1. Recent progress in shuffle-Glide controversy in silicon

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1.1. Dislocation Mobility

At high temperature, it is widely accepted that glide-set dislocation (Figure.1) can move easily than shuffle-set dislocation (Figure.1) from experimental [1,2,3] and theoretical approaches[4,5].

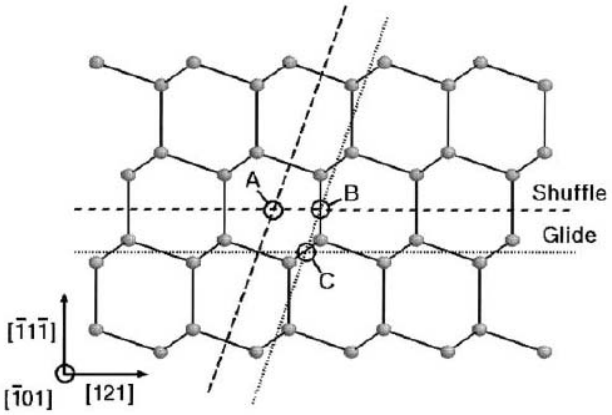

Figure 2. Ball-and-stick representation of the ($\bar{1}01$) plane of the cubic diamond structure. The three circles A, B and C indicate the positions of the dislocation line. Broken (dotted) lines show the 'shuffle' ('glide') {111} planes.

Figure 1: Glide-set and shuffle-set dislocation in silicon

Duesbery pointed out, in usual range of stress ($\tau/\mu<0.01$), the activation energy of partial glide kinks is favored over those of perfect shuffle kinks as shown in below Figure 2.

The kink mechanism of glide-set dislocation was extensively investigated by Bulatov et al.[6,7,8] using atomistic simulation employing SW potential and EDIP potential. They

showed that complicated bond reconstructions on dislocation core and kink play an important role in the dislocation mobility. The resulting activation energies are summarized in Table. 1

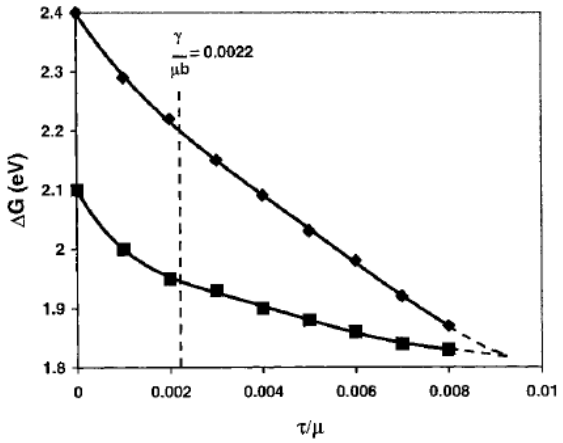

Fig. 10. Free energy for kink pair nucleation and migration for a 30° glide partial (■) and a screw shuffle (◆) dislocation as calculated by Duesbery and Joos [1]. τ_t, the transition stress between the two mechanisms, is about 0.01μ. The minimum stress required for glide partial decorrelation is also indicated

Figure 2: Dependence of activation energies of kinks on stress.

On the other hand, a series of experimental results[9,10,11,12] suggests shuffle-set dislocations nucleate and move below room temperature under hydrostatic pressure (5~15GPa) and high shear stress (~1GPa). Rabier[11,12] pointed out that shuffle-set dislocation could move easier than glide-set one in high stress region (τ/μ<0.01~600MPa). According to his experiment, the shuffle-set dislocations nucleated at low temperature did not move at high temperature 550 C while newly nucleated glide-set dislocations moved easily. Although this result supports his assumption, the conclusion is not still clear.

Shuffle-set dislocation has a lower Peierls stress than glide-set partial dislocation. That was confirmed by atomic calculation with SW potential and Peierls model. According to atomistic calculation with SW potential, Peierls stresses[A] of shuffle-set screw dislocation is 5.5GPa (Koizumi[13] obtained 3GPa using SW potential. Pizzagalli[14] obtained 4.8GPa using ab-initio calculation. Both authors also proved the stability of shuffle-set screw dislocation) and that of glide-set 90 degree dislocation is 18.0GPa[B]. This results supports that shuffle-set dislocation can migrate at low temperature and high stress.

