# Electronic structure of dopant around stacking fault in Si Crystal

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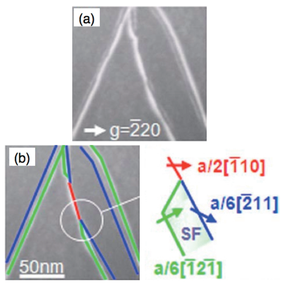
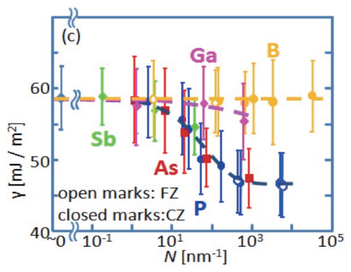
## Experimental observations

Dislocation cores of heavily doped n- and p-type Si crystals have been observed via transmission electron microscopy (TEM) by Ohno et al.[1]. When an n-type dopant (P, As, or Sb) is added, the dissociation width of stacking faults increases with increasing annealing time. Because the dissociation width of the stacking fault is determined by the balance between the stacking fault energy and repulsion of the dislocation cores, an increase in the stacking fault width indicates a decrease in stacking fault energy.

- P, As, Pb(n-type)
  - Stacking fault energy decreases, with increasing the dopant concentration.
  - Dopants segregate in SF region.
- B(p-type)
  - Stacking fault energy remains constant, with increasing the dopant concentration.
  - Dopant does not segregate in SF region.




Y.Ohno, *et al.*, Appl. Phys. Lett. **95** (2009) 091915.

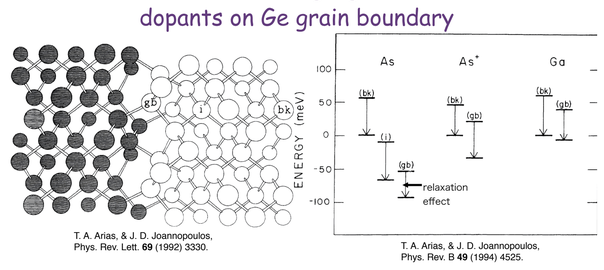



Y. Ohno, *unpublished work.*

Y.Ohno, *et al.*, J. Appl. Phys. **108** (2010) 073514

| | Experiment | Calculation | |
|---|---|---|---|
| | Ohno | Arias & Joannopoulos | Justo |
| Segregate | Ga, P, As, Sb | Donor (N, P, As, Sb) | Donor (N, P, As, Sb) |
| Don't Segregate | B | Acceptor (B, Al, Ga, In) | Acceptor (B, Al, Ga, In) |

### Previous calculations: Segregation behavior of dopants on Ge grain boundary

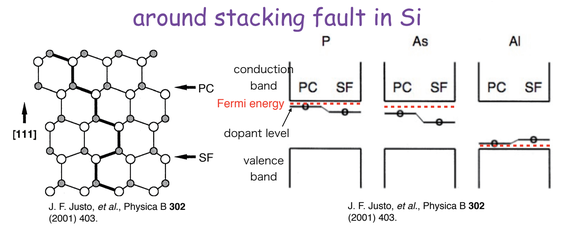



T. A. Arias, & J. D. Joannopoulos, Phys. Rev. Lett. **69** (1992) 3330.

T. A. Arias, & J. D. Joannopoulos, Phys. Rev. B **49** (1994) 4525.

- Comparing ionized As+ and Ga, As is stabilized at GB.
  - ➡ Because donner level drop of n type dopant.
- In perfect lattice(PC) and grain boundary(GB) region, the energy drops due to the relaxation effect are almost same.
  - ➡ Strain around dopant is not main effect on dopant segregation.

### Justo model for electronic structure of dopant around stacking fault in Si




J. F. Justo, *et al.*, Physica B **302** (2001) 403.

J. F. Justo, *et al.*, Physica B **302** (2001) 403.

- P, As(n-type)
  - stabilize the system due to the donor level drop.
- Al(p-type)
  - Do not stabilize the system due to the emptiness of changed acceptor level.
- ➡ Thus, n-type dopants do, but p-type dopants do not segregate in SF region.

