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Microscopic Origin for Electrically Benign Small-angle Grain Boundaries in Low-cost Semiconductors

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As electrically benign, low-cost, near-single-crystalline semiconductors is crucial for large-scale applications, understanding the electrical behavior of small-angle grain-boundaries (GBs), consisting of array of dislocations, becomes important. However, a quantitative microscopic theory is still prohibitively difficult. Here, by developing a multiscale approach combining Monte-Carlo simulation, elasticity theory, first-principles calculation, and grand-canonical statistical modeling, we quantitatively explain the recent experimental observation showing the disappearance of hole transport barrier in poly-Si when the GB angle approaches a critical value of a few degrees. It reveals the microscopic origin for the observation as a transition from electrically harmful dislocations to electrically benign dislocations.

Keywords: Small-Angle Grain Boundary, Dislocations, Electronically Benign Behavior, Multiscale Simulations

In the physics of materials, the objective has often been to find a material that has the desirable physical properties to fit intended applications. Nowadays, however, the paradigm has shifted due to the increased needs for low-cost, low-temperature processing, low-energy consumption during production, large-area application, and the concern for sustainability. It is more than ever that one needs to put low-cost materials to good use. For example, high-efficiency single-crystal semiconductor films are often grown on single-crystalline substrate such as III–V compound semiconductor thin films on Ge for solar cells.[1] However, considering the large-area required for the solar cell and flat panel display, such a single-crystal substrate is too expensive to be practical. As a consequence, polycrystalline semiconductor films,[2,3] grown on non-crystalline substrate such as glass have emerged as an important alternative.

Compared with their single-crystalline counterpart, a polycrystalline device can be low cost but also suffer from low efficiency.[1] One important reason is the existence of abundant boundaries between grains (GBs), which can be detrimental to device performance.[4] For instance, in solar cells, defects associated with GBs can act as recombination centers, to drastically reduce the lifetime

of minority carriers.[2] In thin-film transistors (TFTs), charge trapping at the GBs will result in band bending and consequently undesirable mobility barriers.[3] In general, the ability to fabricate low-temperature, yet low-defect density polycrystalline semiconductors on glass or plastic, is crucial for the development and commercialization of low-cost solar cells, TFTs, and micro-electromechanical systems.

Recently, there have been some experimental indications that high carrier mobility poly-Si films may be made.[5–8] Specifically, Figure 1 shows the results of electrical measurement for well-aligned poly- (or ‘quasi-single crystalline’) p-type Si films possessing both preferred out-of-plane and in-plane orientations (namely, ‘biaxial’). The measured GB mobility barrier (E_B) is found to depend on the total mosaic spread (TMS): $\xi = (\Delta\omega_x^2 + \Delta\omega_y^2 + \Delta\Phi_z^2)^{1/2}$, where $\Delta\omega_x$ ($\Delta\omega_y$, $\Delta\Phi_z$) is the full-width at half-maximum of the rocking curve tilt along the x (y , z) axis. Remarkably, when ξ is below 4° , E_B suddenly vanishes, leading to significantly increased carrier mobility comparable to that of single-crystalline Si, opposed to a gradual decrease. The TMS ξ correlates with GB tilt angle θ . It happens that most of the GBs with $\xi \leq 4^\circ$ belong to small-angle (SA) GBs (SAGBs).

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Despite its importance, no theory has explained the experimental observation. In general, electronic theory and modeling of GBs is rare, in comparison with its point defect counterparts. To quantitatively explain the results of a macroscopic transport measurement based on electronic theory is even scarcer.

To address this difficult problem, we postulate that the macroscopic energy density of hole traps of the SAGB made of dislocations [9] can be formulated as a direct product of four functions: (a) at the μm size scale, the correlation function between ξ and θ , (b) at the sub- μm to 10 s nm size scale, the dislocation core density and (c) their thermal distribution, and (d) at the atomic scale, the energy density of hole traps for individual dislocation. This breakup allows for a calculation of the trap density by a combined Monte Carlo (MC) simulation, elasticity theory (ET), statistical modeling, and first-principles total energy calculations. Remarkable agreement with experiment in Figure 1 is achieved, which validates the assumption. We identify the physical origin for the disappearance of hole transport barrier at $\xi \leq 4^\circ$ as a transition to electrically benign GBs consisting of Frank partial dislocations.[10] We further show that the inclusion of stacking faults as part of the partial dislocation has the effect of delocalizing the wavefunctions of electron traps, which is beneficial to minority carriers in polycrystalline p-type Si solar cells.