[A] It is noted that the Peierls stress is ambiguous in terms of how this value correlates to dislocation nucleation or dislocation mobility. In the present case, it appears to be not related to dislocation mobility but dislocation nucleation.

[B] This result was interpreted that while the sparse bond density on the shuffle-set plane leads to lower Peierls stress, it also hinders possible core reconstruction which is favored at high bond density (glide-set). So there is a systematic core energy advantage to glide-set dislocations, irrespective of partial or full dislocations, this reconstruction energy advantage may pertain to kink processes as well. Their DFT calculation showed that the core of undissociated glide-set screw dislocation has lower energy than that of undissociated shuffle-set dislocation, which might play an important role in cross slip at high T.

TABLE I. Comparison of Peierls stresses in Si obtained from the Peierls-Nabarro model (Ref. 1), σ_p, with those from the atomic relaxation calculation (present work), σ_b (μ=0.4 eV/Å^3, the {111} shear modulus, see Ref. 2).

Dislocation		σ_b (μ)	σ_p (μ)
glide	60°	dissociation	15.63
	screw		19.66
shuffle	60°	0.080	0.076
	screw	0.091	0.103
glide	90°	0.27	0.450
	30°	0.33	0.561

Cai[15] estimated a kink-formation energy at E_k=0.728 eV and a kink migration energy at W_m=0.022eV using the SW potential. Resulting effective activation energy for double-kink nucleation defined by $Q_{nucl}=2E_k+W_m$ (~1.5eV) was much smaller than that of 30 degree partial (2.6eV) on glide set plane and that of Peierls-Nabarro model (2.4eV) estimated by Dusbery[C]. This indicated that shuffle-set dislocation always move faster than glide-set dislocations under all temperature and stress condition[D].

Results are summarized in Table 1.

[C] Experimental activation energy for dislocation motion is 2.2eV in silicon (H. Alexander, Dislocation is Solids, Vol. 7, edited by F. R. N. Nabarro, Amsterdam: North-Holland (1986)). W_m~1.6eV means dislocation dynamics in Si is controlled by the kink migration.

[D] Koizumi et al. (H. Koizumi and T. Suzuki, Mater. Sci. Eng., A **400-401**, 76 (2005)) estimated athermal stress for the mobility of an initially-introduced kink-pair on shuffle-set screw dislocation at 0.0027G using SW potential.

Table 1: Peierls stress and kink formation and migration energies of various types of dislocations in silicon.

*1 [4], *2[W.Cai, unpublished], *3[B. Joos and M. S. Duesbery, PRL78 (1997), 266] *4 [W. Cai, et al., Chapter 64 in Dislocation is Solids, F. R. N. Nabarro and J. P. Hirth ed., Vol. 12 (2004), 1.], *5[15], *6[T. Vegge, K. W. Jacobsen, J. Phys.: Condens. Matter, 14(2002) 2929.], G=68.1GPa(Si)

All results are based on the SW potential (Silicon)

	Peierls stress GPa	Kink mobility eV ( ):exp	
		Kink formation $2E_k$	Kink migration W_m
Glide-set 30 deg.	22.6 *1	1.4 (0.62) *4	1.2 (1.58)*4
Glide-set 90 deg.	18.0 *1	(0.74) *4	(1.55) *4
Shuffle-set 60 deg	4.8*1	-	-
Shuffle-set screw	5.5*1, 3.3*2	1.46*5	0.022 *5

***It should be noted that previous calculation did not see a reaction path of dislocation migration. They obtained a kink-migration energy E_k and a W_m, separately, with different scheme. That method is based on a reaction path assumption shown in Figure 3. Therefore, it is necessary to make sure the validity of the assumption using a whole reaction path, which can be obtained by NEB scheme.

