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

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Although point defects in solids are one of the most promising physical systems to build functioning qubits, it remains challenging to position them in a deterministic array and to integrate them into large networks [1-3]. By means of advanced ab initio calculations we show that undissociated screw dislocations in cubic 3C-SiC, and their associated strain fields, could be used to create a deterministic pattern of relevant point defects (See Fig. 1). Specifically, we present a detailed analysis of the formation energies and electronic structure of the divacancy in 3C-SiC when located in the vicinity of this type of dislocations. Our results show that the divacancy is strongly attracted towards specific and equivalent sites inside the core of the screw dislocations, and would form a one-dimensional arrays along them. Furthermore, we show that the same strain that attracts the divacancy would allow the modulation of the position of its electronic states and of its charge transition levels. Specifically, we find that in the case of the neutral divacancy these modulations result in the loss of its potential as a qubit. However, these same modulations could transform defects with no potential as qubits when located in bulk, into promising defects when located inside the core of the screw dislocations. Since dislocations are still mostly perceived as harmful defects, our findings represent a technological leap as they show that dislocations can be used as active building blocks in future defect-based quantum computers.

References

[1] G. Zhang et al., Applied Physics Reviews 7, 031308 (2020).
[2] A. Chaterjeee et al., Nature Reviews Physics 3, 157 (2021)
[3] G. Wolfowicz et al. Nature Reviews Materials 6, 906 (2021

Figures

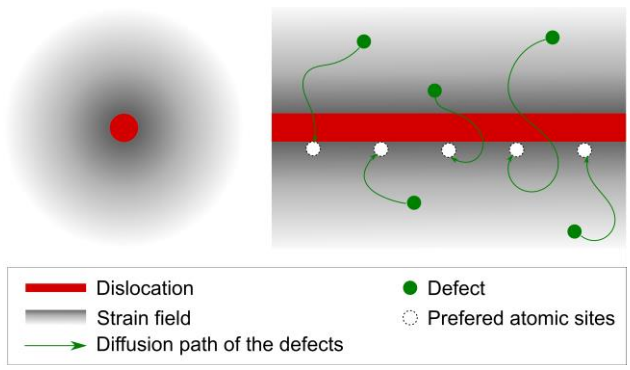

Figure 1: Depiction of a dislocation (red line) attracting defect-based qubits (green dots) due to its induced strain field (gray shaded area).