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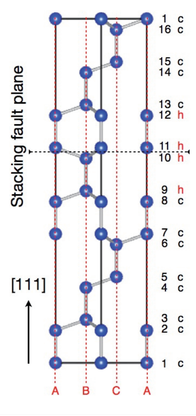
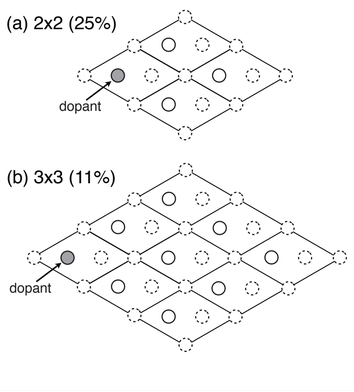
## calculation method

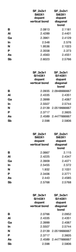



- VASP models
  - $Si_{63}X_1$, $Si_{143}X_1$
    - p-type: B, Al, Ga, In
    - n-type: N, P, A, Sb
  - Solution energy of dopant

$$E_{\text{solution}} = \left(E^{\text{SF}}_{\text{Si}_{63}\text{X}_1} - E^{\text{cubic}}_{\text{Si}_{63}\text{X}_1}\right) - \left(E^{\text{SF}}_{\text{Si}_{64}} - E^{\text{cubic}}_{\text{Si}_{64}}\right)$$

  - Electronic structure at gamma point



To investigate the experimental results of the segregation of dopant atoms around the stacking fault, we performed an energy assessment using Vienna ab initio simulation package (VASP). Our results indicate that both p-type (P, As, Sb) and n-type (Al, Ga, In) dopant atoms reduce the stacking fault energy when these atoms localize around the stacking fault.

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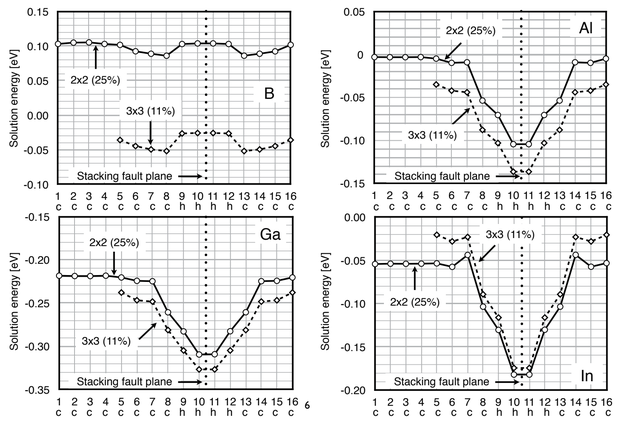
## VASP energy assessment

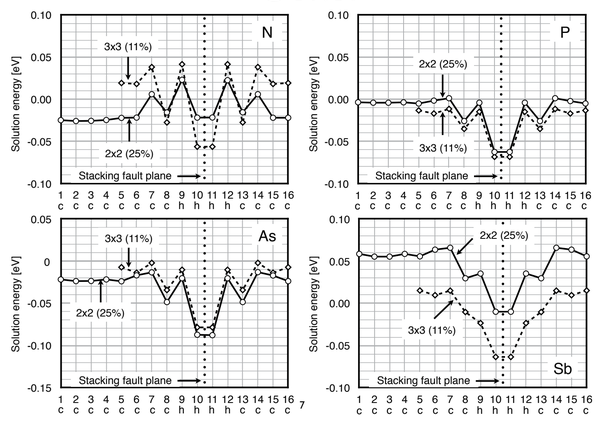
1. Al, Ga, In(p-type), P, As, Sb(n-type) stabilized at SF
2. B stabilized not at SF.
   1. Consistent with the experiments by Ohno

| | Experiment | Calculation | | |
|---|---|---|---|---|
| | Ohno | Arias & Joannopoulos | Justo | This work |
| Segregate | Ga, P, As, Sb | Donor (N, P, As, Sb) | Donor (N, P, As, Sb) | Al, Ga, In, P, As, Sb |
| Don't Segregate | B | Acceptor (B, Al, Ga, In) | Acceptor (B, Al, Ga, In) | B, N |

