b) show the bulk and defective supercells simulated with DFT to investigate the effect induced by the defects on the GaAs electronic properties. Both structures were relaxed using the PBE functional until the force acting on each atom was less than 0.01 eV/Å. The PBE band gap of the bulk GaAs was 0.53 eV, highly underestimated with respect to the 1.43 eV experimentally reported in the literature [52] with a difference of 63%. A single-point calculation with hybrid functional HSE06 was then performed to correct the error, and a band gap of  $\sim 1.14 \text{ eV}$  with a difference of 21% was obtained. This is still underestimated but the value is now closer to the literature [53,54]. The PDOS for the bulk structure is shown in Fig. 3(c). Here and in the other PDOS plots the energy zero is set to the Fermi level, and the projections are normalized to the number of atoms involved. The majority of valence states are equally contributed by both Ga and As atoms, with a



FIG. 3. (a) Bulk structure model of GaAs and (c) associated PDOS plot. Gallium (blue) and arsenic (green) states equally contribute along the whole energy range with a slight difference for the unoccupied states above 2.0 eV only. The first localized state is observed at  $\sim 1.14$  eV. The orbital simulations represented in panel (c) illustrate, along a different zone axis, the Wannier s  $p^3$  orbitals present around the Ga and As atoms. (b) Model used to investigate the DOS projected on the Ga core (blue), As core (green), entire stacking fault (red), and remaining crystal (gray) atoms. The associated PDOS plot (d) shows, with the same color codes, the reduction in energy gap and the presence of valence and conduction band states. All plots are normalized to the involved number of atoms in the projection. The Wannier orbitals (in red) showing the quasi- $s p^2$  geometry are illustrated in panels (e) and (f) for the Ga and As dislocation core, respectively. The black dashed ellipses highlight the position of the stacking faults.

signature of empty antibonding states rising at +1.14 eV. This is visible in Fig. S5 of the Supplemental Material [39]. We note that the lowest unoccupied molecular orbital (LUMO) peak appears isolated from the conduction band, which is in contrast with calculations conducted with a large number of k points (corresponding to a much larger supercell in our real-space representation). However, the presence of such an undesired feature at the bottom of the conduction band can be due to the finite system-size effects [55]. A similar effect has also been reported for GaN in a study by Meng et al. [56]. Figure S4, supporting this explanation, shows the increase in the density of states (with unchanged band gap) near the conduction band for bulk GaAs with two different supercell sizes. We also verified that the character of the first unoccupied states remains unchanged by increasing the system size (not shown). The majority of the unoccupied states contribute above +2.0 eV with a slightly higher intensity from the Ga atoms.

The bonding hybridization simulation (Wannier localization) for the defect-free bulk is shown in the inset of Fig. 3(c). The model is here oriented along the [100] zone axis to exhibit the Wannier orbitals geometry. As expected, four different  $s p^3$ hybrid orbitals separated by 109.5° connecting the Ga atom to the neighboring As atoms are obtained. The same hybridization is also visible for the As atom connected with the four Ga atoms.

The defects suggested by the experiment are then inserted in the structure. The distance between the two dislocations in the modeled defective structure is not equal to the experimental observations due to the complexity to perform the calculations on such big crystal. For this reason, the distance in the simulated model is around 1/3 of the experimental one. Figure 3(b) illustrates how the defect model is divided with different colors into four parts; they correspond to the As core (green), Ga core (blue), intrinsic stacking faults (red), and the remaining atoms in the bulk (gray). Similarly, in Figs. S7(c) and S7(d), the analysis is performed by further dividing the intrinsic stacking fault into three parts: Ga core proximity (pink block 1), intermediate stacking faults (orange block 2), and As core proximity (black block 3). As done previously, the single-point calculation with HSE06 functional was performed for the defective structure. The HSE06 calculated band gap, previously observed at +1.14 eV for the bulk structure, decreases to +0.54 eV [Fig. 3(d)]. The peak, present in all the areas taken into consideration in the structure, suggests an overall influence by the dislocation cores on the electron cloud of the entire modeled crystal. A comparison of the PDOS contributions coming from the Ga and As dislocation core atoms is presented in Fig. 3(d). Ga core atoms (blue line) show a major contribution in the upper part of the valence band (above -0.7 eV) while the projection on the As core atoms (green line) has a predominant distribution in the bottom of the conduction band states with multiple peaks appearing between 0.54 and 1.25 eV.

Major contributions in this interval are due to the As core atoms followed by the contributions from the atoms on the intrinsic stacking faults (red) and then from the remaining atoms (gray line). For the Ga core atoms, the effective contribution to the empty states starts only after +1.7 eV.

