Recombination-Induced Stacking Faults: Evidence for a General Mechanism in Hexagonal SiC

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We report on optically induced nucleation and expansion of stacking faults in hexagonal SiC structures. The activation energy for partial dislocation glide under optical excitation is found to reduce to 0.25 ± 0.05 eV, which is about 2 eV lower than for pure thermal activation. From the measurements of thermal activation and below-gap excitation spectroscopy of dislocation glide, we conclude that the elementary process controlling expansion of stacking faults is kink pair nucleation aided by the phonon-kick mechanism. We propose that solitons on 30° Si(g) partials with a silicon core act as deep 2.4 eV + E_V trap sites, readily providing electron-hole recombination energy to enhance the motion of dislocations. Our results suggest that this is a general mechanism of structural degradation in hexagonal SiC.

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SiC is known to have a very low stacking fault energy γ [1], and this is partly responsible for the occurrence of a variety of polytypes in this material. The formation of stacking faults (SFs) in a crystal is intimately related to the motion of the leading *partial* dislocation on the glide plane of a crystal. Specifically, perfect dislocations—usually formed by the application of a shear stress to the crystal—dissociate into a leading/trailing partial pair that bound a ribbon of stacking fault. The extent of the stacking fault, proportional to the ribbon width, is given by the spacing between the two partial dislocations and is determined by the stacking fault energy γ in the crystal [2]. Dislocation generation and motion are thermally activated processes, and, in a hard material such as SiC, both processes would require relatively large shear stresses in the GPa range at temperatures below 600–700 °C [3]. This is reflected in the large activation barrier for the motion of glide dislocations in SiC, of the order of 2.5 eV [3].

Under electrical injection of carriers, however, the motion of glide dislocations can occur at substantially lower temperatures, in fact even at room temperature. The authors previously reported [4] the very large enhancement of the leading partial dislocation velocity in a 4*H*-SiC *p-i-n* diode under forward biasing. Specifically, the activation enthalpy for partial dislocation motion in bulk 4*H*-SiC was reduced from ~2.5 to ~0.25 eV under electrical stresses. In this Letter, we report on *optically* induced nucleation and expansion of stacking faults in 4*H*- and 6*H*-SiC *at room temperature* under *very low shear stresses*, of the order of kPa. The extra energy provided by recombination of electrons and holes, instead of merely creating photons or phonons, is channeled into aiding dynamic processes through the "recombination-enhanced dislocation glide" (REDG) mechanism [5–7]. In the present case, recombination enhancement is initiated by intense optical excitation of the material resulting in generation of excess carriers that recombine nonradiatively and provide sufficient energy to aid dislocation formation and motion. We have measured the activation energy for partial dislocation glide under optical excitation and found it to be very low, of the order of 0.25 eV, the same magnitude as that caused by electrical biasing. We have also measured the below band gap excitation dependence of recombination-enhanced dislocation glide in 4*H*-SiC and conclude that the elementary process controlling REDG is kink pair nucleation aided by the phonon-kick mechanism. Based on these measurements, we propose that solitons on 30° partials with a silicon core, Si(g), act as sites on the dislocation line for trapping electrons and holes and are the preferential sites for easier nucleation of kink pairs that enhance the motion of dislocations. It is this phonon-kick process that effectively reduces the activation energy for dislocation glide by more than 2 eV. Finally, similar measurements on 6*H*-SiC suggest this phenomenon to be a general mechanism for hexagonal SiC.

Two different hexagonal polytypes of SiC were used, 4*H* and 6*H*, having a band gap of 3.26 and 3.02 eV, respectively. As-received material was in the form of 10–40 μm-thick epitaxial films grown by chemical vapor deposition on commercially available substrate wafers (Cree, Inc.). We studied both *n*- and *p*-type material to find out the effect of doping on optical inducement of SFs and also examined fully processed *p-i-n* devices with top contact metallization removed. A tunable wavelength *ns*-pulsed YAG-Nd laser was used for optical excitation of excess carriers to stimulate REDG. The dislocation glide was probed *in situ* by time-lapse imaging of the background photoluminescence (PL) set off by supplementary, low-intensity excitation from a *cw*-HeCd laser. This all-optical pump-and-probe approach was implemented into a time-resolved imaging spectroscopy setup (see Ref. [8] for more details) to examine REDG. The present experiments also indicate that there is strong REDG in both n-type and p-type SiC and that the doping-defined position of the Fermi level is not a significant factor in degradation of the material under conditions of nonequilibrium electron-hole injection.

