Stability of the Period-Doubled Core of the 90° Partial in Silicon

In a recent Letter [1], Lehto and Öberg (LO) investigated the effects of strain fields on the core structure of the 90° partial dislocation in silicon, especially the influence of the choice of supercell periodic boundary conditions in theoretical simulations. Specifically, they addressed the relative stability of the traditionally accepted single-period (SP) geometry vs our recently proposed double-period (DP) structure [2]. Performing supercell calculations that employed the original Keating potential for Si [3], they reached two main conclusions: (1) that a dipole-cell configuration minimizes the overall cell strain, thus being more adequate for small-cell simulations; (2) that the relative stability of the SP and DP geometries depends on the choice of boundary conditions, with the SP and DP cores being favored for "dipole" and "quadrupole" configurations, respectively. The purpose of the present Comment is not to dispute their first point, with which we agree. Rather, we wish to focus on the more important DP-versus-SP stability issue, because we believe their second conclusion to be incorrect. Below, we show that their results for the relative stability between the two structures are in disagreement with cell-size converged tight-binding total energy (TBTE) calculations, which suggest *the DP core to be more stable, regardless of the choice of boundary condition*. Moreover, we argue that this disagreement is due to their use of a Keating potential.

Clearly, in the limit of sufficiently large supercells, all results should be independent of the choice of boundary conditions. Here, supercell convergence is investigated by performing TBTE and Keating-potential calculations for three different supercell sizes, using both the dipole and quadrupole cells, and two different sets of parameters for the Keating-potential calculations [3,4]. In our larger cell, all dislocation separations are similar to those of the 2048-atom cells studied by LO. The first observation we can draw from the TBTE results in Table I is that, as pointed out by LO, for small cells the dipole boundary condition gives results which are closer to the converged value, while the quadrupole cell has a bias of ~ 10 meV/Å in favor of the DP structure, which decreases by 1 order of magnitude as we approach cell-size convergence. However, Table I also shows that the Keating potential has a much stronger bias in favor of the SP structure. For the 192-atom cell, the results of local-density approximation (LDA) (from Ref. [2]), TETB, and the Keating potentials of Refs. [3] and [4] for $E_{\mathrm{DP}} - E_{\mathrm{SP}}$ are -80, -70, -20, and -15, respectively (in meV/Å, with error bars of $\sim \pm 5$ in each case). Thus, the Keating potential has a systematic bias in favor of SP of ~ 50 meV/Å relative to the more accurate methods. As it happens, going to cell-size convergence shifts all the $E_{\mathrm{DP}} - E_{\mathrm{SP}}$ values by roughly 20 meV/Å. As a result, the converged values for the Keating potentials are close to zero, making the variations with choice of boundary conditions (which, in absolute numbers, are similar to those seen in TBTE) take on an artificial importance. In fact, the $E_{\mathrm{DP}} - E_{\mathrm{SP}}$ values are so small that even the qualitative conclusions about which structure is favored can be seen to depend on the choice of Keating parameters. On the other hand, it seems clear that the more accurate TBTE results would be quite immune from displaying a sign change in $E_{\mathrm{DP}} - E_{\mathrm{SP}}$ as a result of details of the choice of cell size or boundary conditions.

TABLE I. Energy of the DP relative to the SP core, in meV/Å per dislocation, for the 90° partial in Si. Four different approximations (LDA, TBTE, and two different Keating parametrizations) are used to compare quadrupole and dipole boundary conditions. Cell size refers to the DP case.

Cell size (atoms)	192	576	1920
LDA			
Quadrupole	−79		
TETB			
Quadrupole	−74	−63	−55
Dipole	−62	−55	−55
Keating, Ref. [3]			
Quadrupole	−27	−7	1
Dipole	−14	2	5
Keating, Ref. [4]			
Quadrupole	−22	−10	−5
Dipole	−13	−5	−3

Finally, LO also based their conclusions in part on a density-functional calculation for a finite cylindrical sample. However, we suggest that the systematic errors involved in choosing surface boundary conditions for such a geometry may also be severe, and that such results should not be trusted in the absence of careful tests of convergence with respect to sample size.

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