ATOMIC CRACK TIPS IN COVALENT CRYSTAL

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ABSTRACT

Crack tip geometries in covalent crystals were studied by high resolution (HR) TEM. The materials used in the study were SiC, Si crystals and 15R-sialon grain. Cracks were introduced by Vickers indentation in SiC and Si. In 15R-sialon, crack was naturally introduced. It was found that the crack tips were atomically sharp and there was no macroscopic yielding zone. The results of TEM observation are summarized here.

INTRODUCTION

According to continuum fracture mechanics, crack tip is imaged as an elliptical shape and stress becomes infinite at the tip. This large stress accumulation at the tip is modified by mechanism of small scale plastic zone or healing mechanism by cohesive force between two crack walls. But actual materials have discrete and non-elastic natures in an atomic scale, and the crack tip does not seem to be elliptical.

S.M.Wiederhorn et al.[1], B.J.Hockey et al.[2] first observed crack tips which propagated in ceramic materials such as SiC, Al_2O_3 by TEM. They found that there was no macroscopic deformation around the tips and discussed that spontaneous closure and healing behind the tip were an essential mechanism of crack propagation in highly brittle materials.

Another approach to the investigation of crack tip geometry is computer simulations using simplified lattice model. The calculations revealed various aspects of crack propagation. J.E.Sinclair et al.[3] obtained the results showing complete cleavage crack propagation in a diamond structural model. J.H.Weiner et al.[4] calculated dislocation generations at the tip in a two-dimensional crystal model. The features of the calculated crack tips depend largely on bonding potential and lattice structure used in the models. In order to understand the fracture behavior of brittle materials, it is important to observe directly crack tips in the atomic level.

The authors have studied crack tip geometry which propagated in ceramic materials by HR-TEM. This paper summarizes the results of the TEM observations on the cracks in SiC, Si crystals and 15R-sialon grains[5,6].

EXPERIMENTAL PROCEDURE

6H-SiC was obtained from ingot which was industrially produced by Acheson furnace (Taiheiyourundum Co.Ltd.,3N pure). Si was semiconductor grade crystal which was commercially obtained (Nihonsilicon Co.Ltd.,11N pure). The crystal structure of SiC and 15R-sialon is hexagonal, and that of Si is cubic.

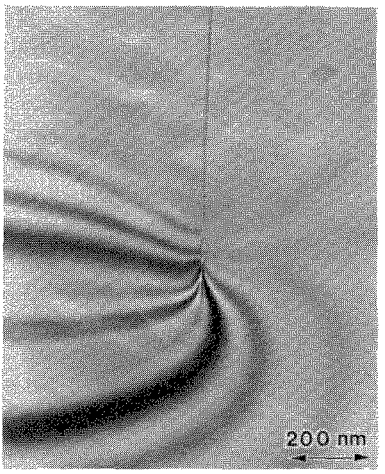
The SiC and Si crystals were cut into small disks, cracks were introduced by Vickers indentation. After thinning by ion bombardment, the samples were observed by TEM (JEM-4000FX,JEOL). 15R-Sialon($SiAl_4O_2N_4$) was prepared by hot-pressing of Si_3N_4, Al_2O_3 and AlN powders. The sample was crashed. It was placed on a holey carbon grid and observed by the TEM. The cracks were found at the edge of the crashed grains.

RESULTS OF CRACK OBSERVATION

1. SiC crystal

Cleavage cracks propagated preferentially in the (0001) and {1120} planes in SiC. HR-TEM photographs of the cracks are shown in Fig.1. It is revealed that the crack is atomically sharp. The crack opens between two adjacent layers. At the tip, lattices of the crystal do not show any disorder. Crack tip blunting does not occur. Another important feature which Fig.1 pointed out is that there were no dislocation generations from the tip. Macroscopic plastic yielding zone does not exist. The fracture of SiC exhibit completely brittle manner.

By close examination of the tip, the lattices are found to be bent or distorted. This distortion extends for a few atomic spacings (about 2-3 nm) in front of the tip. The lattice appears to be partially debonded and the two adjacent debonded lattice planes close here.



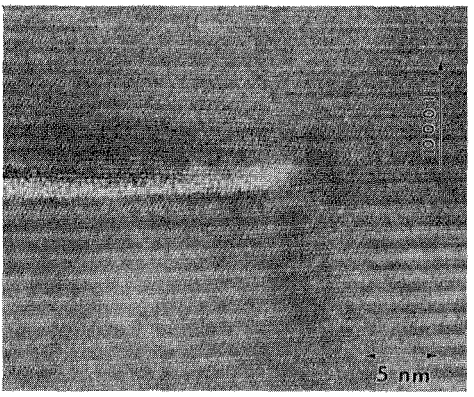


Fig.1 Atomically sharp crack tips in α(6H)-SiC[6].