Figure 1 shows plan-view PL micrographs from the 4H and 6H-SiC exposed to intense optical excitation for several minutes. In each case, the dark triangular shaped features on a light background signify regions with a higher nonradiative recombination rate. Comparison with similar features in forward-biased 4H-SiC diodes [4,9,10] strongly suggests that these are expanding basal plane stacking faults. One can immediately notice that, irrespective of the SiC polytype, generation of excess carriers results in a rapid buildup of multiple SFs. In each case, increasing the duration of illumination resulted in a steady increase of the SF density. It is important to realize that the initial density of basal dislocations in the substrate and the epilayer was about 10^3 cm^{-2} and that at the beginning of the optical excitation experiments hardly any SFs were visible in the areas imaged in Fig. 1. Furthermore, except for a small biaxial stress of a few tens of kPa from the negligible epilayer/substrate lattice mismatch, no other stress existed in the epilayer, and the epilayer temperature during laser irradiation was estimated to be less than 50 °C. Since there is a net motion of dislocations only under a directional shear stress and such a shear stress is absent in the present experiments, it is as though faulting in SiC lowers the energy and optical excitation merely catalyzes the leading partial to glide and expand the SF areas in order to lower the free energy of the crystal [11].

Recently, it has been shown that 4H-SiC bipolar power devices rapidly degrade when electrically stressed [9]. The resulting drift of forward voltage characteristics in p-i-n diodes has been associated with an increase in the density of SFs during operation [10]. Figure 2 shows a similar p-i-n diode and surrounding areas of virginal epilayer after being subjected to a series of intense (50 mJ/cm^2) laser pulses of 355 nm wavelength. Spectral filtration of luminescence exposes key constituents of the structural degradation, basal plane stacking faults, and bounding partial dislocations, as well as interaction of mobile leading partials with fixed threading dislocations. The similarity of this picture with those of diodes degraded under forward biasing [4] proves that the central point in degradation of bipolar devices is the generation of excess carriers that triggers REDG. More importantly, Fig. 2 demonstrates that easy generation of SFs in SiC is an inherent material property irrespective of whether it is processed for device fabrication or is virginal; a bipolar device serves only as a means of generating an excess of carriers, and the solution to the degradation problem must address general materials issues in SiC.

To study REDG in SiC quantitatively, we selected the more relevant polytype, 4H-SiC, and investigated the expansion of SFs as a function of temperature T. In fact, since expansion of an SF is directly related to the motion of its bounding leading partial dislocation, we measured the dislocation velocity v as a function of T from sequential images of the type shown in Fig. 2(b). These experiments were performed under pulsed 50 mJ/cm^2 excitation of a 355 nm wavelength laser beam. Figure 3 shows an Arrhenius plot of the optically stimulated dislocation glide velocity. The linear plot shows that dislocation motion follows the empirical relationship $v = v_0 \exp(-E_i/kT)$ with an activation enthalpy of $E_i = 0.25 \pm 0.05$ eV. The huge decrease of nearly 2 eV from the activation enthalpy for dislocation motion in the dark, $E_d = 2.47$ eV [3], appears to be considerably larger than similar effects seen in other semiconductors, signifying the strength of

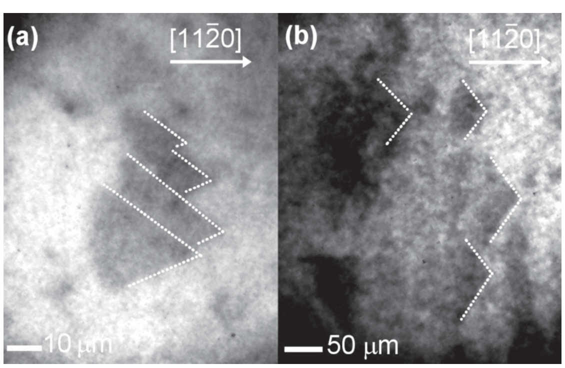

FIG. 1. Plan-view micrographs of integral PL from (a) n-type 4H-SiC and (b) p-type 6H-SiC epilayers after exposure to intense laser pulses of 355 nm wavelength. Dark triangular shaped features are basal plane stacking faults, acting as nonradiative recombination areas for excess carriers (dotted lines are guides for the eyes).

