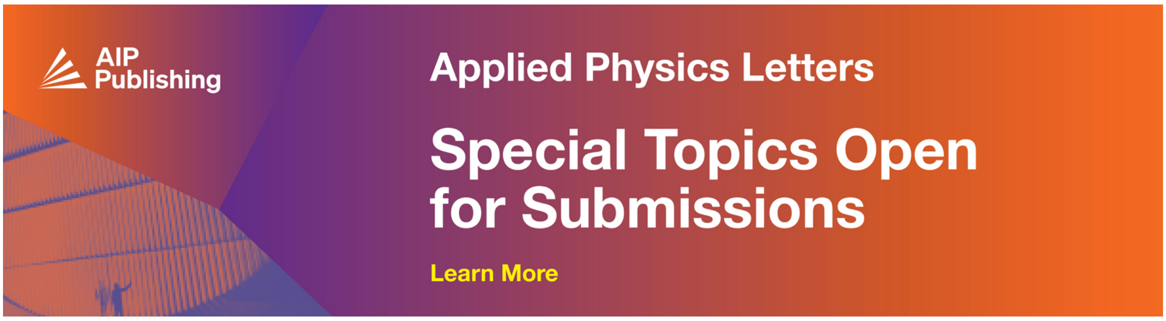
Applied Physics Letters

RESEARCH ARTICLE | NOVEMBER 27 2000

Detection of stacking faults in 6H-SiC by Raman scattering

S. Nakashima; Y. Nakatake; H. Harima; M. Katsuno; N. Ohtani

Appl. Phys. Lett. 77, 3612–3614 (2000)
https://doi.org/10.1063/1.1329629



AIP Publishing

APPLIED PHYSICS LETTERS VOLUME 77, NUMBER 22 27 NOVEMBER 2000

Detection of stacking faults in 6H-SiC by Raman scattering

S. Nakashima[a] and Y. Nakatake
Department of Electrical and Electronics Engineering, Miyazaki University, 1-1 Gakuen-Kibanadai Nishi, Miyazaki 889-2192, Japan

H. Harima
Department of Applied Physics, Graduate School of Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan

M. Katsuno and N. Ohtani
Advanced Technology Research Laboratories, Nippon Steel Corporation, 20-1 Shintomi, Futtsu, Chiba 293-8511, Japan

(Received 20 June 2000; accepted for publication 20 October 2000)

Raman spectra of 6H-SiC crystals including stacking faults have been examined for the *c* face using backscattering geometry. The intensity of the transverse optical phonon band at 796 cm^{-1}, which corresponds to the phonon mode at the Γ point in 3C-SiC, is sensitive to the stacking faults. We found that the intensity of this band depends on the stacking fault density. This is explained based on the bond polarizability model. The spatial distribution of the stacking faults is studied by Raman image measurement. © *2000 American Institute of Physics.* [S0003-6951(00)00249-7]

Silicon carbide has a large number of polytypes for which the stacking sequences of Si–C double atomic planes are different. This fact implies that the stacking faults (SF) are easily generated. In fact the calculated formation energy of the SF is very small compared with that of Si and diamond.[1] It has been pointed out that the SF has strong influence on electrical properties of SiC.[2] So far the SF have been evaluated by x-ray diffraction,[3] high-resolution transmission electron microscopy,[4] and Raman scattering.[5–7] Of these methods Raman scattering is the most desirable since it is nondestructive, simple to use, and the least time consuming. In the present work we study the stacking faults in 6H-SiC by Raman scattering measurement of a transverse phonon mode using a specified experimental geometry. Raman spectra were measured with a backscattering geometry using the 488 nm line of an Ar laser. A triple monochromator with $f=60\,\mathrm{cm}$ equipped with a backillumination type cooled charge coupled device (CCD) detector was used.

Long period SiC polytypes have a number of Raman active modes which arise from the so-called zone folding of the Brillouin zone of the basic polytype (3C polytype).[8,9] The Raman spectra of these phonon modes, especially the folded transverse modes are greatly affected by the SF. Figure 1 shows Raman spectra of 6H-SiC crystals containing low and high densities of the SF. The Raman bands are distorted and broadened for high density of the SF. A striking feature in the spectra is the growth of a Raman band at 796 cm^{-1} at a high density of the SF. Hereafter, we call this the FTO(0) band. We used the FTO(0) band as a monitor of the SF.