We interpret the two peaks at the edges of the valence and conduction bands [blue and green lines in Fig. 3(d)] as signatures of a band localized along the defect channels [see Fig. 4(d), explained below]. Our supercell representation allows us to sample the band only at the gamma point. We note that increasing the size of the supercell along the channel improves the sampling of the band, as it is clearly visible by comparing Figs. S6(b) and S7(b) in the Supplemental Material [39]. As in the defect-free bulk model, the bonding orbitals were simulated in correspondence of the two dislocation cores. The results are illustrated in panel (e) and (f) for the Ga and As single atoms, respectively. The dislocation cores develop a configuration in between  $sp^3$  and  $sp^2$  where three hybrid orbitals separated by 120° are obtained. The presence of an unpaired orbital generates a distortion in the three orbitals geometry not allowing the standard  $s p^2$  planar configuration. This can be connected to the difference in PDOS on the valence and conduction band present in the single Ga and As atoms. These results further made us explore the behavior of the PDOS contribution of the atoms connecting these two



FIG. 4. (a) Electron density map with an isosurface value of  $4.1 \times 10^{-3} \text{ e/Å}^3$  and potential color-gradient scale in red (max) and blue (min) along the [110] zone axis. (b) Distribution of the electrostatic potential in the [001] direction along the stacking fault with average potential energy represented with a magenta line. (c) Graphical representation, along the [111] zone axis perpendicular to the intrinsic stacking fault, of the charge nanochannels generated by the two dislocations. (d) Isosurface (0.012 a.u.) of the integrated charge in the energy interval corresponding to the localized peaks for electrons (red) and holes (blue) in the density of states ["Ga core" and "As core" in Fig. 3(d)], forming the one-dimensional charge channels.

different dislocation cores. Figures S6(d) and S7(d) (supercells of different size along the channel) show the PDOS plots from the atoms in the three different sections as previously described for the structure in Fig. S6(c). The PDOS distribution of block 1 (pink line) is very similar to that of the Ga core atoms where there is a minimum contribution in the conduction band after +1.7 eV and a significant increase in the states below the Fermi level. Similarly, block 3 (black line) follows the trend of the As core atoms where the majority of unoccupied states are concentrated at +1.0 eV and almost zero states in the valence band. Atoms in block 2 (orange line) have a distribution in between the As and Ga core PDOS plots. In fact, both conduction and valence band states are visible with a lower intensity with respect to both block 1 and 3. This effect is probably emphasized as a consequence of the shorter distance, but the same qualitative behavior, with respect to the experimental structure.

Furthermore, an analysis of the electrostatic potential is performed in Fig. 4(a) where the electron density map of the two dislocation cores with potential color scale is shown. Figure 4(b) represents the electrostatic energy along the stacking fault line with the As core showing the highest potential energy acting as LUMO and the Ga core with the lowest potential energy acting as highest occupied molecular orbital (HOMO).

This investigation clearly shows the formation of an electric field between the Ga core and As core confirming the role of the stair-rod dislocation cores as charge wires. This could lead to an improved carrier separation upon doping and a reduction in detrimental recombination.

Since the dislocation cores in both cases are assumed to propagate along the whole length of the nanowire, the highly localized nature of the density of states can induce the formation of charge nanochannels, as shown in Fig. 4(c), and in Fig. 4(d), where we plot the integrated charge (hole) density around the PDOS peaks at the top (bottom) end of the valence (conduction) band (up to the Fermi level in both cases). This suggests the possibility to facilitate the transport of electrons and holes for the Ga and As core, respectively. In this case, since the localized channel states do not close the band gap, doping of the material would be necessary in order to accommodate free carriers in the channels. This phenomenon (this time with the defect band developing within the gap) was recently studied for a different class of materials such as transition-metal dichalcogenide [57]. Even if the electronic states are considerably different with respect to those in GaAs, the simulated physical behavior obtained in this work could be comparable. This could be further analyzed and exploited in the future for the realization of innovative devices where the combination of different growth conditions and materials (including doping) can lead to the formation of preferential paths for improved monodimensional carrier transport. However, these perspectives are beyond the scope of this paper.

#### **IV. CONCLUSIONS**

In conclusion, aberration-corrected STEM has been used to assess the atomic structure of two stair-rod dislocations obtained by merging multiple stacking faults in v-shaped defects. Elemental EDX mapping has been employed to unambiguously identify the nature of the single-atomic columns at the dislocation cores, revealing that they consist of either entirely gallium or arsenic. Their effect on the electronic properties has been investigated by means of DFT calculations showing a reduced energy gap with respect to the bulk material. Furthermore, the development of charge channels along the defect channels, with a corresponding strong electric field between the channels, appear at the edges of valence and conduction bands, probably attributable to the unpaired porbitals in the quasi- $s p^2$  bonding configuration of the singleatomic columns. These results suggest the possibility to obtain strongly localized potential paths within the nanowire which might host free carriers upon appropriate doping and improve the carrier separation along the two dislocation cores.

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