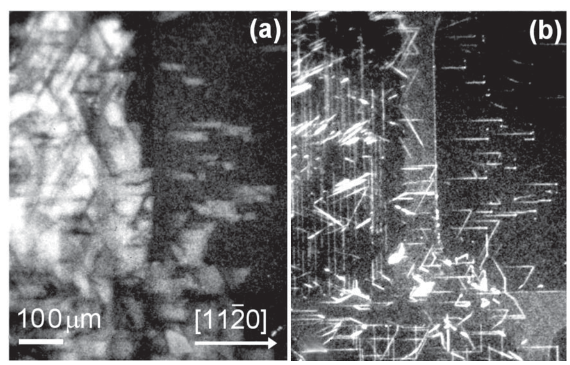

FIG. 2. Spectrally filtered PL images of optically induced structural degradation in 4H-SiC: (a) basal plane stacking faults, seen as an overlay of bright triangles when imaged in the 430 ± 10 nm spectral range; (b) partial dislocations and in-grown threading dislocations, seen correspondingly as bright lines and spots in the wavelength range 778 ± 20 nm. Note that SFs form in both the virginal and processed areas (the darker top-right region comprising half of the p-i-n diode).

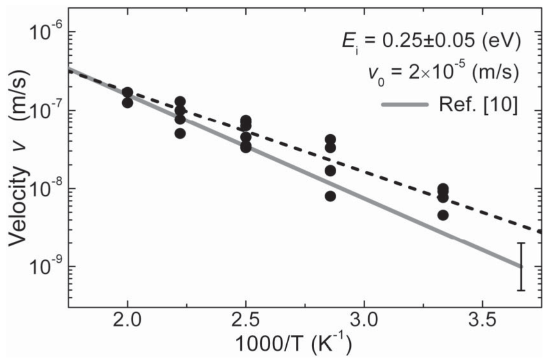

FIG. 3. Arrhenius plot of dislocation glide velocity in $4H$-SiC measured from time-lapse imaging of optically stimulated REDG.

recombination-enhanced defect reactions in SiC (see Table I). An analogous effect was earlier observed during electrical injection measurements on $4H$-SiC *p-i-n* diodes, and the present results justify and confirm the REDG parameters obtained in the past [4].

We had previously proposed [14] that reconstruction defects known as antiphase defects (APDs) [15] or solitons [16] would be likely sites on a partial dislocation to account for trapping of carriers and where local recombination can channel the energy to enhance dislocation motion. Indeed, Heggie and Jones in their theoretical work on doping dependence of dislocation velocity in silicon first suggested that solitons act as preferential sites for nucleation of kink pairs [16]. Moreover, by definition, a soliton is associated with a dangling bond on a reconstructed dislocation line, giving rise to a deep level in the band gap of the semiconductor. We are thus proposing that solitons with an energy level of $(E_d - E_i) \approx 2.25$ eV in the band gap of SiC act as nonradiative recombination sites and are responsible for REDG in this material. In order to verify this model directly, we have performed an excitation-spectrometry type REDG experiment by scanning over deep recombination centers with a tunable below-gap optical excitation from a Nd-YAG:OPO laser system with an average power density per pulse of 0.6 $\mathrm{W/cm^2}$. At a distinct threshold energy, we see an abrupt start of dislocation glide which then continues for all higher energies. This optical activation of dislocation glide occurred when the pump photon energy was gradually increased above 2.58 eV. In view of the dominant phonon-assisted absorption of excitation pulses, the actual energy position of the nonradiative sites is roughly considered to be around 2.4 eV above the valence band.

It is worth mentioning that recent theoretical work by Blumenau *et al.* [17] on dislocations in SiC suggest that only the Si(g) partial dislocation is electrically active with a corresponding band gap level at $E_{\mathrm{Si(g)}} = 0.4\ \mathrm{eV} + E_V$. On the other hand, latest electron-beam-induced–current experiments indicate that both the Si(g) and C(g) partials perform as effective recombination sites [18] even though, according to optical studies [19], the rate of *radiative* transition on the Si(g) partial seems to be much higher than that on the C(g) partial dislocation. The higher mobility of the Si(g) partial in electroluminescence can be made consistent with solitons as the REDG recombination sites if one assumes that only the reconstruction defects on a 30° Si(g) partial dislocation give rise to deep energy levels and act as trapping centers. The REDG model with a single key element, soliton related deep level at $E_S \approx 2.4\ \mathrm{eV} + E_V$, proposed here, can be justified further, considering the optical signature of the electrically active 30° Si(g) partial. Indeed, spatially resolved differential PL spectra obtained from the mobile partial dislocations exhibit two characteristic components, a narrow peak at 2.87 eV and a broad emission band in the region of ~1.8 eV (see Fig. 4). Assuming that dangling bonds on a reconstructed dislocation line give rise to a deep level acting as both radiative and nonradiative sites, the experimental luminescence peaks are consistent with a free-to-bound type $(E_{\mathrm{G}} - E_{\mathrm{Si(g)}}) \sim 2.87$ eV and donor-to-acceptor type $(E_{\mathrm{S}} - E_{\mathrm{Si(g)}}) \sim 2$ eV transitions, respectively. It should be noted that, regardless of the apparently dual nature of the soliton site, only a minor fraction of recombination events on the partial dislocation lines turns out to be radiative [as imaged in Fig. 2(b)].