The barrier E_B , which reflects the amount of band bending caused by charge accumulation at the GB, can be calculated by using the symmetric Schottky barrier model [4,11,12] (inset, Figure 1). We adopt the notion that Fermi level (ϵ_F) is a constant, whereas the valence band maximum (VBM), $\epsilon_{\text{VBM}}(x)$, is position dependent, with

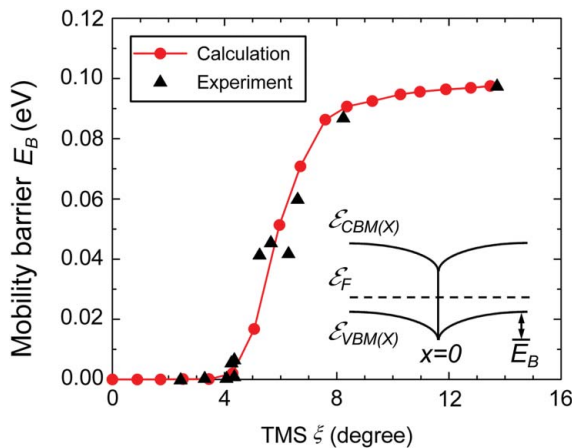


Figure 1. Experimental [6] and theoretical E_B as a function of ξ . Inset is a schematic drawing of the symmetric Schottky barrier model,[4,11] where ϵ_F is the Fermi level, $\epsilon_{\text{VBM}}(x)$ and $\epsilon_{\text{CBM}}(x)$ are the VBM and CBM positions as a function of x due to band bending. Zero is where the GB resides. The curve ‘calculation’ represents the best scenario whose difference with direct calculation is discussed in the main text.

$x = 0$ at the center of the GB. Charge neutrality requires [12] that within the depletion region,

$$e \int_{\epsilon_F}^{\epsilon_T^{\text{max}}} \mathcal{D}(\xi, \epsilon) d\epsilon = (8\epsilon_{\text{Si}}\epsilon_0 N_d E_B)^{1/2}, \quad (1)$$

where ϵ_T^{max} is the maximum energy of hole traps inside the band gap and $\epsilon_{\text{Si}}\epsilon_0$ is the dielectric constant of Si. We calculate ϵ_F from experimentally determined boron doping concentration,[6] $N_d = 1 \times 10^{17} \text{ cm}^{-3}$, to obtain $\epsilon_F = \epsilon_{\text{VBM}} + kT \ln(N_V/N_d) = \epsilon_{\text{VBM}} + 0.12 \text{ eV}$, where $\epsilon_{\text{VBM}} = \epsilon_{\text{VBM}}(\infty)$ and N_V is the effective density of states in the valence band. The integrand, $\mathcal{D}(\xi, \epsilon)$, is the macroscopic areal energy density of hole traps for a given ξ and ϵ ,

$$\mathcal{D}(\xi, \epsilon) = \sum_{i=1}^{N_{\text{DL}}} \int_0^{\theta_c} Q(\xi, \theta) \rho(i, \theta) P(i, \theta) g(i, \epsilon) d\theta, \quad (2)$$

where N_{DL} accounts for different types of dislocations that may exist, $Q(\xi, \theta)$ is the probability to be at GB angle θ when ξ is fixed, $\rho(i, \theta)$ is the dislocation core density, $P(i, \theta)$ is the thermal distribution, $g(i, \epsilon)$ is the hole trap density at a given ϵ , and $\theta_c = 12^\circ$ is a cutoff angle above which $Q(\xi, \theta)$ is approximately zero (See Figure S3 in the Supplemental Material).

Correlation Function $Q(\xi, \theta)$. To simulate the real GB angle θ distribution, $Q(\xi, \theta)$, as a function of mosaic spread ξ requires the use of a system that contains a large number of grains with different orientations. The theoretical approach to study $Q(\xi, \theta)$ is thus the MC simulations. In our study, we generate a large number of grains in a cubic box. A crystallographic orientation is then assigned to each of the grains by using the Gaussian distribution. We take into account the θ dependence of the GB energy and minimize the system energy to mimic experimental annealing process. Detailed discussion can be found in the Supplemental Material and accompanying Figures S1–S3.