The folded mode observed in the Raman scattering of nH polytypes corresponds to a phonon mode with a wave vector of $q=2\pi m/(nc)$ in the basic Brillouin zone of the 3C polytypes in the [111] direction, where n and m are integers $(2m\leqq n)$.[10] The Raman intensities of these folded modes in the transverse optical (FTO) and acoustic (FTA) branches are calculated on the basis of the bond polarizability concept.[8,9]

Under an assumption that the bonding forces between Si(C) and C(Si) atomic planes are the same for hexagonal and cubic environments, the Raman intensity of the FT modes given by Eq. (2) in Ref. 9 is reduced to the following form:[5]

$$W=S[n(\omega)+1]\omega^{-1}|A(q)-B(q)|^2|c(q)|^2$$

and

$$c(q)=N^{-2}\Sigma\alpha_i\exp(iqz_i).$$

Here, S is a constant independent of ω, $n(\omega)$ is the Bose factor, q is the wave vector of phonons, and $A-B$ is the oscillation amplitude of the relative displacement of neighboring Si and C planes. $c(q)$, which is called the Raman structure factor, is given by Fourier transform of the bond Raman polarizability α_i which is equal to the *xx*, *yy*, and *xy* components of the bond Raman polarizability tensor. For the FTO(0) mode, we may put $q=0$. Hence, the arrangement of the bond Raman polarizability along the c axis in a unit cell is represented as[10]

$$\alpha=(\alpha_i)=d(1,1,1,-1,-1,-1)\quad\text{for the 6H polytype.}$$

Accordingly, $\Sigma\alpha_i$ becomes zero. This argument is consistent with the result of the group theory analysis that the FTO(0) mode belongs to the E_1 mode, and *xx*, *yy*, and *xy* Raman tensor components are zero. However, if the SF is present, the arrangement of the bond Raman polarizability becomes random and then the $c(0)=\Sigma\alpha_i$ may be finite unless the coherence length of the phonon modes is infinite. The coherence length of the optical phonon modes inferred from the Raman band width is thought to be less than a few tens of nanometers in SiC. Growth of the FTO(0) band with the SF originates from *stacking fault activated Raman scattering*, which is analogous to disorder activated Raman scattering.[11]

---

[a] Electronic mail: nakashim@pem.miyazaki-u.ac.jp

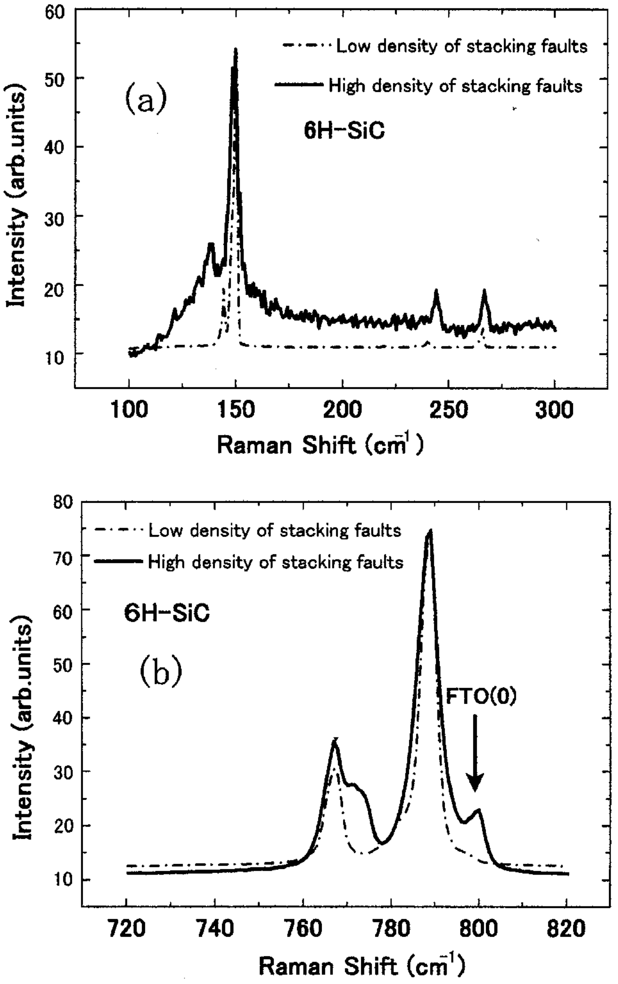


FIG. 1. Raman spectra of the folded transverse modes in 6H-SiC crystals containing stacking faults. (a) Spectra of folded transverse acoustic modes and (b) of the folded transverse optical modes. Solid curves are for high density of the SF and the broken ones are for low density of the SF.