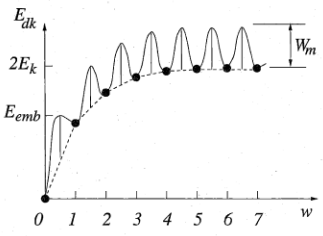

Figure 7-2: Theoretical dependence of the kink pair energy E_{dk} on its width w are shown as dots. For large width it approaches $2E_k$. At finite width w, E_{dk} is a superposition of $2E_k$ and the kink pair interaction energy $W_{int}(w)$. The solid curve illustrates the energy barrier between the neighboring states. E_{emb} is the barrier for nucleating an embryonic double-kink, i.e. transition from state $w = 0$ to $w = 1$.

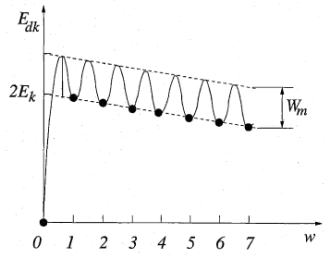

Figure C-1: Kink pair energy E_{dk} as a function of width w, shown as dots. Elastic interactions of between kinks are ignored. The applied stress creates a tilt in the energy landscape.

1.2. Dislocation nucleation

Regarding the dislocation mobility, many researches are done. However, regarding the dislocation nucleation little is known so far.

Unstable stacking fault energy (γ_{us}) would be a material property related to dislocation nucleation. Juan et al.[16] estimated γ_{us} as 1.68 Jm^{-2} for shuffle-set dislocation and 1.89 Jm^{-2} for glide-set dislocation. Godat et al.[17] estimated 0.830 and 3.09 Jm^{-2}, respectively, by using the SW potential and 1.67 and 1.91 Jm^{-2} by the DFT scheme. Those results indicate that shuffle-set dislocation would be nucleated at low temperature. That is in good agreement with experimental results.

The nucleation of shuffle-set perfect dislocation was also obtained using molecular dynamics simulation employing SW potential[18] as well as ab-initio calculations[19].

Question arises: how does glide-set dislocation nucleates? One possibility is the transition of shuffle dislocation to glide dislocation. Rabier showed a perfect dislocation

could be transformed into a dissociated glide one through two basic mechanisms: cross slip and climb as shown in Figure below. Pizzagalli et al. pointed out that transition from shuffle to glide by cross slip appears to be impossible using ab initio and empirical potentials[14]. Rabier[11] carefully observed the nucleation and propagation of perfect shuffle (PS) and dissociated glide (DG) dislocations with TEM observation and showed that there is no evidence of a shuffle to glide transformation[E]. He claimed that PS and DG dislocations in silicon are nucleated and propagate in different range of stress and temperature without any core transformation between two types of core structure of dislocations. Justo et al.[20] denied the possibility of transformation under equilibrium vacancy concentration.

On the other hand, Saka et al.[21,22] reported that the transformation from shuffle-set to glide-set occurred at 400 $°C$ during the heating of dislocations underneath the amorphous phase introduced by Vickers indenter. There is a possibility that sessile shuffle nucleus transform to glissile glide dislocation under large supersaturating of point defects (such as scratch and amorphous region).

[E] He also indicated that glide to shuffle transition is impossible. Pre-existing glide dislocations shows large stacking fault under the high stress at low temperature[11].

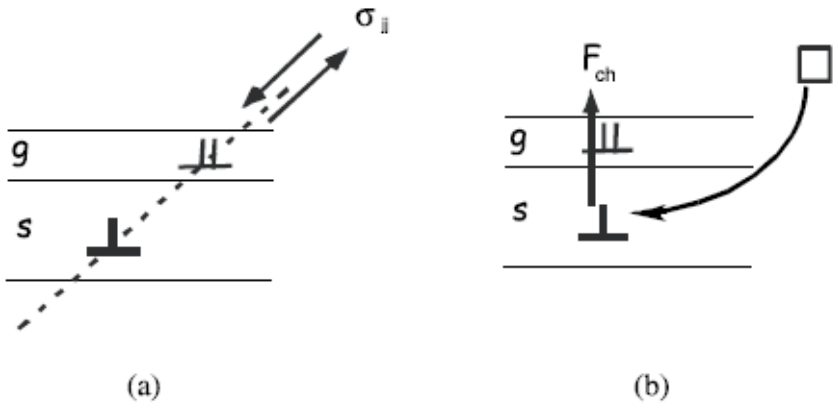

Fig. 3 Transformation from a perfect shuffle into a dissociated glide. The perfect dislocation has moved from one atomic plane in the glide set by: a) cross slip under the action of a mechanical force and b) climb under the action of a chemical force.