Dislocation Core Density $\rho(i, \theta)$. SAGBs are made of dislocation arrays in which the separation d between two adjacent dislocations is given by Frank’s formula: $d = b/\theta$, where b is the component of the Burgers vector $\mathbf{b}$ in the plane perpendicular to the GB tilt axis. Hence, for the i th dislocation (DL- i)

$$\rho(i, \theta) = \frac{1}{d(i, \theta)z(i)}, \quad (3)$$

where $z(i)$ is the periodicity along the dislocation line (e.g. in the [011] direction in Figure S4, Supplemental Material). Bourret [13,14] used the isotropic ET to explain the observed dislocations in tilt SAGBs of Ge, namely DL-A = edge dislocation; DL-B = $30^\circ + 90^\circ$ partial dislocations from dissociation of 60° dislocation; and DL-C = three Frank partial dislocations. The

Burgers vector for each dislocation is also discussed in Figure S4, Supplemental Material. It appears that elemental semiconductors have similar dislocation properties [15–18] and most SAGBs found in poly-Si are tilt GBs.[19]

Thermal Distribution $P(i, \theta)$. A crucial property of the SAGBs is the coexistence of DL-A, B and C. Thermodynamically, portion of the GB composed of DL- i is given by

$$P(i, \theta) = \frac{N_i S_i}{\sum_{i=1}^{N_{DL}} (N_i S_i)}, \quad (4)$$

where N_i and S_i are the number and the cross-section of DL- i , respectively. Note that different dislocations have different cross-sections. The energy to be compared with for different dislocations should be that per unit cross-section area, rather than per dislocation core. This is an analog of comparing the energy of difference surface orientations. To minimize the free energy of the system in its equilibrium configuration, we adopt a grand-canonical ensemble assumption, which yields

$$\frac{N_i}{\sum_{i=1}^{N_{DL}} N_i} = \frac{\exp[(\mu - E_i)S_i/kT]}{\sum_{i=1}^{N_{DL}} \exp[(\mu - E_i)S_i/kT]}, \quad (5)$$

where k is the Boltzmann constant, T is the growth temperature (taken [6] to be 740°C), and E_i is the GB energy for DL- i . The significance of Equation (5) is the introduction of chemical potential μ to represent the average SAGB energy that can be self-consistently determined (Figure S5, Supplemental Material). We employ the isotropic ET to calculate E_i , as previous studies [13,14] showed that such a theory is reasonably accurate for relative dislocation energies when compared with experiments. The results are shown in Figure 2(a). Figure 2(b) shows the energy difference between DL-C and B, which becomes negative and then positive in the SAGB region. Figure 2(c) shows the calculated $P(i, \theta)$. Owing to the negative energy in Figure 2(b), $P(i, \theta)$ shows a population reverse from DL-B to DL-C at $\theta_T = 1.9^\circ$.

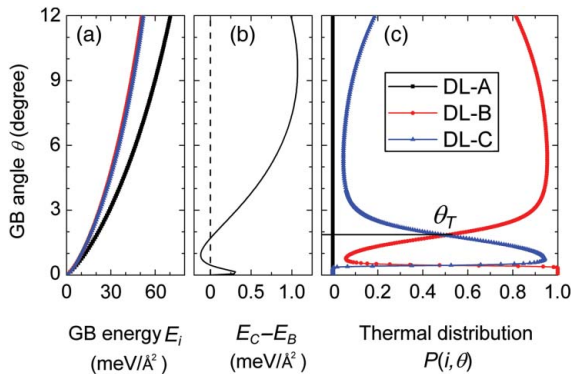


Figure 2. (a) Calculated GB energy for DL-A, B, and C as a function of θ . (b) Energy difference between DL-C and B. (c) Calculated GB distribution at $T = 740^\circ\text{C}$.

Trap Density of State $g(i, \epsilon)$. All dislocations considered here are line defects, extending along the $z = [011]$ direction. In the orthogonal x and y directions, the lattice distortion caused by the dislocation will relax. We simulate the dislocation by a supercell-cluster hybrid model [15] which preserves the periodicity along z , but is finite in the (x, y) -plane. A 12 Å-thick vacuum region is used to separate the dislocation with its images. Hydrogen is used to passivate the dangling bands at surfaces. Our model avoids the usual dislocation–dislocation dipole error and is straightforward in computing energy level alignment. We have tested the results to be convergent to be within 0.02 eV for supercells containing approximately 1,000 atoms.

First-principles density functional theory (DFT) calculations were performed within the local-density approximation (LDA).[20,21] The exchange–correlation functional of Ceperley and Alder [22], as parameterized by Perdew and Zunger,[23] and the ultrasoft pseudopotentials [24,25] for electron–ion interactions, as implemented in the Vienna *ab initio* simulation package,[26] were used. We used a plane wave energy cutoff of 15 Ry to converge the system total energy to within 0.01 eV. Six k -points along the z -direction (with a periodicity of about 7.6 Å) are used in Brillouin zone integration. All structures are fully relaxed until forces on individual atoms are less than 0.025 eV/Å. To check the LDA results, the HSE functional [27] was applied to the dislocation supercell with 236 atoms. It was found that the change in defect levels is within 0.05 eV.