Presently, besides shear stress, the only other driving force for partial dislocation motion could be an electronic one arising because of the quantum-well nature of stacking

TABLE I. Parameters of the recombination-enhanced dislocation glide in some semiconductors observed *in situ* by: optical excitation (this work); electroluminescence using forward current injection through a *p-n* junction [4]; transmission electron microscopy at 200 kV [12]; scanning electron microscopy [7]; transmission electron microscopy at 1 MV [13].

Material (dislocation)	Injection method	In the dark E_d (eV)	Under injection E_i (eV)	$\Delta E = E_d - E_i$ ΔE (eV)	Band gap E_{G} (eV)	References
$4H$-SiC (30°)	Optical	2.47	0.22	2.25	3.26	This work
$4H$-SiC (30°)	Electrical	2.47	0.25	2.22	3.26	[4]
ZnS (α, β)	*e*-beam	1.15	0.3	0.85	3.6	[12]
GaP (α)	*e*-beam	1.5	0.4	1.1	2.26	[7]
GaAs (β)	*e*-beam	1.7	0.6	1.1	1.42	[7]
Si (60°)	*e*-beam	2.2	1.6	0.6	1.11	[13]

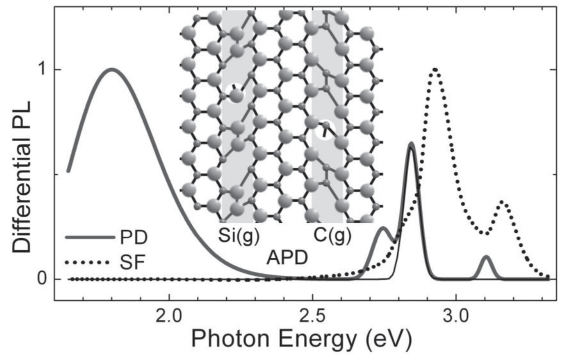

FIG. 4. Spectral signatures of mobile Si(g) partial dislocation (PD) and stacking fault (SF) revealed by spatially resolved differential PL. The inset shows atomic configuration of APDs on 30° C(g) and 30° Si(g) partial dislocations, each containing a dangling bond.

faults [11]. Indeed, Lindefeldt *et al.* [20] showed that a single-layer SF in 4*H*-SiC gives rise to a narrow energy band at about 0.2 eV below the conduction band. Similarly, a double-layer SF forms a deeper band at approximately $E_C - 0.6$ eV. Since the electronic energy of the system may be decreased by the conduction electrons occupying the lower energy states in these quantum wells, formation of SFs would stabilize the system [20]. For this to occur, however, the Fermi energy of the material must be higher than the SF energy level, implying that the crystal must be highly *n*-doped. Such an effect does in fact occur in highly *n*-doped 4*H*-SiC, which after annealing fills up with double-layer SFs [21,22]. However, the SFs formed under optical excitation or by forward biasing are predominantly the single-layer type [19]. Furthermore, our observation of the rapid buildup of SF density in *p*-type SiC, similar to *n*-type material, and a recently reported degradation of electrically stressed *p*-*i*-*n* diodes in which the active layer was *p*-type [23], calls for a more elaborate explanation. Clearly, stress alone cannot explain the formation and multidirection expansion of SFs under carrier injection in SiC, implying that other driving forces must be operating in the crystal [23]. One possibility would be a transient nonequilibrium raising of the quasi-Fermi level by carrier injection to above the single-layer SF level. In this way, the free energy of the faulted crystal would be temporarily lowered, thus providing a driving force for glide of the leading partials and expansion of the stacking faults.

In summary, we found that stacking faults fill the volume of 4*H*- and 6*H*-SiC crystals under optical excitation at room temperature. The SF areas expand by the motion of partial dislocations that glide on the (0001) planes with a very low activation energy, measured to be $\sim$0.25 eV. The drastic lowering of about 2 eV is by the mechanism of recombination-enhanced dislocation glide. This low activation threshold agrees well with observations in forward operating *p*-*n*-junction devices, implying that radiation enhanced dislocation glide is a general phenomenon in hexagonal SiC polytypes.

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