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LETTER TO THE EDITOR

Experimental determination of the intrinsic stacking-fault energy of SiC crystals

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Abstract. The intrinsic stacking fault in the (111) plane of SiC, which is closed by two Shockley partial dislocations, has been observed by high-resolution electron microscopy. The energy of the intrinsic stacking-fault of SiC is experimentally determined and compared with the theoretical value calculated by Denteneer *et al*.

The microstructure of SiC crystals has been studied by many researchers. The important structural character of SiC is its existence as many polytypes, not only in its bulk crystal but also in its whisker form [1]. The influence of stacking faults on the growth of polytype structures was discussed by Pandey *et al* [2]. Actually, the polytype structures are formed by introducing various possible configurations of stacking faults. Therefore the determination of the stacking-fault energy of SiC is significant to the understanding of the structural character of SiC. Denteneer *et al* [3] calculated the stacking-fault energies of β-SiC theoretically and obtained the values: $\gamma_{ISF} = 12$ mJ m^{-2} and $\gamma_{ESF} = -15$ mJ m^{-2} (ISF and ESF standing for intrinsic and extrinsic stacking faults, respectively). The results, however, could not be compared with the experimental values because at that time the stacking-fault energy of β-SiC had not been experimentally determined. In this letter the experimental value of the intrinsic stacking-fault energy of SiC will be given in what follows.

The 60° dislocation in the (111) plane of a FCC structural crystal with low stacking-fault energy will be dissociated into an extended dislocation. The extended dislocation consists of two Shockley partials and an intrinsic or extrinsic stacking fault between the two partials. The intrinsic stacking-fault energy for such a configuration of extended dislocation can be calculated by considering the dislocations in anisotropic elastic media [4]:

$$\gamma_I = [\mu_{eff}/(1 - \nu_{eff})] \cdot (b^2/4\pi d) \tag{1}$$

where

$$[\mu_{eff}/(1 - \nu_{eff})] = (C + C_{12})(C + 2C_{11})\sqrt{C_{44}(C - C_{12})}/3C\sqrt{C_{11}(C_{11} + C_{12} + 2C_{44})} \tag{2}$$

$$C = \sqrt{(C_{11} + C_{12} + 2C_{44})C_{11}/2}. \tag{3}$$

C_{11}, C_{12} and C_{44} are elastic constants. b is the Burgers vector of Shockley partial

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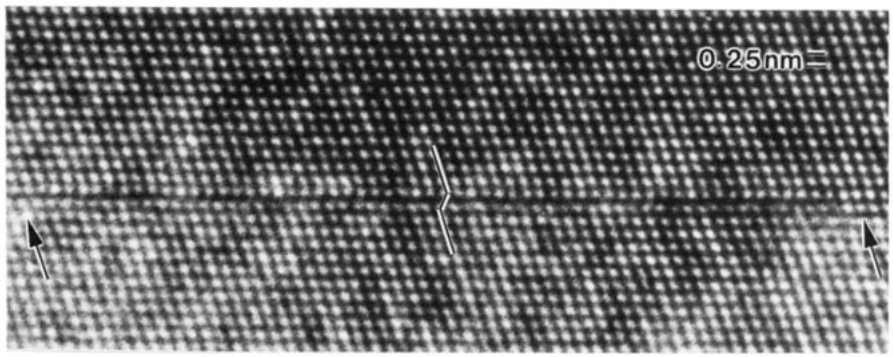

Figure 1. A high-resolution image of an extended dislocation in the (111) plane of SiC viewed along the [110] direction.

dislocations which is equal to $a/\sqrt{6}$ (a is the crystal constant). d is the width of the intrinsic stacking fault between two Shockley partials. The stacking-fault energy can be determined as long as d can be experimentally obtained.

Figure 1 shows such an extended dislocation in the (111) plane of SiC viewed along the $[\bar{1}10]$ direction. The images were taken using a JEOL-200CX high resolution electron microscope with an interpretable resolution of about 0.25 nm. The width of the intrinsic stacking fault can be obtained from figure 1, and is about 16 nm.

For SiC, C_{11}, C_{12} and C_{44} are 35.23, 14.04 and 23.29 $\times$ 10^{10} N m^{-2} respectively [5]. The crystal constant, a, of SiC is 0.43589 nm. Substituting all of the relevant values for SiC into the equations (1), (2) and (3), we can obtain the experimental value of the intrinsic stacking-fault energy, which is about 34 mJ m^{-2}. The difference between the experimental and theoretical (12 mJ m^{-2}) values is serious in a sense. The theoretical values of intrinsic stacking-fault energies given by Denteneer *et al* are sometimes much lower than the experimental results. The theoretical value for Si, for example, is nearly 50% lower than the experimental one (theoretical value: 33 mJ m^{-2}; experimental one: 69 mJ m^{-2}). Only for three crystals i.e. Si, Ge and SiC was the stacking-fault energy calculated. Therefore the theoretical method for calculating the stacking-fault energy needs improvement if it is to meet the experimental results.

Actually, it should be very unlikely for a SiC crystal to contain dislocations or extended dislocations [6] despite there being fewer intrinsic stacking faults. This is the case here, where the SiC crystal observed was a whisker (SiC_w) in an Al/SiC_w composite [7]. Anyway, our result is of significance to the improvement of the theoretical calculation method to some extent, although the statistical study for SiC crystals will be rather difficult. In our observations of SiC crystal microstructure the intrinsic stacking faults were really rather few, as implied by Denteneer *et al* [3], but the extrinsic stacking faults appeared frequently. Figure 2 shows some extrinsic stacking faults in SiC indicated by the arrows. This phenomenon indicates that the energy of the extrinsic stacking fault in SiC is indeed lower than that of intrinsic stacking, which is in agreement with the predication of Denteneer *et al* [3].

In conclusion, the experimental value of the intrinsic stacking-fault energy of SiC has been given for the first time in this letter, having been obtained by high-resolution electron microscopy. Comparison with the theoretical calculation shows that the result given by Denteneer *et al* [3] is reasonable to some extent. The theoretical method needs improving if it is to model experiment, for example for Si and SiC.

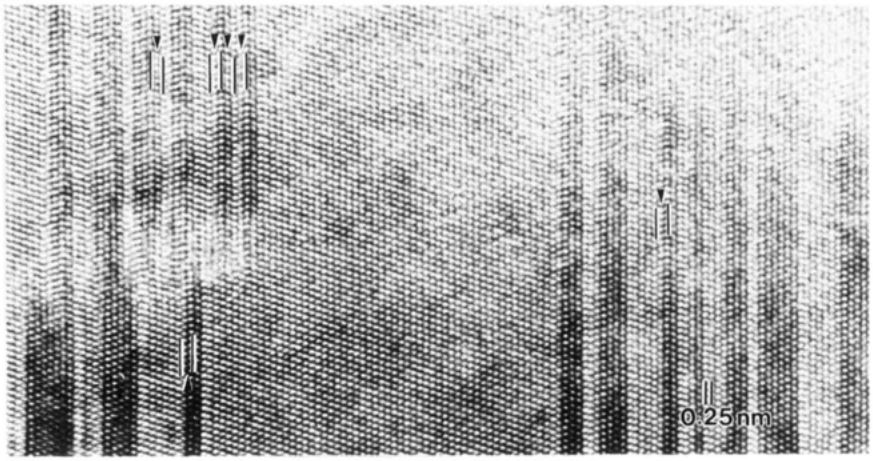

Figure 2. Extrinsic stacking faults in the (111) planes of SiC viewed along the [110] direction, which is indicated by the arrows.

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