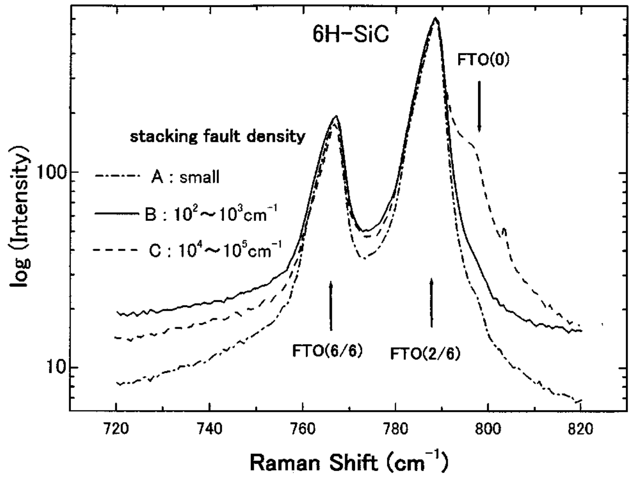


FIG. 2. High frequency portion of the Raman spectra of samples with different SF densities. The SF densities of samples B and C are 10^3-10^4 and 10^4-10^5 cm^{-1}, respectively. The intensity is plotted on logarithmic scale.

Ion-implanted semiconductors[12,13] or mixed crystals[11] often show additional Raman bands at frequencies corresponding to those of zone-edge phonon modes.

The earlier hypothesis is experimentally verified by Raman measurements of crystals with different SF densities which are determined beforehand. SiC crystals containing high and low density of stacking faults were cut from a 6H-SiC ingot grown in a direction perpendicular and parallel to the *c* axis, respectively.[14] The SF density was determined from etch-pit-density measurements. The *c* face was examined with backscattering geometry. No polarization measurement was made. Figure 2 shows Raman spectra of 6H-SiC crystals with relatively low SF densities, the intensity being plotted on the log scale. Since the SF density of the two samples is not heavy, the FTO(0) band is weak and not well separated from the FTO(2/6) band. The intensity of the FTO(0) band increases with increasing SF density, but the FTO(2/6) and FTO(6/6) bands show no remarkable change with this density; the figure in parenthesis denotes the reduced wave vector of the corresponding phonon in 3C-SiC. Note that the band shape of the FTO(2/6) and FTO(6/6) modes are almost independent of the SF density except for the tail regions. This fact suggests that SF has not much influence on the phonon lifetime, but it does affect the Raman activity through extinction of the periodicity. Judging from the Raman spectra shown in Fig. 2, the lower detection limit of the SF density by Raman measurements may be about 10^3 cm^{-1}.

In Fig. 3 we show an example of one dimensional Raman images of a commercial base 6H-SiC wafer grown by a chemical vapor deposition method, which contains relatively high density of stacking faults. The image was obtained by a line illumination method and a CCD detector. The laser beam expanded linearly by a cylindrical lens was focused on the sample surface. The illumination region on the sample was 70×2000 μm. The spectra are plotted with steps of 65 μm. The intensity of the FTO(0) mode varies with the position, indicating that the SF density is not uniform in this wafer.