Figure 3 (upper panel) shows the energy positions of trap states inside bulk Si band gap at their extremes, namely, ϵ_{VBM}^{DL} and ϵ_{CBM}^{DL} , where CBM stands for conduction band minimum. It shows that DL-A introduces a relatively deep empty band (electron traps), whereas DL-B introduces a relatively deep occupied band (hole traps) at its 30° partial. The integration of $D(\xi, \epsilon)$ in Equation (1) is from $\epsilon_F = 0.12$ eV to $\epsilon_T^{\max} = \epsilon_{VBM}^{DL}$. By examining Figure 3, we see that one only needs to consider DL-B for $g(i, \epsilon)$. Figure 4(a) shows the energy dispersion of the gap states for DL-B 30° partial and Figure 4(b) shows $g(DL-B, \epsilon)$ for hole traps, from which we determine $\epsilon_{VBM}^{DL-B} = 0.18$ eV.

Note that various approaches with different levels of accuracy have been used in applying Equations (1)–(5), it may thus make sense to find $\epsilon_T^{\max}(\text{fit})$ and $E_i(\text{fit})$ that best reproduce experimental results. This yields $\epsilon_T^{\max}(\text{fit}) = 0.22$ eV, $E_A(\text{fit}) = E_A(\text{ET})$, $E_B(\text{fit}) = E_B(\text{ET})$, and $E_C(\text{fit}) = E_C(\text{ET}) - 0.5$ meV/Å². The difference between direct calculated ϵ_{VBM}^{DL-B} and $\epsilon_T^{\max}(\text{fit})$ is 0.04 eV. Besides numerical uncertainty and DFT errors, several additional factors may contribute: (1) our model is based on the assumption of symmetrical tilt GBs, made of evenly spaced dislocation arrays. Neither twist nor asymmetrical tilt boundaries are considered; (2) the classical

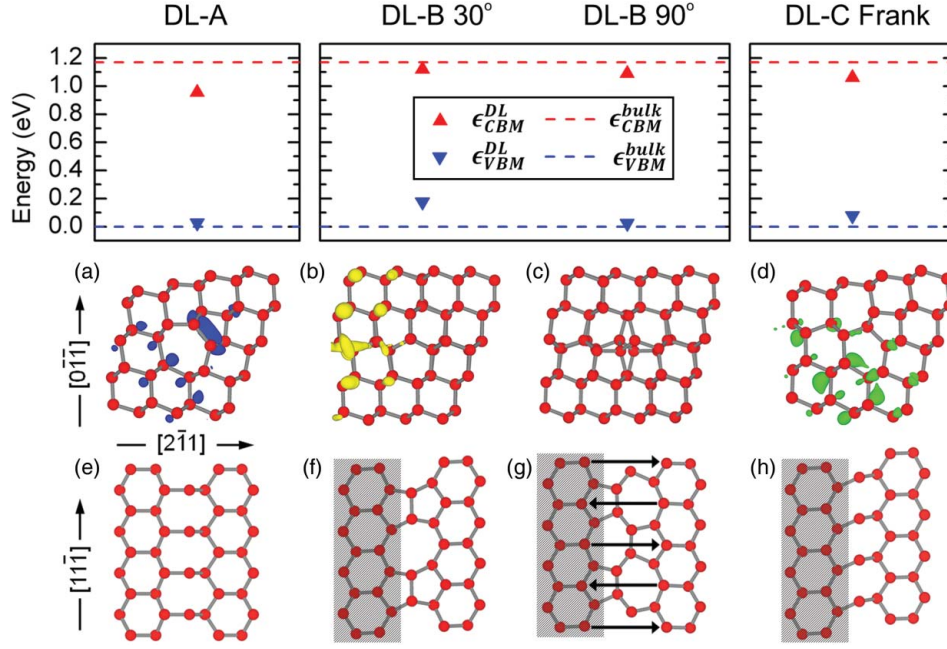


Figure 3. (Upper panel) Calculated ϵ_{VBM}^{DL} (blue triangle) and ϵ_{CBM}^{DL} (red triangle) with respect to bulk Si. The ϵ_{CBM}^{bulk} and ϵ_{VBM}^{DL} have been rigidly shifted to match experimental bulk band gap (Lower panels). The corresponding dislocation core structures projected onto (011) and (111) planes. The charge density at different contour levels of (blue = 0.0015, green = 0.001, and yellow = 0.0005 $e/\text{\AA}^3$) are plotted for the ϵ_{CBM}^{DL} states in (a), (d), and for the ϵ_{VBM}^{DL} state in (b). Shaded region denotes stacking fault. Arrows in (g) show alternating stacking of the heptagon–pentagon pairs.