Dislocation behavior in different temperature and stress regions is summarized in Table 2 below.

Table 2 Dislocation behaviors in different temperature and stress regions (Peierls stress of shuffle-set dislocation is lower than that of glide-set dislocation. At low stress, glide-set dislocation has lower double-kink energy. At high stress, shuffle-set dislocation has lower energy. Shuffle-set dislocation is immobile under low stress.)

	Low Temp. < 300K	High Temp.>800K
Low Stress < 20MPa	• Nothing happens	• 30 deg. Glide-set dislocations van migrate and move with double-kink pair mechanism • Cross-slip takes places at pre-existing constrictions[23]. (Hard to move) • Shuffle-set dislocations cannot move.
High Stress > 1GPa	• Perfect shuffle-set dislocations nucleate and move. • Cross-slip takes place frequently • Pre-existing glide-set dislocations get to extend largely.	Not known

[1] K. Wessel and H. Alexander, Philo. Mag. **35**, 1523 (1977).

[2] A. Gomez, D. J. H. Cockayne, P. B. Hirsch, and V. Vitek, Phio. Mag. **31**, 105 (1975).

[3] K. Sato, K. Hiraga, and K. Sumino, Jpn. J. Appl. Phys. **19**, L155 (1980).

[4] Q. Ren, B. Joos, and M. S. Duesbery, Phys. Rev. B **52**, 13223 (1995). Erratum, Phys. Rev. B**53**, 11883 (1996).

[5] M. S. Duesbery and B. Joos, Philos. Mag. Lett. **74**, 253 (1996).

[6] V. V. Bulatov, S. Yip, and A. S. Argon, Philos. Mag. A **72**, 453 (1995).

[7] V. V. Bulatov, J. F. Justo, W. Cai, S. Yip, A. S. Argon, L. Lenosky, M. de Koning, and T. Diaz de la Rubia, Philos. Mag. A **81**, 1257 (2001).

[8] V. V. Bulatov, Script. Mater., **45**, 1247 (2001).

[9] T. Suzuki, T. Yasutomi, T. Tokuoka, and I. Yonenaga, Phys. Rev. A **79**, 2637 (1999).

[10] J. Rabier, J. L. Demenet, Phys. Status Solidi B **222**, 63 (2000).

[11] J. Rabier and J. L. Demenet, Phys. Status Solidi A **202**, 944 (2005).

[12] J. Rabier, Phys. Status Solidi A **204**, 2248 (2007).

[13] H. Koizumi, Y. Kamimura, T. Suzuki, Philos. Mag. A **80**, 609 (2000).

[14] L. Pizzagalli, P. Beauchamp, Philos. Mag Lett.. **84**, 729 (2004).

[15] W. Cai, Doctoral thesis, MIT, (2001).

[16] Y. Juan, E. Kaxiras, Philos. Mag A **74**, 1367 (1996).

[17] J. Godet, L. Pizzagalli, S. Brochard, and P. Beauchamp, J. Phys.: Condens. Matter. **15**, 6943 (2003).

[18] J. Godet, L. Pizzagalli, S. Brochard, and P. Beauchamp, Phys. Rev. B **70**, 054109 (2004).

[19] J. Godet, S. Brochard, L. Pizzagalli, P. Beauchamp, and J. M. Soler, Phys. Rev. B **73**, 092105 (2006).

[20] J. F. Justo, M. Koning, W. Cai, V. V. Bulatov, Phys. Rev. Lett, **84**, 2172 (2000).

[21] K. Asaoka, T. Umeda, S. Arai, H. Saka, Mater. Sci. Eng. A, **400-401**, 93 (2005).

[22] H. Saka, K. Yamamoto, S. Arai, K. Kuroda, Philos. Mag.. **86**, 29 (2006).

[23] F. Vallino, A. Jacques, J. George, Phys. Status Solidi B **222**, 51 (2000).