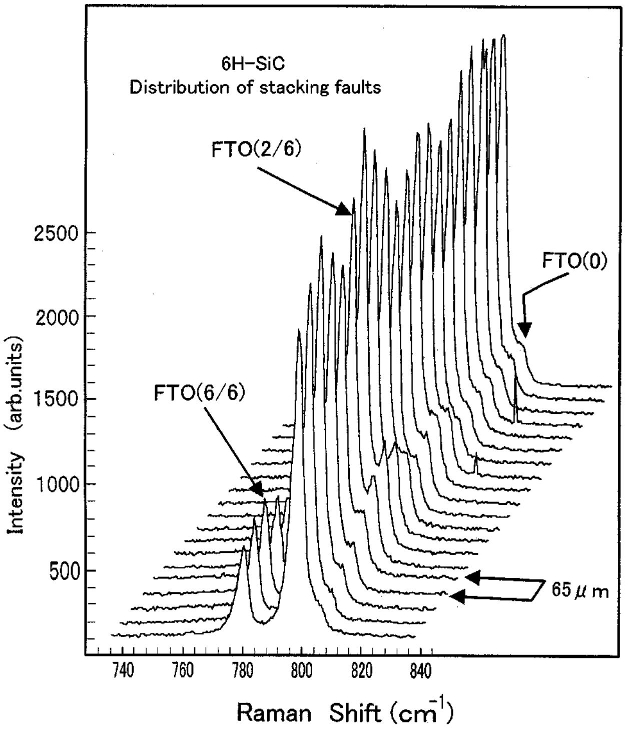


FIG. 3. Spatial variation of the intensity of the FTO(0) band in a 6H-SiC crystal which includes SF.

It should be noted that in order to observe the FTO(0) mode sensitive to the SF we should employ the back scattering geometry using the *c* face of SiC crystals. In this geometry the intensity of the FTO(0) mode is very weak provided there is no stacking fault. Accordingly, this band is sensitive to the presence of the SF. However, in the backscattering geometry using the *ac* face, $x(yz)\overline{x}$, the FTO(0) band is strongly observed, because the Raman tensor component α_{xz} or α_{yz} is not zero even when the stacking fault density is zero. The presence of this band may prevent the detection of the SF. When laser light is obliquely incident on a sample surface, leakage signal of the Raman band related to the tensor component α_{xz} prevents observation of the FTO(0) mode sensitive to the SF. In fact, when we used an objective lens with a large numerical aperture in the Raman microscope, a Raman band was distinctly observed at 796 cm^{-1}, but this band did not depend on the SF density. The approach mentioned earlier can also be applied to the 4H polytype. Raman analyses of the 4H polytype are now under way.

In summary, Raman spectra of 6H-SiC crystals containing stacking faults are measured using the backscattering geometry for the *c* face. We have found that the Raman band at 796 cm^{-1} is sensitive to the stacking faults and that this band can be used as a measure of the SF. Our results demonstrate that Raman spectroscopy is useful to characterize the SF in a nondestructive and simple manner.

This work has been supported in part by the NEDO of Japan and Research Project of Grant-In-Aid for Scientific Research, Japan.

[1] P. Käckell, J. Furthmüller, and F. Bechstedt, Phys. Rev. B **58**, 1326 (1998).
[2] J. Takahashi, N. Ohtani, M. Matsumoto, and S. Shinoyama, J. Cryst. Growth **181**, 229 (1997).
[3] V. V. Pujar and J. D. Cawley, J. Am. Ceram. Soc. **80**, 1653 (1997).
[4] F. R. Chien, S. R. Nutt, J. M. Carulli, Jr., N. Buchan, C. P. Beetz, Jr., and W. S. Yoo, J. Mater. Res. **9**, 2086 (1994).
[5] S. Nakashima, H. Ohta, M. Hangyo, and B. Palosz, Philos. Mag. B **70**, 971 (1994).
[6] S. Nakashima, K. Kisoda, H. Niizuma, and H. Harima, Physica B **219&220**, 371 (1996).
[7] S. Rohmfeld, M. Hundhausen, and L. Ley, Phys. Rev. B **58**, 9858 (1998).
[8] S. Nakashima, K. Katahama, Y. Nakakura, and A. Mitsuishi, Phys. Rev. B **33**, 5721 (1986).
[9] S. Nakashima and K. Tahara, Phys. Rev. B **40**, 6339 (1989).
[10] S. Nakashima and M. Hangyo, Solid State Commun. **80**, 21 (1991).
[11] P. Parayanthal, F. H. Pollak, and J. M. Woodall, Appl. Phys. Lett. **41**, 961 (1982).
[12] W. Limmer, W. Ritter, R. Sauer, B. Mensching, C. Liu, and B. Rauschenbach, Appl. Phys. Lett. **72**, 2589 (1998).
[13] R. Cusco, G. Talamas, L. Artus, J. M. Martin, and G. Gonzalez-Diaz, J. Appl. Phys. **79**, 3927 (1996).
[14] J. Takahashi and N. Ohtani, Phys. Status Solidi B **202**, 163 (1997).