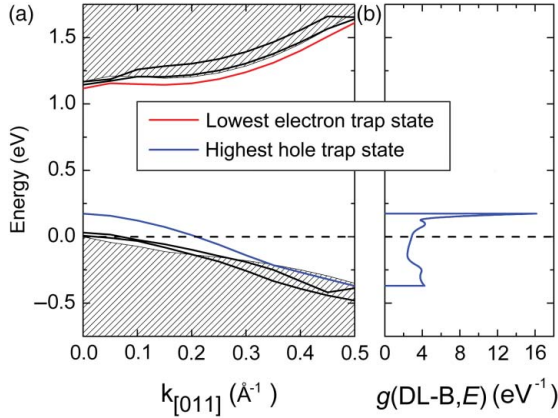


Figure 4. Electronic structure of DL-B 30° partial. (a) Band structure. Red and blue lines denote lowest electron and highest hole trap states, respectively. Shaded areas denote the projected Si bulk bands. (b) Calculated density of states for the hole traps.

ET is unable to capture the energy cusps at low-energy coincident site lattices (CSL) boundaries [9]; and (3) the limitation of the isotropic medium assumption. Despite the limitations of the current model, it demonstrates that transition from electrically harmful dislocations to electrically benign dislocations is responsible for the disappearance of E_B at $\theta \leq \theta_T$.

Physical Origin for Deep Traps. There have been considerable efforts in determining the electrical properties of dislocations. The results are, however, often

controversial.[19,28–30] Among them, recently Chen et al. [19,28] showed that SAGBs in clean as-grown polycrystalline Si have weak electron beam-induced current (EBIC) contrast at room temperature, which implies low recombination activity in such samples. Figure 3(a)–(h) shows atomic structures of dislocation cores, among which the DL-B 90° partial takes a complex double-period core structure.[31,32] Often, one explains the trap level position in terms of bond distortion, as reflected by the length of the Burgers vector. Indeed, $|\mathbf{b}_A| = a/\sqrt{2}$ is the largest, which results in charge localization around DL-A core, in agreement with Chan et al. [18] and Liu et al.[17] However, while DL-B 90° partial with $|\mathbf{b}_{B-90^\circ}| = a/\sqrt{6}$ has the shallowest levels, DL-B 30° partial with $|\mathbf{b}_{B-30^\circ}| = |\mathbf{b}_{B-90^\circ}|$ still has the highest ϵ_{VBM}^{DL} . Thus, atomic detail matters. We believe the shallowness of the DL-B 90° partial is caused by its pentagon–heptagon pairs, which form alternating dipoles along [211], as indicated by arrows in Figure 3(g), to relax strain.

Our analysis further reveals that stacking faults (shaded in Figure 3) play a crucial role in mitigating the severity of traps by delocalizing their wavefunctions. Taking DL-A and DL-C as examples, they have similar atomic structures, except that DL-C contains a stacking fault. Charge contour plots in Figure 3(a), 3(b), and 3(d) shows clearly that stacking fault delocalizes the wavefunctions. In Si, the stacking fault VBM is about 0.1 eV above bulk VBM, whereas the stacking fault CBM is very

close to bulk CBM.[33] For a good approximation, therefore, the mixing of dislocation states with stacking fault states raises the trap levels of DL-C from those of DL-A, as can be seen from Figure 3 (upper panel). Note that it is this DL-C with stacking fault that accounts for the electrical benign behavior of SAGBs. For DL-B 30° partial, which also contains a stacking fault, a similar effect of wavefunction delocalization is also observed. However, the compressed bonds, not on but near the stacking fault, may be responsible for the remaining deepness of the hole traps.

In summary, a multiscale approach, rooted in first-principles theory, can account for the macroscopic electrical properties of SAGBs. We identify the DL-B 30° partials as the origin for hole transport barrier. A transition from DL-B to electrically benign DL-C takes place at a mosaic spread $\xi \leq 4^\circ$. The prospect of low-cost high-efficiency quasi-single-crystal group IV semiconductors raises the hope to replace expensive single-crystalline substrates for electronics and optoelectronics. We note that the lattice dislocations for SAGBs and the secondary GB dislocations for near-CSL GBs may bear some similarities, which raises the question if the electrically benign behavior here can be extended to the vicinity of electronically benign CSL GBs, e.g. Si $\Sigma 3\{111\}$ twin GBs.[10,34]

Supplementary online material Supplementary online material. A more detailed information on experiments is available at <http://dx.doi.org/10.1080/21663831.2013.859639>

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