2. 15R-sialon grain

Crack tips in 15R-sialon were shown in Fig.2. Completely brittle crack tip feature, that is, no evidence of plasticity, was observed again in 15R-sialon grain. At the tip, lattice spacing of 15R-sialon expands slightly. Fig.2 shows more clearly the atomically sharp cracks in 15R-sialon than in SiC.

3. Si crystal

Cleavage cracks in Si always propagate in <111> plane (Fig.3). Although the crack tip in Si crystal is not so clear as those of SiC and 15R-sialon, it is also atomically sharp. In Si, however, small dislocation segments were found around the periphery of the crack and the tip. It is considered that the dislocations were formed owing to the stress around the tip concentrated when the crack propagated and the successive ion-bombardment of Si crystal.

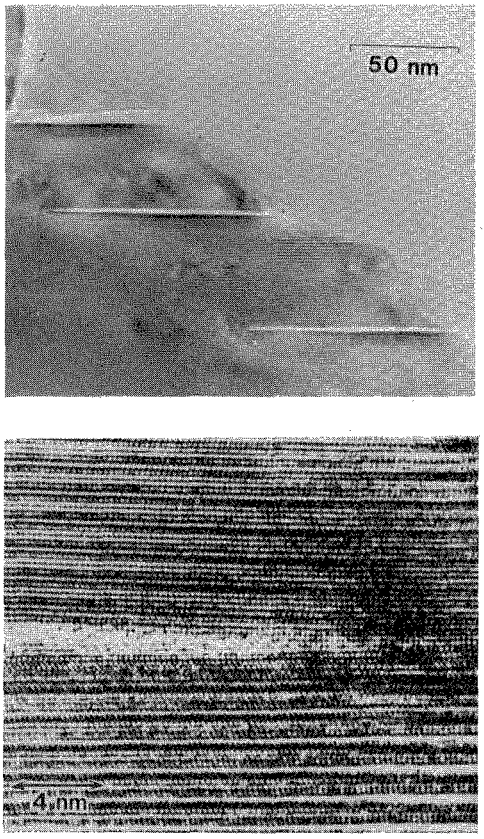


Fig.2 Crack tip in 15R-sialons[5]. The crack propagates in C plane.

DISCUSSION

Atomic fracture process has been studied by many computer

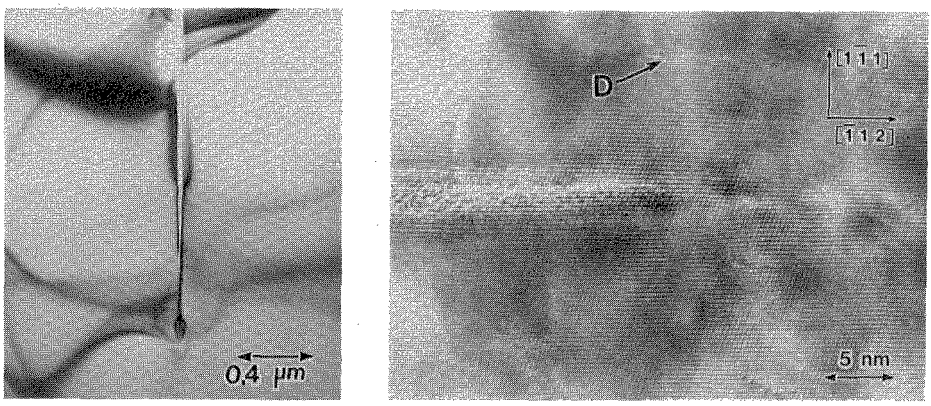


Fig.3 Crack tips in Si crystal[6]. Crack propagates in (111) plane. D:dislocation segment around the tip.

calculations[3,4]. J.E. Sinclair et al.[3] simulated a completely brittle fracture. They used a model which had diamond lattice structure and covalent bonding potential. The calculation showed that the crack propagated in a cleavage manner. Non-linear lattice deformation was limited in a very small region at the tip, dislocation generation was less stable than cleaving of the lattice, and there was no cohesive interaction between two crack planes behind the tip.

The results of TEM observation (Figs.1,2 and 3) suggest that the crack tip features in the covalent crystals correspond basically to the result of Sinclair et al.'s calculation[3]. This means that the crack tips in the covalent crystals are atomically sharp and the crack blunting or the macroscopic yielding around the crack tip do not occur. In Si crystals, however, dislocation segments, a wake of fracture, were found

around the tip. It should be noticed that Si crystal is not completely brittle. The atomically sharp crack tip feature observed in this work leads to conclusion that fracture behavior must be considered not only in terms of energy balance theory but of kinetics of debonding of lattice, as S.M.Weiderhorn[1] pointed out.

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