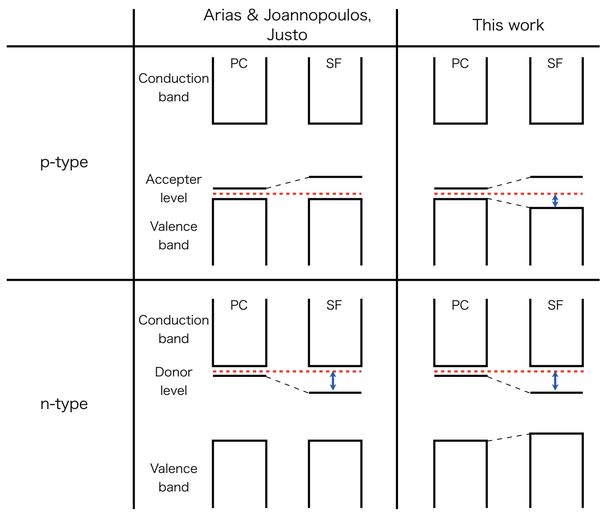
### Acceptor



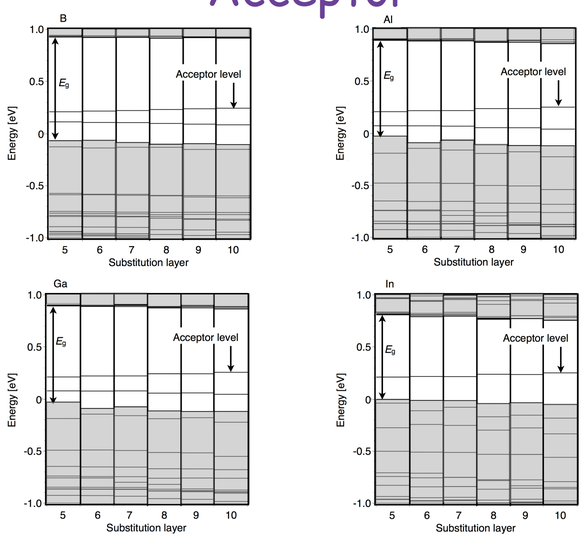

### Donor



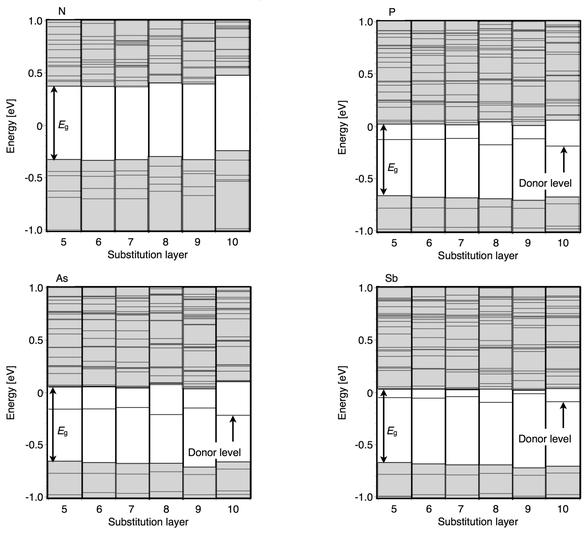

## Electronic structure




### Acceptor




### Donor




## Summary

- **Energy assessment of dopant segregation in Si**
  1. Al, Ga, In(acceptor, n-type), P, As, Sb(donor, p-type) stabilize the system when segregate at stacking faults.
  2. B stable at next layer of SF.
  3. N behavior depends on the concentration.
- **Electronic structure change due to dopant replacement**
  4. Al, Ga, and In(acceptor) stabilize due to the valence band drop.
  5. P, As, and Sb(donor) stabilize due to the dopant level drop.

To describe the dopant behavior in the stacking fault region in Si crystal, we proposed a new model as illustrated in Fig.[1][2]. When the n-type dopant atoms are substituted at the stacking fault region (SF), the donor levels and total energy are shifted to lower energies. Conversely, when the p-type dopant atoms are substituted at the stacking fault, the system is unaffected by the change in the acceptor level because of the acceptor level do not contain any electrons, whereas the valence band shifts to lower energies and reduces the total energy.